Spectral Learning Techniques for Weighted Automata, Transducers, and Grammars

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Status Quo

- Composable/composite objects (strings and trees) are ubiquitous in NLP
- Latent variables provide powerful mechanisms for learning the relevant information needed to solve tasks from composable data
- Classical learning paradigms are Expectation–Maximization and Split–Merge

An Alternative Approach

Spectral Methods in General...

- Provide tools for learning latent variable models with strong algorithmic and statistical guarantees
- Facilitate the connection of latent variable models with (multi-)linear algebra commonly used in machine learning
- In practice are faster than iterative methods, and not prone to local minima
- Implementations can readily benefit from latest developments in numerical linear algebra in a black-box fashion

This Tutorial in Particular...

- Emphasize the relation of spectral methods and recursive computations performed by classical weighted automata and grammars
- Show how the language of Hankel matrices seamlessly applies to string and tree computations

Outline

1. Weighted Automata and Hankel Matrices
2. Spectral Learning of Probabilistic Automata
3. Spectral Methods for Transducers and Grammars
   - Sequence Tagging
   - Finite-State Transductions
   - Tree Automata
4. Hankel Matrices with Missing Entries
5. Conclusion
6. References

Outline

Compositional Functions and Bilinear Operators

- Compositional functions defined in terms of recurrence relations
- Consider a sequence $abaccb$

$$f(abaccb) = \boldsymbol{\alpha}_f(ab) \cdot \boldsymbol{\beta}_f(accb)$$

where

- n is the dimension of the model
- $\boldsymbol{\alpha}_f$ maps prefixes to $\mathbb{R}^n$
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f(abaccb) &= \boldsymbol{\alpha}_f(ab) \cdot \boldsymbol{\beta}_f(accb) \\
&= \boldsymbol{\alpha}_f(ab) \cdot \mathbf{A}_a \cdot \boldsymbol{\beta}_f(ccb)
\end{aligned}
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where

- n is the dimension of the model
- $\boldsymbol{\alpha}_f$ maps prefixes to $\mathbb{R}^n$
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- $\mathbf{A}_a$ is a bilinear operator in $\mathbb{R}^{n \times n}$

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Problem

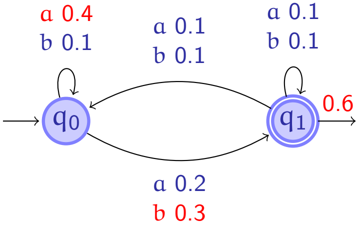
How to estimate $\boldsymbol{\alpha}_f(\lambda)$, $\boldsymbol{\beta}_f(\lambda)$ and $\mathbf{A}_{\mathtt{a}}, \mathbf{A}_{\mathtt{b}}, \ldots$ from "samples" of f?

Weighted Finite Automata (WFA)

An algebraic model
for compositional functions on strings

Weighted Finite Automata (WFA)

Example with 2 states and alphabet $\Sigma = \{a, b\}$



Operator Representation

$$\boldsymbol{\alpha}_0 = \begin{bmatrix} 1.0 \\ 0.0 \end{bmatrix}$$

$$\boldsymbol{\alpha}_\infty = \begin{bmatrix} 0.0 \\ 0.6 \end{bmatrix}$$

$$\mathbf{A}_a = \begin{bmatrix} 0.4 & 0.2 \\ 0.1 & 0.1 \end{bmatrix}$$

$$\mathbf{A}_b = \begin{bmatrix} 0.1 & 0.3 \\ 0.1 & 0.1 \end{bmatrix}$$

$$f(ab) = 0.4 \times 0.3 \times 0.6 + 0.2 \times 0.1 \times 0.6 = 0.084$$

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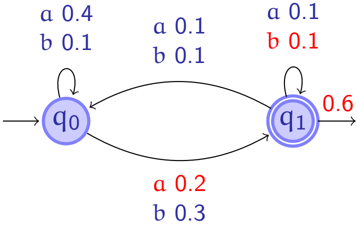

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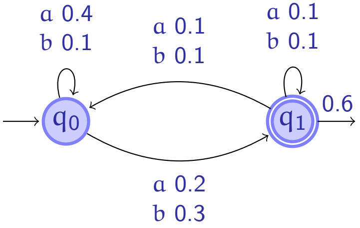

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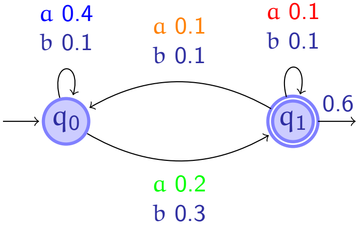

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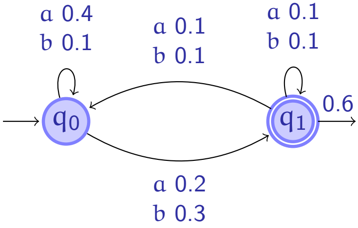

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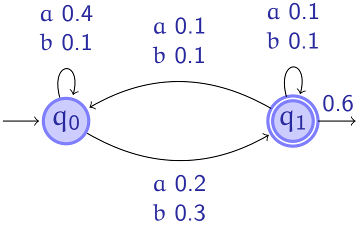

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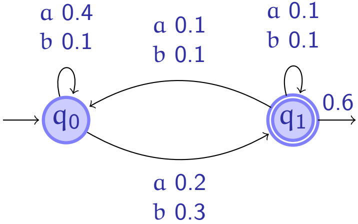

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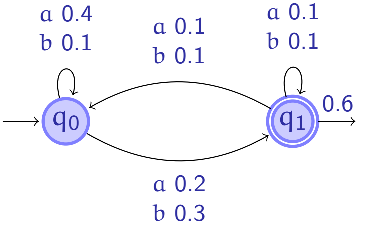

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Notation:

- Σ: alphabet – finite set
- n: number of states – positive integer
- α_0: initial weights – vector in $\mathbb{R}^n$ (features of empty prefix)
- α_∞: final weights – vector in $\mathbb{R}^n$ (features of empty suffix)
- $\mathbf{A}_\sigma$: transition weights – matrix in $\mathbb{R}^{n \times n}$ ($\forall \sigma \in \Sigma$)

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Definition: WFA with n states over Σ

$$A = \langle \boldsymbol{\alpha}_0, \boldsymbol{\alpha}_\infty, \{\mathbf{A}_\sigma\} \rangle$$

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Compositional Function: Every WFA A defines a function $f_A : \Sigma^\star \to \mathbb{R}$

$$f_A(x) = f_A(x_1 \dots x_T) = \boldsymbol{\alpha}_0^\top \mathbf{A}_{x_1} \cdots \mathbf{A}_{x_T} \boldsymbol{\alpha}_\infty = \boldsymbol{\alpha}_0^\top \mathbf{A}_x \boldsymbol{\alpha}_\infty$$

Example – Hidden Markov Model

- Assigns probabilities to strings $f(x) = \mathbb{P}[x]$
- Emission and transition are conditionally independent given state

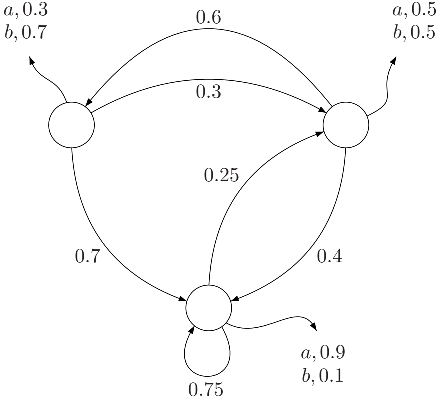
$$\boldsymbol{\alpha}_0^\top = [0.3 \;\; 0.3 \;\; 0.4]$$

$$\boldsymbol{\alpha}_\infty^\top = [1 \;\; 1 \;\; 1]$$

$$\mathbf{A}_a = \mathbf{O}_a \cdot \mathbf{T}$$

$$\mathbf{T} = \begin{bmatrix} 0 & 0.7 & 0.3 \\ 0 & 0.75 & 0.25 \\ 0.6 & 0.4 & 0 \end{bmatrix}$$

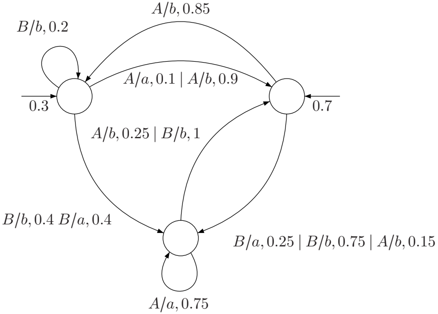
$$\mathbf{O}_a = \begin{bmatrix} 0.3 & 0 & 0 \\ 0 & 0.9 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}$$



Example – Probabilistic Tagger

- $\Sigma = \mathcal{X} \times \mathcal{Y}$, where $\mathcal{X}$ input alphabet and $\mathcal{Y}$ output alphabet
- Assigns conditional probabilities $f(x, y) = \mathbb{P}[y|x]$ to pairs $(x, y) \in \Sigma^\star$

$$\mathcal{X} = \{A, B\}$$
$$\mathcal{Y} = \{a, b\}$$
$$\boldsymbol{\alpha}_0^\top = [0.3 \;\; 0 \;\; 0.7]$$
$$\boldsymbol{\alpha}_\infty^\top = [1 \;\; 1 \;\; 1]$$
$$\mathbf{A}_B^b = \begin{bmatrix} 0.2 & 0.4 & 0 \\ 0 & 0 & 1 \\ 0 & 0.75 & 0 \end{bmatrix}$$



Other Examples of WFA

Automata-theoretic:

- Probabilistic Finite Automata (PFA)
- Deterministic Finite Automata (DFA)

Dynamical Systems:

- Observable Operator Models (OOM)
- Predictive State Representations (PSR)

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Disclaimer: All weights in $\mathbb{R}$ with usual addition and multiplication (*no semi-rings!*)

Applications of WFA

WFA Can Model:

- Probability distributions $f_A(x) = \mathbb{P}[x]$
- Binary classifiers $g(x) = \mathrm{sign}(f_A(x) + \theta)$
- Real predictors $f_A(x)$
- Sequence predictors $g(x) = \mathrm{argmax}_y f_A(x, y)$ (with $\Sigma = \mathcal{X} \times \mathcal{Y}$)

Used In Several Applications:

- Speech recognition [Mohri et al., 2008]
- Machine translation [de Gispert et al., 2010]
- Image processing [Albert and Kari, 2009]
- OCR systems [Knight and May, 2009]
- System testing [Baier et al., 2009]

Useful Intuitions About f_A

$$f_A(x) = f_A(x_1 \ldots x_T) = \boldsymbol{\alpha}_0^\top \mathbf{A}_{x_1} \cdots \mathbf{A}_{x_T} \boldsymbol{\alpha}_\infty = \boldsymbol{\alpha}_0^\top \mathbf{A}_x \boldsymbol{\alpha}_\infty$$

- Sum-Product: $f_A(x)$ is a sum–product computation

$$\sum_{i_0, i_1, \ldots, i_T \in [n]} \boldsymbol{\alpha}_0(i_0) \left(\prod_{t=1}^{T} \mathbf{A}_{x_t}(i_{t-1}, i_t) \right) \boldsymbol{\alpha}_\infty(i_T)$$

- Forward-Backward: $f_A(x)$ is dot product between forward and backward vectors

$$f_A(ps) = \left(\boldsymbol{\alpha}_0^\top \mathbf{A}_p \right) \cdot \left(\mathbf{A}_s \boldsymbol{\alpha}_\infty \right) = \boldsymbol{\alpha}_p \cdot \boldsymbol{\beta}_s$$

- Compositional Features: $f_A(x)$ is a linear model

$$f_A(x) = \left(\boldsymbol{\alpha}_0^\top \mathbf{A}_x \right) \cdot \boldsymbol{\alpha}_\infty = \boldsymbol{\phi}(x) \cdot \boldsymbol{\alpha}_\infty$$

where $\boldsymbol{\phi} : \Sigma^\star \to \mathbb{R}^n$ *compositional features* (i.e. $\boldsymbol{\phi}(x\sigma) = \boldsymbol{\phi}(x)\mathbf{A}_\sigma$)

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Forward–Backward Equations for $\mathbf{A}_\sigma$

Any WFA A defines *forward* and *backward* maps

$$\boldsymbol{\alpha}_A, \boldsymbol{\beta}_A : \Sigma^\star \to \mathbb{R}^n$$

such that for any splitting $x = p \cdot s$ one has

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Example

- In HMM coordinates of $\boldsymbol{\alpha}_A$ and $\boldsymbol{\beta}_A$ have probabilistic interpretation:

$$[\boldsymbol{\alpha}_A(p)]_i = \mathbb{P}[p\,,\, h_{+1} = i]$$
$$[\boldsymbol{\beta}_A(s)]_i = \mathbb{P}[s \mid h = i]$$

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Key Observation

Comparing $f_A(ps)$ and $f_A(p\sigma s)$ reveals information about $\mathbf{A}_\sigma$:

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Hankel matrices help organize and solve these equations!

