Spectral Learning of Weighted Automata: from theory to practice

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Context

- 10+ years of research:
  - Premise: [François Denis, Aurélien Lemay, Alain Terlutte. Learning regular languages using RFSAs. 2004]
  - Breakthrough:
    [Raphaël Bailly, François Denis, Liva Ralaivola: Grammatical inference as a principal component analysis problem. 2009]
    and
    [Daniel Hsu, Sham M. Kakade, Tong Zhang. A Spectral Algorithm for Learning Hidden Markov Models. 2009]
  - Readable survey: [Borja Balle, Xavier Carreras, Franco M. Luque, Ariadna Quattoni. Spectral learning of weighted automata - A forward-backward perspective. 2014]
  - To go beyond: [Hadrien Glaude. Méthodes des moments pour l'inférence de systèmes séquentiels linéaires rationnels, PhD thesis, 2016]

Context

- 10+ years of research (lot of researchers - not me)
- 1+ year of programming developments founded by the Laboratoire d'Excellence Archimède (ANR-11-LABX-0033):
  - 2 (part time) research engineers: Denis Arrivault & Dominique Benielli (Archimède Development team)
  - 2 (very part time) researchers: François Denis & myself
  - A first release as a baseline for the SPiCe competition `http://spice.lif.univ-mrs.fr/index.php` (April 2016)
  - Final release as a Scikit-Learn compatible toolbox (version 1.0: October 2016; version 1.2: May 2018)
  - [Denis Arrivault, Dominique Benielli, François Denis, Rémi Eyraud. Scikit-SpLearn: a toolbox for the spectral learning of weighted automata compatible with scikit-learn. 2017]

Outline

Spectral Learning of Weighted Automata (WA)

Scikit SpLearn toolbox

Conclusion and Future developments

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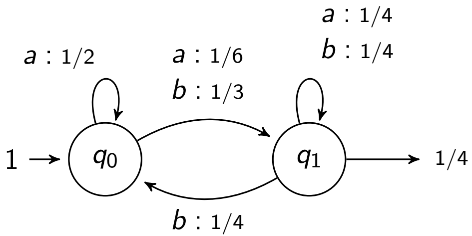
Linear representation of Weigthed Automata



$$\alpha_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \alpha_\infty = \begin{bmatrix} 0 \\ 1/4 \end{bmatrix}$$

$$M_a = \begin{bmatrix} 1/2 & 1/6 \\ 0 & 1/4 \end{bmatrix} \qquad M_b = \begin{bmatrix} 0 & 1/3 \\ 1/4 & 1/4 \end{bmatrix}$$

WA and linear projection

To compute the weight given to $w = \sigma_1 \dots \sigma_m$:

$$\alpha_0^\top M_w \alpha_\infty = \alpha_0^\top M_{\sigma_1} \dots M_{\sigma_m} \alpha_\infty$$

Example in previous WA: $r(bba) = \alpha_0^\top M_b M_b M_a \alpha_\infty = 5/576$

Let $\alpha^i(w)$ such that $\alpha^0(w) = \alpha_0^\top$ and $\alpha^{i+1}(w) = \alpha^i(w) M_{\sigma_i}$.
The jth component of vector α^i is the sum of the weights of all paths that arrive to the state j given the corresponding prefix.

$\alpha^i(w)$ can be seen as a linear projection into $\mathbb{R}^{nb\_states}$. The automaton is then computing the inner product $\langle \alpha^{|w|}, \alpha_0 \rangle$.

Hankel matrix

$$\mathcal{H}_r = \begin{bmatrix} r(\epsilon \cdot \epsilon) & r(\epsilon \cdot a) & r(\epsilon \cdot b) & r(\epsilon \cdot aa) & r(\epsilon \cdot ab) & \dots \\ r(a \cdot \epsilon) & r(a \cdot a) & r(a \cdot b) & r(a \cdot aa) & r(a \cdot ab) & \dots \\ r(b \cdot \epsilon) & r(b \cdot a) & r(b \cdot b) & r(b \cdot aa) & r(b \cdot ab) & \dots \\ r(aa \cdot \epsilon) & r(aa \cdot a) & r(aa \cdot b) & r(aa \cdot aa) & r(aa \cdot ab) & \dots \\ r(ab \cdot \epsilon) & r(ab \cdot a) & r(ab \cdot b) & r(ab \cdot aa) & r(ab \cdot ab) & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ & & & & & \end{bmatrix}$$

Theorem [Carlyle & Paz,1971; Flies, 1974]:
A rational series $r : \Sigma^* \to \mathbb{R}$ can be defined by a WA iff the rank of its Hankel matrix is finite. In that case this rank is the minimal number of states of any WA that computes r.

Hankel Basis

- Only finite sub-blocks of a Hankel matrix are of interest
- Defined over a basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$
  - $\mathcal{P}$ is a set of rows (prefixes)
  - $\mathcal{S}$ is a set of columns (suffixes)
- $H_{\mathcal{B}}$ is the Hankel matrix restricted to $\mathcal{B}$
- 2 important properties:
  - prefix-close
  - complete

From a Hankel matrix to a WA

[Bailly et al., 2009; Hsu et al.