The Hankel Matrix

Two Equivalent Representations

- Functional: $f : \Sigma^\star \to \mathbb{R}$
- Matricial: $\mathbf{H}_f \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star}$, the *Hankel matrix* of f

Definition: p prefix, s suffix $\quad \Rightarrow \quad \mathbf{H}_f(p, s) = f(p \cdot s)$

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Example $f(x) = |x|_a$
(number of a's in x)

$$\mathbf{H}_f = \begin{array}{c c} & \begin{array}{ccccc} \lambda & a & b & aa & \cdots \end{array} \\ \begin{array}{c} \lambda \\ a \\ b \\ aa \\ \vdots \end{array} & \begin{bmatrix} 0 & 1 & 0 & 2 & \cdots \\ 1 & 2 & 1 & 3 & \\ 0 & 1 & 0 & 2 & \\ 2 & 3 & 2 & 4 & \\ \vdots & & & & \ddots \end{bmatrix} \end{array}$$

The Hankel Matrix

Two Equivalent Representations

- Functional: $f : \Sigma^\star \to \mathbb{R}$
- Matricial: $\mathbf{H}_f \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star}$, the *Hankel matrix* of f

Definition: p prefix, s suffix $\quad \Rightarrow \quad \mathbf{H}_f(p, s) = f(p \cdot s)$

Example $f(x) = |x|_a$

(number of a's in x)

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$\mathbf{H}_f(\lambda, aa) = \mathbf{H}_f(a, a) = \mathbf{H}_f(aa, \lambda) = 2$

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Properties

- $|x| + 1$ entries for $f(x)$
- Depends on ordering of $\Sigma^\star$
- Captures structure

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A Fundamental Theorem about WFA

Relates the rank of $\mathbf{H}_f$

and the number of states of WFA computing f

A Fundamental Theorem about WFA

Theorem [Carlyle and Paz, 1971, Fliess, 1974]

Let $f : \Sigma^\star \to \mathbb{R}$ be any function

1. If $f = f_A$ for some WFA A with n states $\Rightarrow$ $\mathrm{rank}(\mathbf{H}_f) \leqslant n$
2. If $\mathrm{rank}(\mathbf{H}_f) = n$ $\Rightarrow$ exists WFA A with n states s.t. $f = f_A$

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Because proof of (2) gives an algorithm for recovering A from the Hankel matrix of f_A

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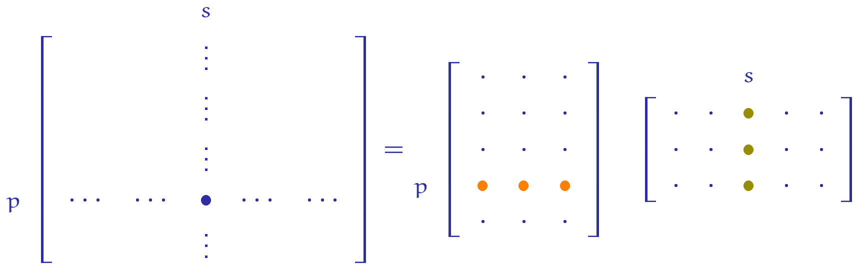
Why Fundamental?

Because proof of (2) gives an algorithm for recovering A from the Hankel matrix of f_A

Example: Can recover an HMM from the probabilities it assigns to sequences of observations

Structure of Low-rank Hankel Matrices

$\mathbf{H}_{f_A} \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star}$ $\quad\quad$ $\mathbf{P} \in \mathbb{R}^{\Sigma^\star \times n}$ $\quad\quad$ $\mathbf{S} \in \mathbb{R}^{n \times \Sigma^\star}$



$$f_A(p_1 \cdots p_T \cdot s_1 \cdots s_{T'}) = \underbrace{\boldsymbol{\alpha}_0^\top \mathbf{A}_{p_1} \cdots \mathbf{A}_{p_T}}_{\boldsymbol{\alpha}_A(p)} \underbrace{\mathbf{A}_{s_1} \cdots \mathbf{A}_{s_{T'}} \boldsymbol{\alpha}_\infty}_{\boldsymbol{\beta}_A(s)}$$

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$$\begin{array}{cc} & s \\ p & \left[\begin{array}{ccccc} & & \vdots & & \\ & & \vdots & & \\ & & \vdots & & \\ \cdots & \cdots & \bullet & \cdots & \cdots \\ & & \vdots & & \end{array}\right] \end{array} = \begin{array}{cc} & \\ & \left[\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \bullet & \bullet & \bullet \\ \cdot & \cdot & \cdot \end{array}\right] \\ p & \end{array} \begin{array}{c} s \\ \left[\begin{array}{ccccc} \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \end{array}\right] \end{array}$$

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$$\boldsymbol{\alpha}_A(p) = \mathbf{P}(p, \cdot) \qquad \boldsymbol{\beta}_A(s) = \mathbf{S}(\cdot, s)$$

Hankel Factorizations and Operators

$$\mathbf{H}_{\sigma} \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star}$$

$$\begin{array}{cc} & \begin{array}{ccccc} & & s & & \end{array} \\ p & \begin{bmatrix} & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ & & \cdot & & \end{bmatrix} \end{array}$$

$$f_A(p_1 \cdots p_T \cdot \sigma \cdot s_1 \cdots s_{T'})$$

Hankel Factorizations and Operators

$$\mathbf{H}_\sigma \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star} \qquad \mathbf{P} \in \mathbb{R}^{\Sigma^\star \times n} \qquad \mathbf{A}_\sigma \in \mathbb{R}^{n \times n} \qquad \mathbf{S} \in \mathbb{R}^{n \times \Sigma^\star}$$

$$\begin{array}{cc} & s \\ & \\ & \\ & \\ p & \\ & \end{array}\!\!\begin{array}{c} \\ \left[\begin{array}{ccccc} & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ & & \cdot & & \end{array}\right]\end{array} = \begin{array}{c} \\ \\ \\ p \\ \\ \end{array}\left[\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \color{orange}\bullet & \color{orange}\bullet & \color{orange}\bullet \\ \cdot & \cdot & \cdot \end{array}\right] \left[\begin{array}{ccc} \color{red}\bullet & \color{red}\bullet & \color{red}\bullet \\ \color{red}\bullet & \color{red}\bullet & \color{red}\bullet \\ \color{red}\bullet & \color{red}\bullet & \color{red}\bullet \end{array}\right] \begin{array}{c} \begin{array}{ccccc} & & s & & \end{array} \\ \left[\begin{array}{ccccc} \cdot & \cdot & \color{olive}\bullet & \cdot & \cdot \\ \cdot & \cdot & \color{olive}\bullet & \cdot & \cdot \\ \cdot & \cdot & \color{olive}\bullet & \cdot & \cdot \end{array}\right] \end{array}$$

$$f_A(p_1 \cdots p_T \cdot \sigma \cdot s_1 \cdots s_{T'}) = \underbrace{\boldsymbol{\alpha}_0^\top \mathbf{A}_{p_1} \cdots \mathbf{A}_{p_T}}_{\color{orange}\boldsymbol{\alpha}_A(p)} \cdot {\color{red}\mathbf{A}_\sigma} \cdot \underbrace{\mathbf{A}_{s_1} \cdots \mathbf{A}_{s_{T'}} \boldsymbol{\alpha}_\infty}_{\color{olive}\boldsymbol{\beta}_A(s)}$$

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$$\mathbf{H}_\sigma \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star} \qquad \mathbf{P} \in \mathbb{R}^{\Sigma^\star \times n} \qquad \mathbf{A}_\sigma \in \mathbb{R}^{n \times n} \qquad \mathbf{S} \in \mathbb{R}^{n \times \Sigma^\star}$$

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Note: Works with finite sub-blocks as well (assuming $\mathrm{rank}(\mathbf{P}) = \mathrm{rank}(\mathbf{S}) = n$)

General Learning Algorithm for WFA

General Learning Algorithm for WFA

Key Idea: The Hankel Trick

1. Learn a low-rank Hankel matrix that *implicitly* induces "latent" states
2. Recover the states from a decomposition of the Hankel matrix

Limitations of WFA

Invariance Under Change of Basis

For any invertible matrix $\mathbf{Q}$ the following WFA are equivalent:

- $A = \langle \boldsymbol{\alpha}_0, \boldsymbol{\alpha}_\infty, \{\mathbf{A}_\sigma\} \rangle$
- $B = \langle \mathbf{Q}^\top \boldsymbol{\alpha}_0, \mathbf{Q}^{-1} \boldsymbol{\alpha}_\infty, \{\mathbf{Q}^{-1} \mathbf{A}_\sigma \mathbf{Q}\} \rangle$

$$
\begin{aligned}
f_A(x) &= \boldsymbol{\alpha}_0^\top \mathbf{A}_{x_1} \cdots \mathbf{A}_{x_T} \boldsymbol{\alpha}_\infty \\
&= (\boldsymbol{\alpha}_0^\top \mathbf{Q})(\mathbf{Q}^{-1} \mathbf{A}_{x_1} \mathbf{Q}) \cdots (\mathbf{Q}^{-1} \mathbf{A}_{x_T} \mathbf{Q})(\mathbf{Q}^{-1} \boldsymbol{\alpha}_\infty) = f_B(x)
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\end{aligned}
$$

Example

$$
\mathbf{A}_a = \begin{bmatrix} 0.5 & 0.1 \\ 0.2 & 0.3 \end{bmatrix} \qquad \mathbf{Q} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \qquad \mathbf{Q}^{-1} \mathbf{A}_a \mathbf{Q} = \begin{bmatrix} 0.3 & -0.2 \\ -0.1 & 0.5 \end{bmatrix}
$$

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\end{aligned}
$$

Consequences

- There is no *unique* parametrization for WFA
- Given A it is *undecidable* whether $\forall x \; f_A(x) \geqslant 0$
- Cannot expect to recover a *probabilistic* parametrization

Outline

Spectral Learning of Probabilistic Automata

Basic Setup:

- Data are strings sampled from probability distribution on $\Sigma^\star$
- Hankel matrix is estimated by empiricial probabilities
- Factorization and low-rank approximation is computed using SVD

The Empirical Hankel Matrix

Suppose $S = (x^1, \ldots, x^N)$ is a sample of N i.i.d. strings

Empirical distribution

$$\hat{f}_S(x) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}[x^i = x]$$

Empirical Hankel matrix

$$\hat{\mathbf{H}}_S(p, s) = \hat{f}_S(ps)$$

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Example:

$$S = \left\{ \begin{array}{c} aa,\ b,\ bab,\ a, \\ b,\ a,\ ab,\ aa, \\ ba,\ b,\ aa,\ a, \\ aa,\ bab,\ b,\ aa \end{array} \right\} \longrightarrow \hat{f}_S(aa) = \frac{5}{16} \approx 0.31$$

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Example:

$$S = \left\{ \begin{array}{c} aa,\ b,\ bab,\ a, \\ b,\ a,\ ab,\ aa, \\ ba,\ b,\ aa,\ a, \\ aa,\ bab,\ b,\ aa \end{array} \right\} \longrightarrow \hat{\mathbf{H}}_S = \begin{array}{c} \\ \lambda \\ a \\ b \\ ba \end{array} \begin{array}{c} \begin{array}{cc} a & b \end{array} \\ \begin{bmatrix} .19 & .25 \\ .31 & .06 \\ .06 & .00 \\ .00 & .13 \end{bmatrix} \end{array}$$

(Hankel with rows $\mathcal{P} = \{\lambda, a, b, ba\}$ and columns $\mathcal{S} = \{a, b\}$)

Finite Sub-blocks of Hankel Matrices

Parameters:

- Set of rows (prefixes) $\mathcal{P} \subset \Sigma^\star$
- Set of columns (suffixes) $\mathcal{S} \subset \Sigma^\star$

$\mathbf{h}_{\lambda,\mathcal{S}}$ $\quad$ $\mathbf{H}$ $\quad$ $\mathbf{H}_a$ $\quad$ $\mathbf{h}_{\mathcal{P},\lambda}$

$$\begin{array}{cc}
 & \begin{array}{cccccc} & \overbrace{\quad\quad\quad}^{\mathcal{S}} & & & & \\ \lambda & a & b & aa & ab & \dots \end{array} \\
\begin{array}{c} \Sigma^\star \\ \lambda \\ \mathcal{P}\left\{\begin{array}{c} a \\ b \end{array}\right. \\ aa \\ ab \\ \vdots \end{array} &
\begin{bmatrix}
1 & 0.3 & 0.7 & 0.05 & 0.25 & \dots \\
0.3 & 0.05 & 0.25 & 0.02 & 0.03 & \dots \\
0.7 & 0.6 & 0.1 & 0.03 & 0.2 & \dots \\
0.05 & 0.02 & 0.03 & 0.017 & 0.003 & \dots \\
0.25 & 0.23 & 0.02 & 0.11 & 0.12 & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
\end{array}$$

- $\mathbf{H} \in \mathbb{R}^{\mathcal{P}\times\mathcal{S}}$ for finding $\mathbf{P}$ and $\mathbf{S}$
- $\mathbf{H}_\sigma \in \mathbb{R}^{\mathcal{P}\times\mathcal{S}}$ for finding $\mathbf{A}_\sigma$
- $\mathbf{h}_{\lambda,\mathcal{S}} \in \mathbb{R}^{1\times\mathcal{S}}$ for finding $\boldsymbol{\alpha}_0$
- $\mathbf{h}_{\mathcal{P},\lambda} \in \mathbb{R}^{\mathcal{P}\times 1}$ for finding $\boldsymbol{\alpha}_\infty$

Low-rank Approximation and Factorization

Will use the singular value decomposition (SVD) as the main building block

Hence the name spectral!

Low-rank Approximation and Factorization

Parameters:

- Desired number of states n
- Block $\mathbf{H} \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}}$ of the empirical Hankel matrix

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Low-rank Approximation: compute truncated SVD of rank n

$$\underbrace{\mathbf{H}}_{\mathcal{P} \times \mathcal{S}} \approx \underbrace{\mathbf{U}_n}_{\mathcal{P} \times n} \underbrace{\mathbf{\Lambda}_n}_{n \times n} \underbrace{\mathbf{V}_n^\top}_{n \times \mathcal{S}}$$

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Factorization: $\mathbf{H} \approx \mathbf{P}\mathbf{S}$ given by SVD, pseudo-inverses are easy

$$\begin{aligned} \mathbf{P} &= \mathbf{U}_n \mathbf{\Lambda}_n & \Rightarrow \quad & \mathbf{P}^+ = \mathbf{\Lambda}_n^{-1} \mathbf{U}_n^\top \quad \left(= (\mathbf{H}\mathbf{V}_n)^+\right) \\ \mathbf{S} &= \mathbf{V}_n^\top & \Rightarrow \quad & \mathbf{S}^+ = \mathbf{V}_n \end{aligned}$$

Computing the WFA

Parameters:

- Factorization $\mathbf{H} \approx (\mathbf{U}\boldsymbol{\Lambda}) \cdot \mathbf{V}^\top = \mathbf{P} \cdot \mathbf{S}$
- Hankel blocks $\mathbf{H}_\sigma$, $\mathbf{h}_{\lambda,\mathcal{S}}$, $\mathbf{h}_{\mathcal{P},\lambda}$

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Parameters:

- Factorization $\mathbf{H} \approx (\mathbf{U}\boldsymbol{\Lambda}) \cdot \mathbf{V}^\top = \mathbf{P} \cdot \mathbf{S}$
- Hankel blocks $\mathbf{H}_\sigma$, $\mathbf{h}_{\lambda,\mathcal{S}}$, $\mathbf{h}_{\mathcal{P},\lambda}$

Equations:

$$
\begin{aligned}
\mathbf{A}_\sigma &= \mathbf{P}^+ \mathbf{H}_\sigma \mathbf{S}^+ = \boldsymbol{\Lambda}^{-1} \mathbf{U}^\top \mathbf{H}_\sigma \mathbf{V} \quad \big(= (\mathbf{H}\mathbf{V})^+ \mathbf{H}_\sigma \mathbf{V}\big) \\
\boldsymbol{\alpha}_0^\top &= \mathbf{h}_{\lambda,\mathcal{S}} \mathbf{S}^+ = \mathbf{h}_{\lambda,\mathcal{S}} \mathbf{V} \\
\boldsymbol{\alpha}_\infty &= \mathbf{P}^+ \mathbf{h}_{\mathcal{P},\lambda} = \boldsymbol{\Lambda}^{-1} \mathbf{U}^\top \mathbf{h}_{\mathcal{P},\lambda} \quad \big(= (\mathbf{H}\mathbf{V})^+ \mathbf{h}_{\mathcal{P},\lambda}\big)
\end{aligned}
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\end{aligned}
$$

Full Algorithm

1. Estimate empirical Hankel and retrieve sub-blocks $\mathbf{H}, \mathbf{H}_\sigma, \mathbf{h}_{\lambda,\mathcal{S}}, \mathbf{h}_{\mathcal{P},\lambda}$
2. Perform SVD of $\mathbf{H}$
3. Solve for $\mathbf{A}_\sigma$, $\boldsymbol{\alpha}_0$, $\boldsymbol{\alpha}_\infty$ with pseudo-inverses

Computational and Statistical Complexity

Running Time:

- Empirical Hankel matrix: $O(|\mathcal{PS}| \cdot N)$
- SVD and linear algebra: $O(|\mathcal{P}| \cdot |\mathcal{S}| \cdot n)$

Statistical Consistency:

- By law of large numbers, $\hat{\mathbf{H}}_S \to \mathbb{E}[\mathbf{H}]$ when $N \to \infty$
- If $\mathbb{E}[\mathbf{H}]$ is Hankel of some WFA A, then $\hat{A} \to A$
- Works for data coming from PFA and HMM

PAC Analysis: (assuming data from A with n states)

- With high probability, $\|\hat{\mathbf{H}}_S - \mathbf{H}\| \leqslant O(1/\sqrt{N})$
- When $N \geqslant O(n|\Sigma|^2 T^4/\varepsilon^2 \mathfrak{s}_n(\mathbf{H})^4)$, then

$$\sum_{|x| \leqslant T} |f_A(x) - f_{\hat{A}}(x)| \leqslant \varepsilon$$

Proofs can be found in [Hsu et al., 2009, Bailly, 2011, Balle, 2013]

Practical Considerations

Basic Setup:

- Data are strings sampled from probability distribution on $\Sigma^\star$
- Hankel matrix is estimated by empiricial probabilities
- Factorization and low-rank approximation is computed using SVD

Advanced Implementations:

- Choice of parameters $\mathcal{P}$ and $\mathcal{S}$
- Scalable estimation and factorization of Hankel matrices
- Smoothing and variance normalization
- Use of prefix and substring statistics

Choosing the Basis

Definition: The pair $(\mathcal{P}, \mathcal{S})$ defining the sub-block is called a *basis*

Intuitions:

- Basis should be choosen such that $\mathbb{E}[\mathbf{H}]$ has full rank
- $\mathcal{P}$ must contain strings reaching each possible state of the WFA
- $\mathcal{S}$ must contain string producing different outcomes for each pair of states in the WFA

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Popular Approaches:

- Set $\mathcal{P} = \mathcal{S} = \Sigma^{\leqslant k}$ for some $k \geqslant 1$ [Hsu et al., 2009]
- Choose $\mathcal{P}$ and $\mathcal{S}$ to contain the K most frequent prefixes and suffixes in the sample [Balle et al., 2012]
- Take all prefixes and suffixes appearing in the sample [Bailly et al., 2009]

Scalable Implementations

Problem: When $|\Sigma|$ is large, even the simplest basis become huge

Hankel Matrix Representation:

- Use hash functions to map $\mathcal{P}$ ($\mathcal{S}$) to row (column) indices
- Use sparse matrix data structures because statistics are usually sparse
- Never store the full Hankel matrix in memory

Efficient SVD Computation:

- SVD for sparse matrices [Berry, 1992]
- Approximate randomized SVD [Halko et al., 2011]
- On-line SVD with rank 1 updates [Brand, 2006]

Refining the Statistics in the Hankel Matrix

Smoothing the Estimates

- Empirical probabilities $\hat{f}_S(x)$ tend to be sparse
- Like in n-gram models, smoothing can help when Σ is large
- Should take into account that strings in $\mathcal{P}\mathcal{S}$ have different lengths
- Open Problem: How to smooth empirical Hankels properly

Refining the Statistics in the Hankel Matrix

Smoothing the Estimates

- Empirical probabilities $\hat{f}_S(x)$ tend to be sparse
- Like in n-gram models, smoothing can help when Σ is large
- Should take into account that strings in $\mathcal{PS}$ have different lengths
- Open Problem: How to smooth empirical Hankels properly

Row and Column Weighting

- More frequent prefixes (suffixes) have better estimated rows (columns)
- Can scale rows and columns to reflect that
- Will lead to more reliable SVD decompositions
- See [Cohen et al., 2013] for details

Substring Statistics

Problem: If the sample contains strings with wide range of lengths, small basis will ignore most of the examples

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String Statistics (occurence probability):

$$S = \left\{ \begin{array}{c} aa,\ b,\ bab,\ a, \\ bbab,\ abb,\ babba,\ abbb, \\ ab,\ a,\ aabba,\ baa, \\ abbab,\ baba,\ bb,\ a \end{array} \right\} \longrightarrow \quad \hat{\mathbf{H}} = \begin{array}{c} \\ \lambda \\ a \\ b \\ ba \end{array} \begin{array}{c} \begin{array}{cc} a & b \end{array} \\ \left[\begin{array}{cc} .19 & .06 \\ .06 & .06 \\ .00 & .06 \\ .06 & .06 \end{array} \right] \end{array}$$

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Substring Statistics (expected number of occurences as substring):

$$\text{Empirical expectation} = \frac{1}{N} \sum_{i=1}^{N} [\text{number of occurences of } x \text{ in } x^i]$$

$$S = \left\{ \begin{array}{c} aa,\ b,\ bab,\ a, \\ bbab,\ abb,\ babba,\ abbb, \\ ab,\ a,\ aabba,\ baa, \\ abbab,\ baba,\ bb,\ a \end{array} \right\} \longrightarrow \hat{\mathbf{H}} = \begin{array}{c} \\ \lambda \\ a \\ b \\ ba \end{array} \begin{array}{c} \begin{array}{cc} a & b \end{array} \\ \begin{bmatrix} 1.31 & 1.56 \\ .19 & .62 \\ .56 & .50 \\ .06 & .31 \end{bmatrix} \end{array}$$

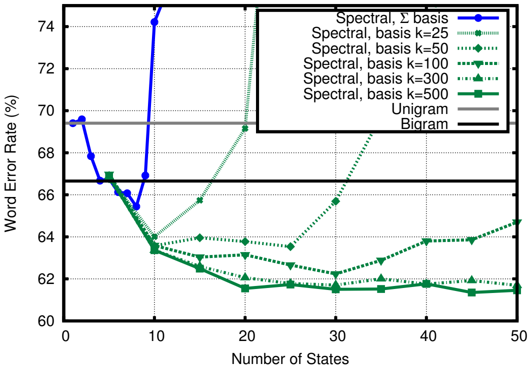
Substring Statistics

Theorem [Balle et al., 2014]
If a probability distribution f is computed by a WFA with n states, then the corresponding substring statistics are also computed by a WFA with n states

Learning from Substring Statistics

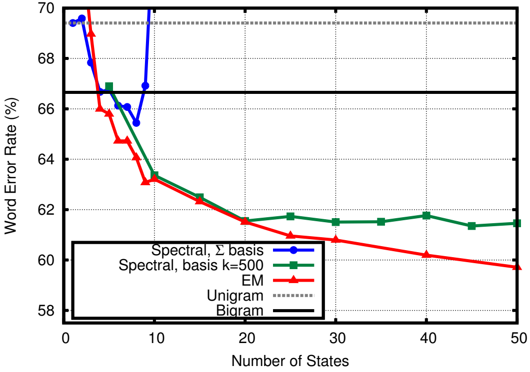
- Can work with smaller Hankel matrices
- But estimating the matrix takes longer

Experiment: PoS-tag Sequence Models



- PTB sequences of simplified PoS tags [Petrov et al., 2012]
- Configuration: expectations on frequent substrings
- Metric: error rate on predicting next symbol in test sequences

Experiment: PoS-tag Sequence Models



- Comparison with a bigram baseline and EM
- Metric: error rate on predicting next symbol in test sequences
- At training, the Spectral Method is > 100 faster than EM

Outline

Sequence Tagging and Transduction

- Many applications involve pairs of input-output sequences:
  - Sequence tagging (one output tag per input token)
    e.g.: part of speech tagging

output:	NNP	NNP	VBZ	NNP	.
input:	Ms.	Haag	plays	Elianti	.

  - Transductions (sequence lenghts might differ)

    e.g.: spelling correction

output: a p p l e
input: a p l e

- Finite-state automata are classic methods to model these relations. Spectral methods apply naturally to this setting.

Sequence Tagging

- Notation:
  - Input alphabet $\mathcal{X}$
  - Output alphabet $\mathcal{Y}$
  - Joint alphabet $\Sigma = \mathcal{X} \times \mathcal{Y}$
- Goal: map input sequences to output sequences of the same length
- Approach: learn a function

$$f : (\mathcal{X} \times \mathcal{Y})^{\star} \to \mathbb{R}$$

Then, given an input $x \in \mathcal{X}^T$ return

$$\operatorname*{argmax}_{y \in \mathcal{Y}^T} f(x, y)$$

(note: this maximization is not tractable in general)

Weighted Finite Tagger

- Notation:
  - $\mathcal{X} \times \mathcal{Y}$: joint alphabet – finite set
  - n: number of states – positive integer
  - $\boldsymbol{\alpha}_0$: initial weights – vector in $\mathbb{R}^n$ (features of empty prefix)
  - $\boldsymbol{\alpha}_\infty$: final weights – vector in $\mathbb{R}^n$ (features of empty suffix)
  - $\mathbf{A}_a^b$: transition weights – matrix in $\mathbb{R}^{n \times n}$ ($\forall a \in \mathcal{X}, b \in \mathcal{Y}$)

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- Definition: WFTagger with n states over $\mathcal{X} \times \mathcal{Y}$

$$A = \langle \boldsymbol{\alpha}_0, \boldsymbol{\alpha}_\infty, \{\mathbf{A}_a^b\} \rangle$$

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$$A = \langle \boldsymbol{\alpha}_0, \boldsymbol{\alpha}_\infty, \{\mathbf{A}_a^b\} \rangle$$

- Compositional Function: Every WFTagger defines a function $f_A : (\mathcal{X} \times \mathcal{Y})^\star \to \mathbb{R}$

$$f_A(x_1 \dots x_T, y_1 \dots y_T) = \boldsymbol{\alpha}_0^\top \mathbf{A}_{x_1}^{y_1} \cdots \mathbf{A}_{x_T}^{y_T} \boldsymbol{\alpha}_\infty = \boldsymbol{\alpha}_0^\top \mathbf{A}_x^y \boldsymbol{\alpha}_\infty$$

The Spectral Method for WFTaggers

Data → *Low-rank matrix estimation* → **Hankel matrix** → *Factorization and linear algebra* → **WFA**

- Assume $f(x, y) = \mathbb{P}(x, y)$
  - Same mechanics as for WFA, with $\Sigma = \mathcal{X} \times \mathcal{Y}$
  - In a nutshell:
    1. Choose set of prefixes and suffixes to define Hankel
       $\rightarrow$ in this case they are bistrings
    2. Estimate Hankel with prefix-suffix training statistics
    3. Factorize Hankel using SVD
    4. Compute α and β projections,
       and compute operators $\langle \boldsymbol{\alpha}_0, \boldsymbol{\alpha}_\infty, \{\mathbf{A}_\sigma\} \rangle$
- Other cases:
  - $f_A(x, y) = \mathbb{P}(y \mid x)$ — see [Balle et al., 2011]
  - $f_A(x, y)$ non-probabilistic — see [Quattoni et al., 2014]

Prediction with WFTaggers

- Assume $f_A(x, y) = \mathbb{P}(x, y)$
- Given $x_{1:T}$, compute most likely output tag at position t:

$$\operatorname*{argmax}_{a \in \mathcal{Y}} \mu(t, a)$$

where

$$\mu(t, a) \triangleq \mathbb{P}(y_t = a \mid x) \;\; \propto \sum_{y = y_1 \ldots a \ldots y_T} \mathbb{P}(x, y)$$

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where

$$\begin{aligned}
\mu(t, a) \triangleq \mathbb{P}(y_t = a \mid x) &\propto \sum_{y = y_1 \dots a \dots y_T} \mathbb{P}(x, y) \\
&\propto \sum_{y = y_1 \dots a \dots y_T} \boldsymbol{\alpha}_0^\top \mathbf{A}_x^y \boldsymbol{\alpha}_\infty \\
&\propto \underbrace{\boldsymbol{\alpha}_0^\top \left(\sum_{y_1 \dots y_{t-1}} \mathbf{A}_{x_{1:t-1}}^{y_{1:t-1}} \right)}_{\alpha_A^\star(x_{1:t-1})} A_{x_t}^a \underbrace{\left(\sum_{y_{t+1} \dots y_T} \mathbf{A}_{x_{t+1:T}}^{y_{i+1:T}} \right) \boldsymbol{\alpha}_\infty}_{\beta_A^\star(x_{t+1:T})}
\end{aligned}$$

$$\alpha_A^\star(x_{1:t}) = \alpha_A^\star(x_{1:t-1}) \left(\sum_{b \in \mathcal{Y}} \mathbf{A}_{x_t}^b \right) \qquad \beta_A^\star(x_{t:T}) = \left(\sum_{b \in \mathcal{Y}} \mathbf{A}_{x_t}^b \right) \beta_A^\star(x_{t+1:T})$$

Prediction with WFTaggers (II)

- Assume $f_A(x, y) = \mathbb{P}(x, y)$
- Given $x_{1:T}$, compute most likely output bigram ab at position t:

$$\operatorname*{argmax}_{a,b \in \mathcal{Y}} \mu(t, a, b)$$

where

$$\begin{aligned} \mu(t, a, b) &= \mathbb{P}(y_t = a, y_{t+1} = b \mid x) \\ &\propto \alpha_A^\star(x_{1:t-1}) \mathbf{A}_{x_t}^a \mathbf{A}_{x_{t+1}}^b \beta_A^\star(x_{t+2:T}) \end{aligned}$$

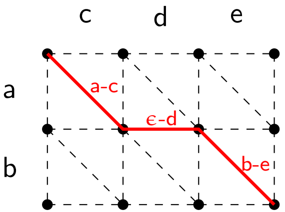
- Compute most likely full sequence y – intractable

In practice, use Minimum Bayes-Risk decoding:

$$\operatorname*{argmax}_{y \in \mathcal{Y}^T} \sum_t \mu(t, y_t, y_{t+1})$$

Finite State Transducers

(ab,cde)



- A WFTransducer evaluates aligned strings,
  using the empty symbol ϵ to produce one-to-one alignments:

$$f\binom{c\ d\ e}{a\ \epsilon\ b} = \boldsymbol{\alpha}_0^\top \mathbf{A}_a^c \mathbf{A}_\epsilon^d \mathbf{A}_b^e \boldsymbol{\alpha}_\infty$$

- Then, a function g can be defined on unaligned strings by aggregating alignments

$$g(ab, cde) = \sum_{\pi \in \Pi(ab,cde)} f(\pi)$$

Finite State Transducers: Main Problems

- Prediction: given an FST A, how to ...
  - Compute $g(x, y)$ for unaligned strings?
  - Compute marginal quantities $\mu(\text{edge}) = \mathbb{P}(\text{edge} \mid x)$?
  - Compute most-likely y for given x?

Finite State Transducers: Main Problems

- Prediction: given an FST A, how to ...
  - Compute $g(x, y)$ for unaligned strings?
    $\rightarrow$ using edit-distance recursions
  - Compute marginal quantities $\mu(\text{edge}) = \mathbb{P}(\text{edge} \mid x)$?
    $\rightarrow$ also using edit-distance recursions
  - Compute most-likely y for given x?
    $\rightarrow$ use MBR-decoding with marginal scores

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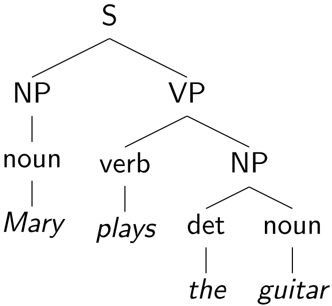
- Unsupervised Learning: learn an FST from pairs of unaligned strings
  - Unlike with EM, the spectral method can not recover latent structure such as alignments
    (recall: alignments are needed to estimate Hankel entries)
  - See [Bailly et al., 2013b] for a solution based on Hankel matrix completion

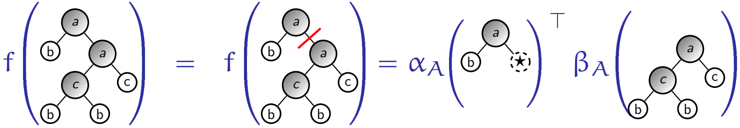
Spectral Learning of Tree Automata and Grammars



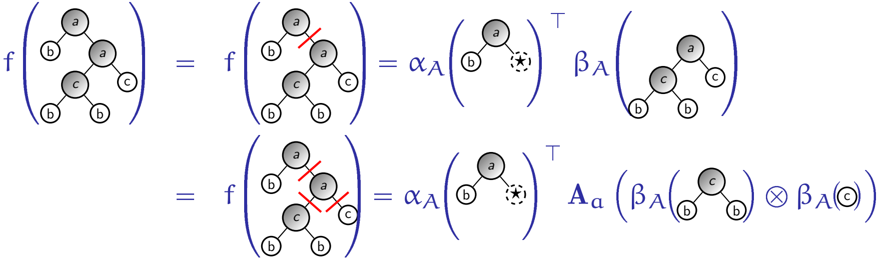
Some References:

- Tree Series: [Bailly et al., 2010, Bailly et al., 2010]
- Latent-annotated PCFG: [Cohen et al., 2012, Cohen et al., 2013]
- Dependency parsing: [Luque et al., 2012, Dhillon et al., 2012]
- Unsupervised learning of WCFG: [Bailly et al., 2013a, Parikh et al., 2014]
- Synchronous grammars: [Saluja et al., 2014]

Compositional Functions over Trees



Compositional Functions over Trees



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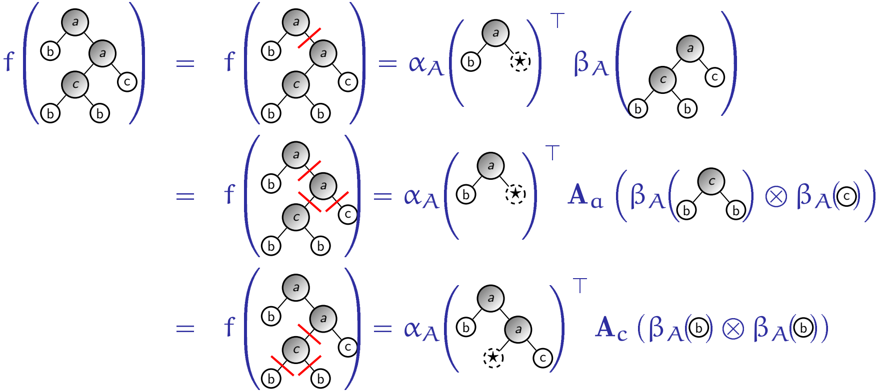
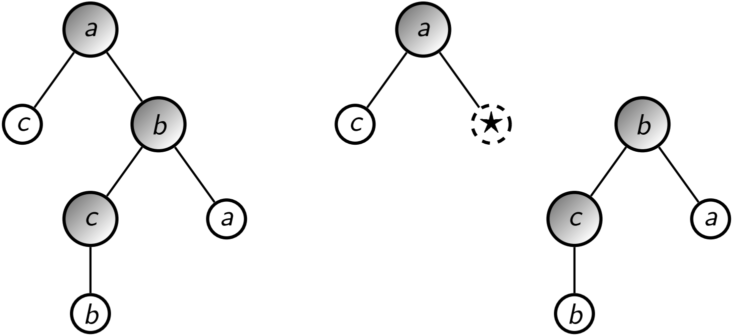


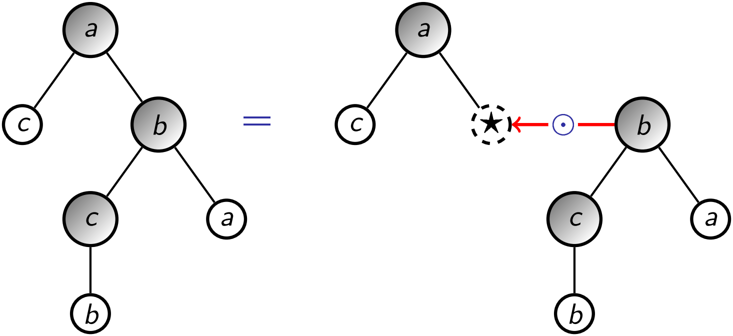
Inside-Outside Composition of Trees



$$t = t_o \odot t_i$$

note: i-o composition generalizes the notion of concatenation in strings, i.e., outside trees are prefixes, inside trees are suffixes

Inside-Outside Composition of Trees



$$t = t_o \odot t_i$$

note: i-o composition generalizes the notion of concatenation in strings, i.e., outside trees are prefixes, inside trees are suffixes

Weighted Finite Tree Automata (WFTA)

An algebraic model for compositional functions on trees

WFTA Notation (I)

Labeled Trees

- $\{\Sigma^k\} = \{\Sigma^0, \Sigma^1, \ldots, \Sigma^r\}$ – ranked alphabet
- $\mathcal{T}$ – space of labeled trees over some ranked alphabet

Tree:

- $t \in \mathcal{T} = \langle V, E, l(v) \rangle$: a labeled tree
- $V = \{1, \ldots, m\}$: the set of vertices
- $E = \{\langle i, j \rangle\}$: the set of edges forming a tree
- $l(v) \rightarrow \{\Sigma^k\}$: returns the label of v – (i.e. a symbol in $\{\Sigma^k\}$)

WFTA Notation (II)

Labeled Trees

- $\{\Sigma^k\} = \{\Sigma^0, \Sigma^1, \dots, \Sigma^r\}$ – ranked alphabet
- $\mathcal{T}$ – space of labeled trees over some ranked alphabet

Leaf Trees and Inside Compositions:

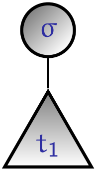
leaf tree

$\sigma \in \Sigma^0$

$t = \sigma$

unary composition

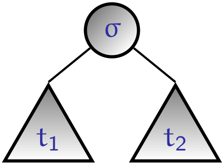
$\sigma \in \Sigma^1,\ t_1 \in \mathcal{T}$



$t = \sigma[t_1]$

binary composition

$\sigma \in \Sigma^2,\ t_1, t_2 \in \mathcal{T}$



$t = \sigma[t_1, t_2]$

Notation for Matrices and Tensors

Kronecker product:

- for $v_1 \in \mathbb{R}^n$ and $v_2 \in \mathbb{R}^n$:
- $v_1 \otimes v_2 \in \mathbb{R}^{n^2}$ contains all products between elements of v_1 and v_2
- Example:
  - $v_1 = [a, b]$
  - $v_2 = [c, d]$
  - $v_1 \otimes v_2 = [ac, ad, bc, bd]$

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Simplifying assumption:

- We consider trees with maximum arity 2
- We think of matrices and tensors as functions:
  - Vectors $\mathbf{v} \in \mathbb{R}^n$
  - Matrices $\mathbf{A}^1 \in \mathbb{R}^{n \times n}$: take one vector $\mathbf{v} \in \mathbb{R}^n$ and produce another vector $\mathbf{A}^1\,\mathbf{v} \in \mathbb{R}^n$
  - Tensors $\mathbf{A}^2 \in \mathbb{R}^{n \times n^2}$: take two vectors $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^n$ and produce another vector $\mathbf{A}^2(\mathbf{v}_1 \otimes \mathbf{v}_2) \in \mathbb{R}^n$

Weighted Finite Tree Automata (WFTA)

$\Sigma = \{\Sigma^0, \Sigma^1, \Sigma^2\}$: ranked alphabet of order 2 – finite set

Definition: WFTA with n states over Σ

$$A = \langle \boldsymbol{\alpha}_\star, \{\boldsymbol{\beta}_\sigma\}, \{\mathbf{A}_\sigma^1\}, \{\mathbf{A}_\sigma^2\} \rangle$$

- n: number of states – positive integer
- $\boldsymbol{\alpha}_\star \in \mathbb{R}^n$: root weights
- $\boldsymbol{\beta}_\sigma \in \mathbb{R}^n$: leaf weights – $(\forall \sigma \in \Sigma^0)$
- $\mathbf{A}_\sigma^1 \in \mathbb{R}^{n \times n}$: node weights – $(\forall \sigma \in \Sigma^1)$
- $\mathbf{A}_\sigma^2 \in \mathbb{R}^{n \times n^2}$: node weights – $(\forall \sigma \in \Sigma^2)$
- Note: $\mathbf{A}_\sigma^2$ is a tensor in $\mathbb{R}^{n \times n \times n}$ packed as a matrix

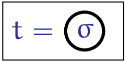
WFTA: Inside Function

Definition: Any WFTA A defines an inside function:

$$\beta_A : \mathcal{T} \to \mathbb{R}^n$$ – maps a tree to a vector in $\mathbb{R}^n$

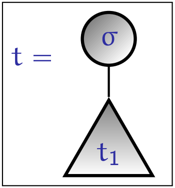
- if $t = \sigma$ is a leaf:

$$\beta_A(t) = \boldsymbol{\beta}_\sigma$$



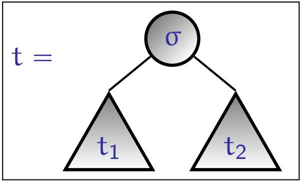
- if $t = \sigma[t_1]$ results from a unary composition:

$$\beta_A(t) = \mathbf{A}^1_\sigma \beta_A(t_1)$$



- if $t = \sigma[t_1, t_2]$ results from a binary composition:

$$\beta_A(t) = \mathbf{A}^2_\sigma \left(\beta_A(t_1) \otimes \beta_A(t_2)\right)$$



WFTA Function:

Every WFTA A defines a function

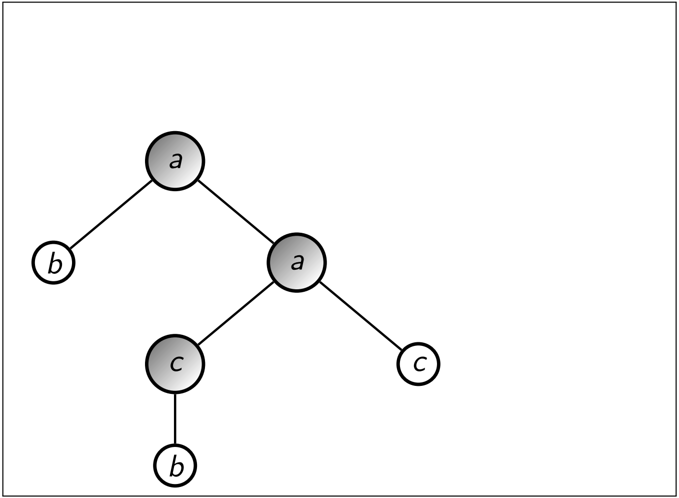
$$f_A : \mathcal{T} \to \mathbb{R}$$

computed as:

$$f_A(t) = \boldsymbol{\alpha}_\star^\top \beta_A(t)$$

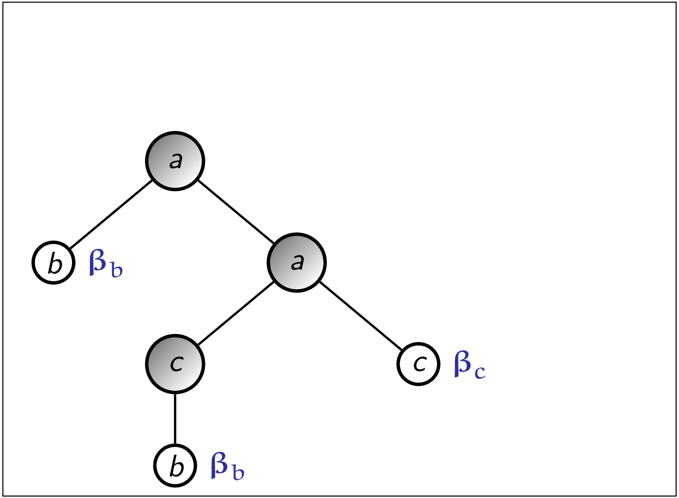
Weighted Finite Tree Automaton (WFTA)

Example of inside computation:



Weighted Finite Tree Automaton (WFTA)

Example of inside computation:



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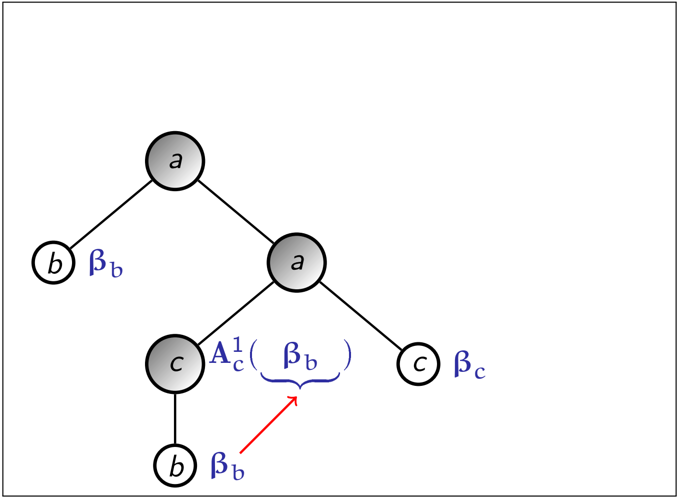

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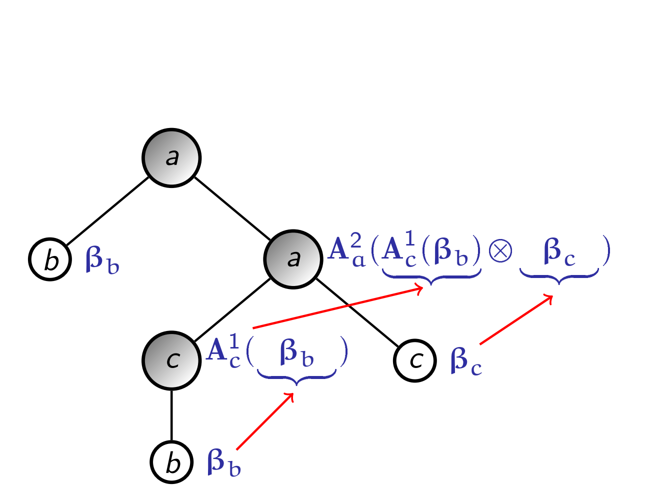
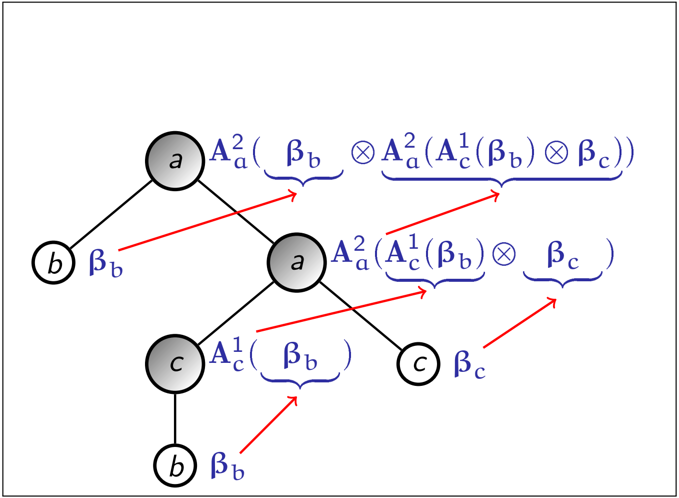


Weighted Finite Tree Automaton (WFTA)

Example of inside computation:



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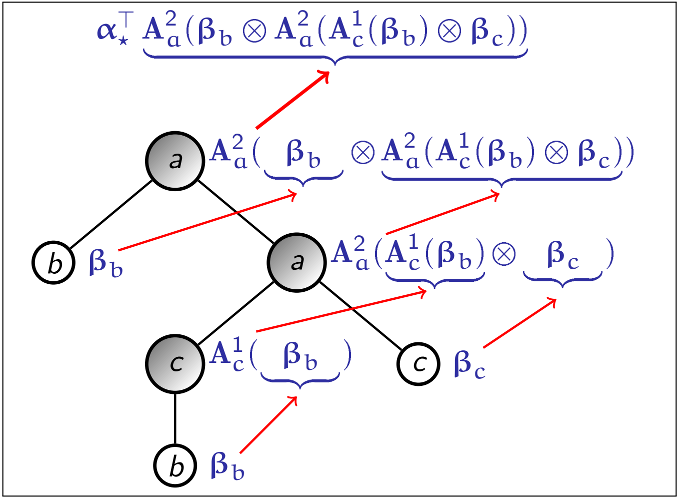

Useful Intuition: Latent-variable Models as WFTA

$$f_A(t) = \alpha_\star^t \beta_A(t)$$

- Each labeled node v is *decorated* with a latent variable $h_v \in [n]$
- $f_A(t)$ is a sum–product computation:

$$\sum_{h_0,h_1,\dots,h_{|V|}\in[n]} \left(\alpha_\star(h_0) \prod_{v\in V:a(v)=0} \beta_{l(v)}[h_v] \times \prod_{v\in V:a(v)=1} \mathbf{A}^1_{l(v)}[h_v, h_{c(t,v)}] \times \prod_{v\in V:a(v)=2} \mathbf{A}^2_{l(v)}[h_v, h_{c_1(t,v)}, h_{c_2(t,v)}] \right)$$

- $f_A(t)$ is a linear model in the latent space defined by $\beta_A : \mathcal{T} \to \mathbb{R}^n$

$$f_A(t) = \sum_{i=1}^{n} \alpha_\star[i]\ \beta_A(t)[i]$$

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$$\times \prod_{v \in V : a(v) = 1} \mathbf{A}^1_{l(v)}[h_v, h_{c(t,v)}]$$
$$\left. \times \prod_{v \in V : a(v) = 2} \mathbf{A}^2_{l(v)}[h_v, h_{c_1(t,v)}, h_{c_2(t,v)}] \right)$$

- $f_A(t)$ is a linear model in the latent space defined by $\beta_A : \mathcal{T} \to \mathbb{R}^n$

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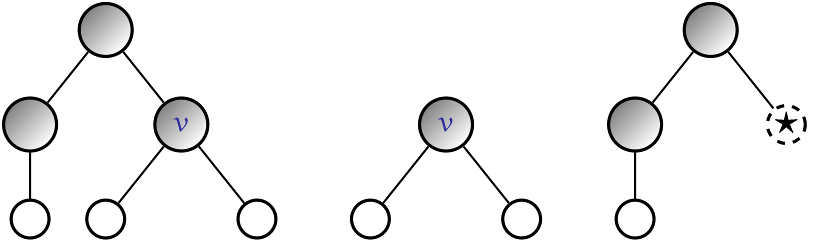
Inside/Outside Decomposition

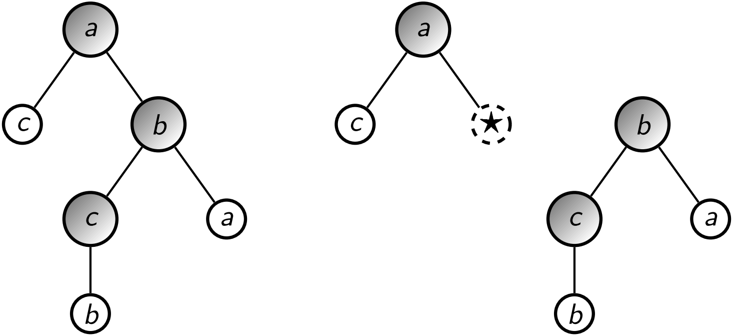


tree t inside tree $t[v]$ outside tree $t \backslash v$

Consider a tree t and one node v:

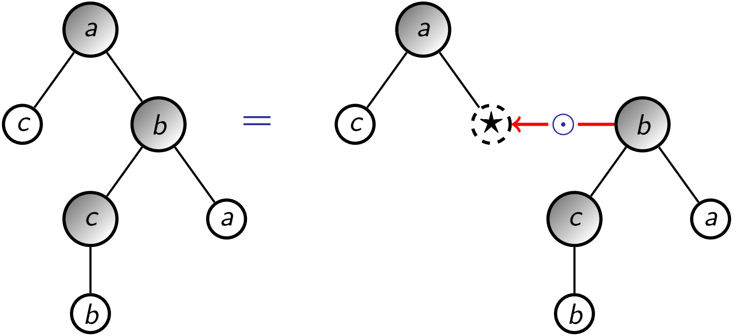
- Inside tree $t[v]$: the subtree of t rooted at v
  - $t[v] \in \mathcal{T}$
- Outside tree $t \backslash v$: the rest of t when removing $t[v]$
  - $\mathcal{T}_\star$: the space of outside trees, i.e. $t \backslash v \in \mathcal{T}_\star$
  - Foot node $\star$: a tree insertion point (a special symbol $\star \notin \{\Sigma^k\}$)
  - An outside tree has exactly one foot node in the leaves

Inside/Outside Composition



- A tree is formed by composing an outside tree with an inside tree
  $\longrightarrow$ generalizes prefix/suffix concatenation in strings
- Multiple ways to decompose a full tree into inside/outside trees
  $\longrightarrow$ as many as nodes in a tree

Inside/Outside Composition



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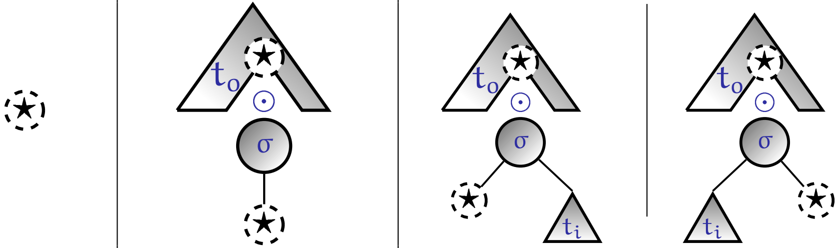
Outside Trees

- Outside trees $t_\star \in \mathcal{T}_\star$ are defined recursively using compositions:

foot node	unary composition	binary composition	
	$t_o \in \mathcal{T}_\star,\ \sigma \in \Sigma^1$	$t_o \in \mathcal{T}_\star,\ \sigma \in \Sigma^2,\ t_i \in \mathcal{T}$	



$t_\star = \star$	$t_\star = t_o \odot \sigma[\star]$	$t_\star = t_o \odot \sigma[\star, t_i]$	$t_\star = t_o \odot \sigma[t_i, \star]$

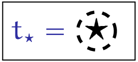
WFTA: Outside Function

Definition: Any WFTA A defines an outside function:

$$\alpha_A : \mathcal{T}_\star \to \mathbb{R}^n$$ – maps an outside tree to a vector in $\mathbb{R}^n$

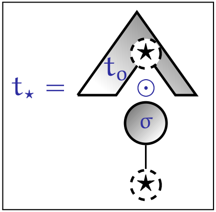
- if $t_\star = \star$ is a foot node:

$$\alpha_A(t_\star) = \boldsymbol{\alpha}_0$$



- if $t_\star = t_o \odot \sigma[\star]$ results from a unary composition:

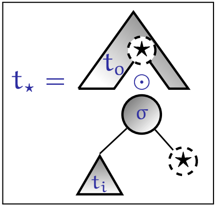
$$\alpha_A(t_\star) = \alpha_A(t_o)^\top \mathbf{A}_\sigma^1$$



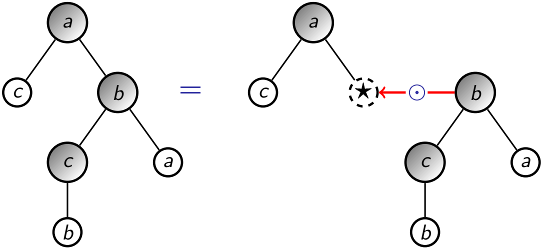
- if $t_\star = t_o \odot \sigma[t_i, \star]$ results from a binary composition:

$$\alpha_A(t_\star) = \alpha_A(t_o)^\top \mathbf{A}_\sigma^2 (\beta_A(t_i) \otimes \mathbf{1}^n)$$

(note: similar expression for $t_\star = t_o \odot \sigma[\star, t_i]$)



WFTA are fully compositional



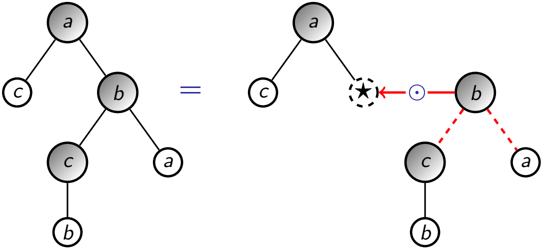
For any inside-outside decomposition of a tree:

$$f_A(t) = \alpha_A(t_o)^\top \beta_A(t_i) \qquad \text{(let } t = t_o \odot t_i\text{)}$$

Consequences:

- We can isolate the α_A and β_A vector spaces

WFTA are fully compositional



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$$= \alpha_A(t_o)^\top \mathbf{A}_\sigma^2(\beta_A(t_1) \otimes \beta_A(t_2)) \qquad \text{(let } t_i = \sigma[t_1, t_2]\text{)}$$

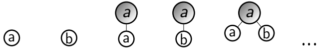
Consequences:

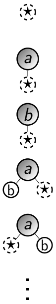
- We can isolate the α_A and β_A vector spaces
- Given α_A and β_A, we can isolate the operators $\mathbf{A}_\sigma^k$

Hankel Matrices of functions over Labeled Trees

Two Equivalent Representations

- Functional: $f_A : \mathcal{T} \to \mathbb{R}$
- Matricial: $H_{f_A} \in \mathbb{R}^{|\mathcal{T}_\star| \times |\mathcal{T}|}$ *(the Hankel matrix of* f_A*)*





$$
\begin{bmatrix}
0 & 1 & -1 & 2 & 3 & \dots \\
-1 & 2 & 1 & -1 & \cdots & \\
4 & 1 & 6 & 2 & & \\
0 & -1 & -3 & -7 & & \\
3 & \vdots & & & & \\
\vdots & & & & &
\end{bmatrix}
$$

- Definition:
  $H(t_o, t_i) = f(t_o \odot t_i)$
- Sublock for σ:
  $H_\sigma(t_o, \sigma[t_1, t_2]) = f(t_o \odot \sigma[t_1, t_2])$
- Highly redundant,
  i.e., $|V| + 1$ entries for $f(t)$

A Fundamental Theorem about WFTA

Relates the rank of $\mathbf{H}_f$

and the number of states of WFTA computing f

A Fundamental Theorem about WFTA

Let $f : \mathcal{T} \to \mathbb{R}$ be any function over labeled trees.

1. If $f = f_A$ for some WFTA A with n states $\Rightarrow$ $\mathrm{rank}(\mathbf{H}_f) \leqslant n$
2. If $\mathrm{rank}(\mathbf{H}_f) = n \Rightarrow$ exists WFTA A with n states s.t. $f = f_A$

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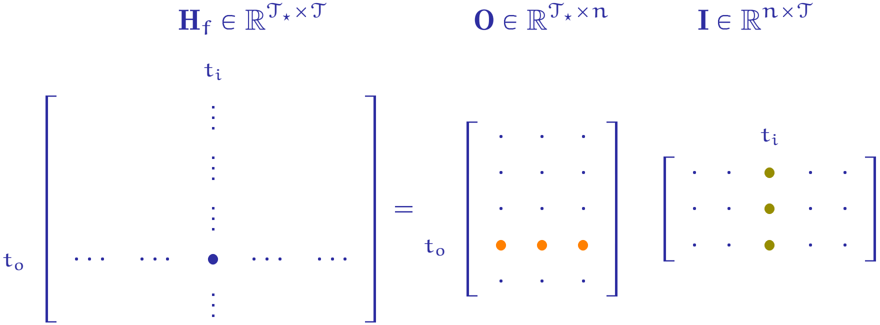
Why Fundamental?

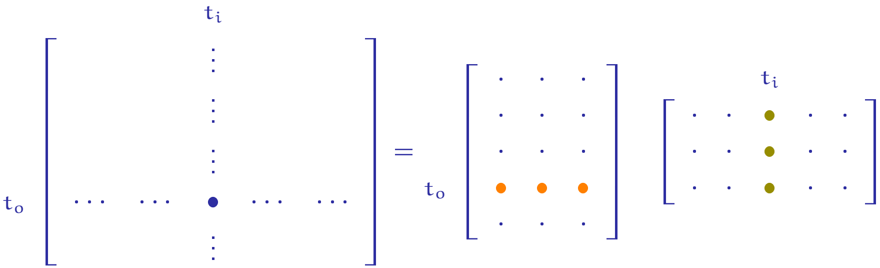
Proof of (2) gives an algorithm for "recovering" A from the Hankel matrix of f_A

Structure of Low-rank Hankel Matrices



Structure of Low-rank Hankel Matrices

$\mathbf{H}_f \in \mathbb{R}^{\mathcal{T}_\star \times \mathcal{T}}$ $\quad$ $\mathbf{O} \in \mathbb{R}^{\mathcal{T}_\star \times n}$ $\quad$ $\mathbf{I} \in \mathbb{R}^{n \times \mathcal{T}}$



$$f(t_o \odot t_i) = \alpha_A(t_o)^\top \beta_A(t_i)$$

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$$\begin{array}{cc} & t_i \\ t_o & \left[\begin{array}{ccccc} & & \vdots & & \\ & & \vdots & & \\ & & \vdots & & \\ \cdots & \cdots & \bullet & \cdots & \cdots \\ & & \vdots & & \end{array}\right] \end{array} = \begin{array}{cc} & \\ t_o & \left[\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \bullet & \bullet & \bullet \\ \cdot & \cdot & \cdot \end{array}\right] \end{array} \begin{array}{c} t_i \\ \left[\begin{array}{ccccc} \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \end{array}\right] \end{array}$$

$$f(t_o \odot t_i) = \alpha_A(t_o)^\top \beta_A(t_i)$$

$$\alpha_A(t_o) = \mathbf{O}(t_o, \cdot) \qquad \beta_A(t_i) = \mathbf{I}(\cdot, t_i)$$

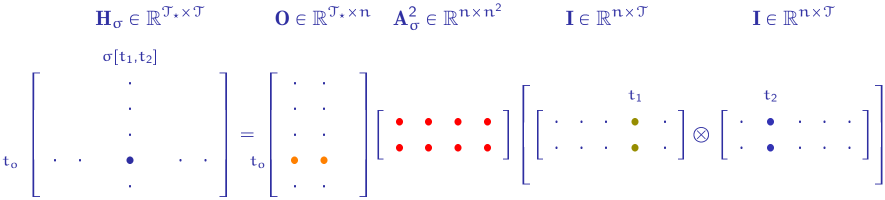
Hankel Factorizations and Operators

$$\mathbf{H}_{\sigma} \in \mathbb{R}^{\mathcal{T}_\star \times \mathcal{T}}$$

$$\begin{array}{cc} & \sigma[t_1, t_2] \\ t_o & \left[\begin{array}{ccccc} & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ & & \cdot & & \end{array}\right] \end{array}$$

$$f(t_o \odot \underbrace{\sigma[t_1, t_2]}_{t_i})$$

Hankel Factorizations and Operators



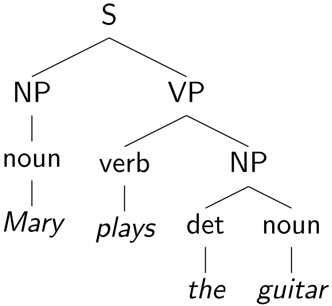
$$f(t_o \odot \underbrace{\sigma[t_1, t_2]}_{t_i}) = \alpha_A(t_o)^\top \underbrace{\mathbf{A}_\sigma^2(\beta_A(t_1) \otimes \beta_A(t_2))}_{\beta_A(t_i)}$$

Hankel Factorizations and Operators

$$\mathbf{H}_\sigma = \mathbf{O}\ \mathbf{A}_\sigma^2\ [\mathbf{I} \otimes \mathbf{I}] \quad \Longrightarrow \quad \mathbf{A}_\sigma^2 = \mathbf{O}^+\ \mathbf{H}_\sigma\ [\mathbf{I} \otimes \mathbf{I}]^+$$

Note: Works with finite sub-blocks as well
(assuming $\mathrm{rank}(\mathbf{O}) = \mathrm{rank}(\mathbf{I}) = n$)

WFTA: Application to Parsing



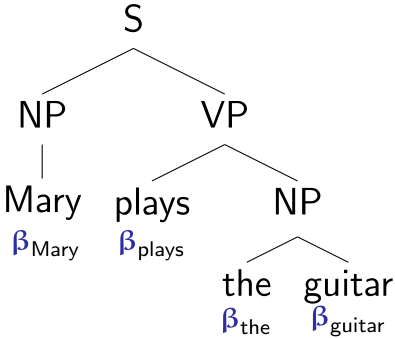
Some intuitions:

- Derivation = Labeled Tree
- Learning compositional functions over derivations
  $\Longrightarrow$ learning functions over trees
- We are interested in functions computed by WFTA

WFTA for Parsing: Key Questions

- What is the latent state representing?
  - e.g., latent real-valued embeddings of words and phrases
- What form of supervision do we get?
  - Full Derivations (labeled trees)
    i.e., supervised learning of latent-variable grammars
  - Derivation skeletons (unlabeled trees)
    e.g. [Pereira and Schabes, 1992]
  - Yields from the grammar (only sentences)
    i.e., grammar induction

Parsing and Tree Automaton



- Vectors β_σ associated with terminal symbols
- Matrices and tensors $\mathbf{A}_\sigma^k$ associated with non-terminals
- Bottom-up computation embeds inside trees into vectors in $\mathbb{R}^n$

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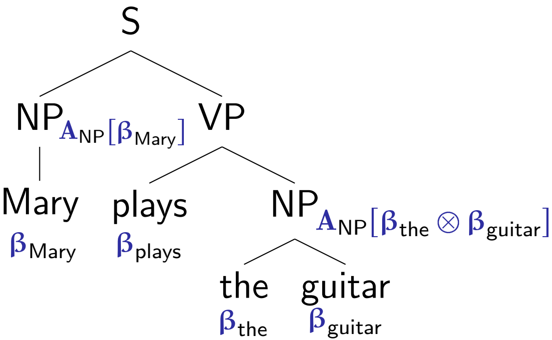

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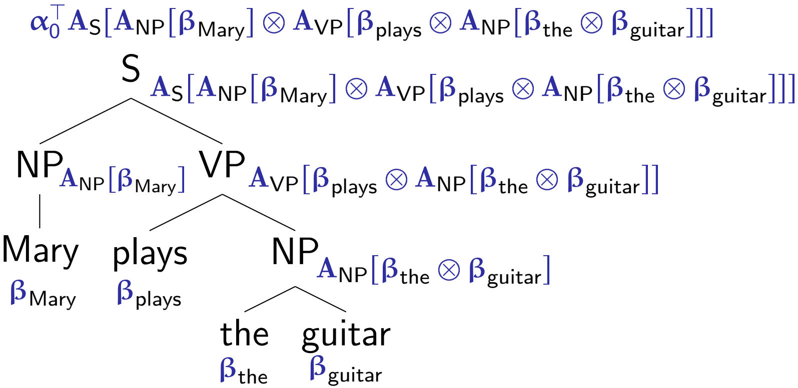

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- Bottom-up computation embeds inside trees into vectors in $\mathbb{R}^n$

WFTA on Parse Trees

- WFTA $A = \langle \boldsymbol{\alpha}_\star, \{\boldsymbol{\beta}_w\}, \{\mathbf{A}^1_{\mathrm{N}}\}, \{\mathbf{A}^2_{\mathrm{N}}\} \rangle$
  - n: number of states; i.e. dimensionality of the embedding
  - Ranked alphabet:
    - $\Sigma^0 = \{$*the*, *Mary*, *plays*, $\dots\}$ – terminal words
    - $\Sigma^1 = \{$noun, verb, det, NP, VP, $\dots\}$ – unary non-terminals
    - $\Sigma^2 = \{$S, NP, VP, $\dots\}$ – binary non-terminals
  - $\boldsymbol{\alpha}_\star$ – initial weights
  - $\{\boldsymbol{\beta}_w\}$ for all $w \in \Sigma^0$ – word embeddings
  - $\{\mathbf{A}^1_{\mathrm{N}}\}$ for all $\mathrm{N} \in \Sigma^1$ – compute embedding of unary phrases
  - $\{\mathbf{A}^2_{\mathrm{N}}\}$ for all $\mathrm{N} \in \Sigma^2$ – compute embedding of binary phrases

WFTA on Parse Trees

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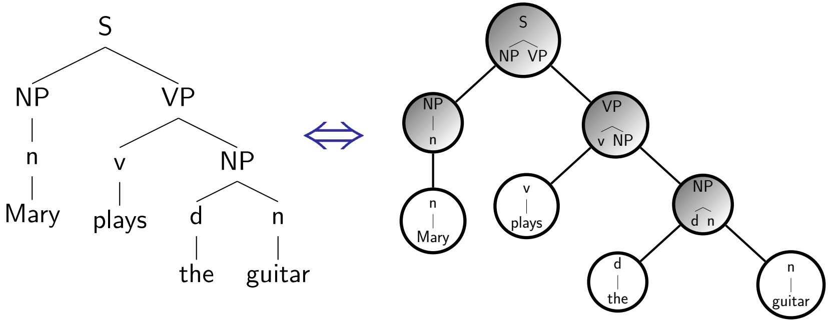
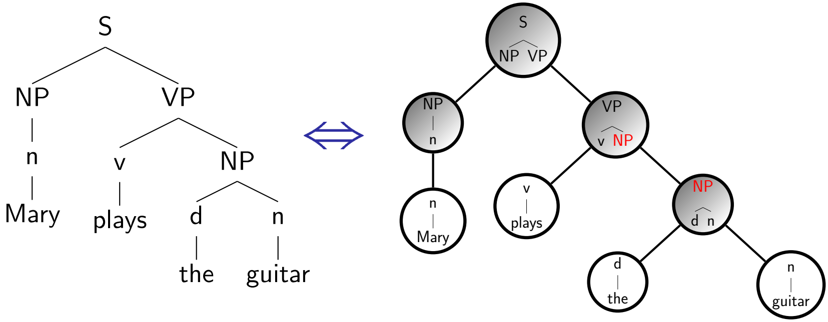
  - $\{\mathbf{A}^1_N\}$ for all $N \in \Sigma^1$ – compute embedding of unary phrases
  - $\{\mathbf{A}^2_N\}$ for all $N \in \Sigma^2$ – compute embedding of binary phrases
- If $t = t_o \odot t_i$
  - $f_A(t) = \alpha_A(t_o)^\top \beta_A(t_i)$
  - $\beta_A(t_i)$: an n-dimensional embedding of an inside tree t_i
    i.e., maps inside trees to similar vectors if they are *replaceable*
  - $\alpha_A(t_o)$: an n-dimensional embedding of an outside tree t_o
    i.e., maps outside trees to similar vectors if they accept similar *arguments*

Production Parse Trees



- A production parse tree represents the edges of a parse tree, i.e. the context-free productions

WFTA on Production Parse Trees



- WFTA operators associated with rule productions
  - i/o compositions constrained by overlapping non-terminal
  - The WFTA induces a separate n-dimensional space per non-terminal, i.e. observed non-terminals are refined
- WFTA on production parse trees include:
  - classic WCFG, for $n = 1$
  - PCFG-LA, for $n > 1$ [Matsuzaki et al 2005, Petrov et al 2006, Cohen et al 2012]

Spectral Learning of Tree Automata

- WFTA are a general algebraic framework for compositional functions
- WFTA can exploit real-valued embeddings
- There are simple algorithms for learning WFTA from samples

Outline

Learning WFA in More General Settings

Data $\longrightarrow$ *Low-rank matrix estimation* $\longrightarrow$ **Hankel matrix** $\longrightarrow$ *Factorization and linear algebra* $\longrightarrow$ **WFA**

Question: How do we use these approach to learn $f : \Sigma^\star \to \mathbb{R}$ where $f(x)$ does not have a probabilistic interpretation?

Learning WFA in More General Settings

Data → *Low-rank matrix estimation* → **Hankel matrix** → *Factorization and linear algebra* → **WFA**

Question: How do we use these approach to learn $f : \Sigma^\star \to \mathbb{R}$ where $f(x)$ does not have a probabilistic interpretation?

Examples:

- Classification $f : \Sigma^\star \to \{+1, -1\}$
- Unconstrained real-valued predictions $f : \Sigma^\star \to \mathbb{R}$
- General scoring functions for tagging: $f : (\Sigma \times \Delta)^\star \to \mathbb{R}$

Example: Hankel Matrices with Missing Entries

When learning probabilistic functions...

entries in $\mathbf{H}_f$ are estimated from empirical counts, e.g. $f(x) = \mathbb{P}[x]$

$$\left\{ \begin{array}{c} \text{aa, b, bab, a,} \\ \text{b, a, ab, aa,} \\ \text{ba, b, aa, a,} \\ \text{aa, bab, b, aa} \end{array} \right\} \longrightarrow \begin{array}{c} \\ \epsilon \\ a \\ b \\ ba \end{array} \begin{array}{c} \begin{array}{cc} a & b \end{array} \\ \begin{bmatrix} .19 & .25 \\ .31 & .06 \\ .06 & .00 \\ .00 & .13 \end{bmatrix} \end{array}$$

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But in a general regression setting...

entries in $\mathbf{H}_f$ are labels observed in the sample, and many may be missing

$$\left\{ \begin{array}{c} \text{(bab,1)} \\ \text{(bbb,0)} \\ \text{(aaa,3)} \\ \text{(a,1)} \\ \text{(ab,1)} \\ \text{(aa,2)} \\ \text{(aba,2)} \\ \text{(bb,0)} \end{array} \right\} \longrightarrow \begin{array}{c c} & \begin{array}{ccc} \epsilon & a & b \end{array} \\ \begin{array}{c} a \\ b \\ aa \\ ab \\ ba \\ bb \end{array} & \left[\begin{array}{ccc} 1 & 2 & 1 \\ \cdot & \cdot & 0 \\ 2 & 3 & \cdot \\ 1 & 2 & \cdot \\ \cdot & \cdot & 1 \\ 0 & \cdot & 0 \end{array} \right] \end{array}$$

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When learning probabilistic functions. . .

entries in $\mathbf{H}_f$ are estimated from empirical counts, e.g. $f(x) = \mathbb{P}[x]$

$$\left\{ \begin{array}{c} \text{aa, b, bab, a,} \\ \text{b, a, ab, aa,} \\ \text{ba, b, aa, a,} \\ \text{aa, bab, b, aa} \end{array} \right\} \longrightarrow \begin{array}{c} \\ \epsilon \\ a \\ b \\ ba \end{array} \begin{array}{c} \begin{array}{cc} a & b \end{array} \\ \begin{bmatrix} .19 & .25 \\ .31 & .06 \\ .06 & .00 \\ .00 & .13 \end{bmatrix} \end{array}$$

But in a general regression setting...

entries in $\mathbf{H}_f$ are labels observed in the sample, and many may be missing

$$\left\{ \begin{array}{c} \text{(bab,1)} \\ \text{(bbb,0)} \\ \text{(aaa,3)} \\ \text{(a,1)} \\ \text{(ab,1)} \\ \text{(aa,2)} \\ \text{(aba,2)} \\ \text{(bb,0)} \end{array} \right\} \longrightarrow \begin{array}{c} \\ a \\ b \\ aa \\ ab \\ ba \\ bb \end{array} \begin{array}{c} \begin{array}{ccc} \epsilon & a & b \end{array} \\ \begin{bmatrix} 1 & 2 & 1 \\ ? & ? & 0 \\ 2 & 3 & ? \\ 1 & 2 & ? \\ ? & ? & 1 \\ 0 & ? & 0 \end{bmatrix} \end{array}$$

Inference of Hankel Matrices

Goal: Learn a Hankel matrix $\mathbf{H} \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}}$ from partial information, *then apply the Hankel trick*

Why is this even possible?

Need only $O((n+m)r)$ coefficients to represent $n \times m$ matrix with rank r

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SVD $$\underbrace{\mathbf{M}}_{n \cdot m} = \underbrace{\mathbf{U}}_{n \cdot r} \underbrace{\mathbf{\Lambda}}_{r} \underbrace{\mathbf{V}^\top}_{m \cdot r}$$

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What partial information about $\mathbf{H}$ *can we hope to gather?*

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Information Models:

- Subset of entries: $\{\mathbf{H}(p, s) | (p, s) \in I\}$
- Linear measurements: $\{\mathbf{H}\mathbf{v} | \mathbf{v} \in V\}$
- Bilinear measurements: $\{\mathbf{u}^\top \mathbf{H}\mathbf{v} | \mathbf{u} \in U, \mathbf{v} \in V\}$
- Constraints between entries: $\{\mathbf{H}(p, s) \geqslant \mathbf{H}(p', s') | (p, s, p', s') \in I\}$
- *Noisy versions of all the above*

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What a priori information about $\mathbf{H}$ do we have?

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Constraints and Inductive Bias:

- Hankel constraints $\mathbf{H}(p, s) = \mathbf{H}(p', s')$ if $ps = p's'$
- Constraints on entries $|\mathbf{H}(p, s)| \leqslant C$
- Low-rank constraints/regularization $\mathrm{rank}(\mathbf{H})$

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Empirical Risk Minimization Approach

Formalize the problem

"find Hankel matrix that agrees with data"

[Balle and Mohri, 2012]

Empirical Risk Minimization Approach

Data: $\{(x^i, y^i)\}_{i=1}^N$, $x^i \in \Sigma^\star$, $y^i \in \mathbb{R}$

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Optimization (constrained formulation):

$$\underset{\mathbf{H} \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}}}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} \ell(y^i, \mathbf{H}(x^i)) \text{ subject to } \operatorname{rank}(\mathbf{H}) \leqslant R$$

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Note: These optimization problems are *non-convex*!

Nuclear Norm Relaxation

Nuclear Norm: matrix $\mathbf{M}$, $\|\mathbf{M}\|_* = \sum \mathfrak{s}_i(\mathbf{M})$

In machine learning, minimizing the nuclear norm is a commonly used convex surrogate for minimizing the rank

Convex Optimization for Hankel matrix estimation

$$\operatorname*{argmin}_{H \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}}} \frac{1}{N} \sum_{i=1}^{N} \ell(y^i, \mathbf{H}(x^i)) + \lambda \|\mathbf{H}\|_*$$

Optimization Algorithms for Hankel Matrix Estimation

Optimizing the Nuclear Norm Surrogate

- Projected/Proximal sub-gradient (e.g. [Duchi and Singer, 2009])
- Frank–Wolfe [Jaggi and Sulovsk, 2010]
- Singular value thresholding [Cai et al., 2010]

Non-Convex "Heuristics"

- Alternating minimization (e.g. [Jain et al., 2013])

Applications of Hankel Matrix Estimation

- Max-margin taggers [Quattoni et al., 2014]
- Unsupervised transducers [Bailly et al., 2013b]
- Unsupervised WCFG [Bailly et al., 2013a]

Outline

Conclusion

- Spectral methods provide new tools to learn compositional functions by means of algebraic operations
- Key result:

  forward-backward recursions $\Leftrightarrow$ low-rank Hankel matrices
- Applicable to a wide range of compositional formalisms: finite-state automata and transducers, context-free grammars, ...
- Relation to loss-regularized methods, by means of matrix-completion techniques

Spectral Learning Techniques for Weighted Automata, Transducers, and Grammars

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TUTORIAL @ EMNLP 2014

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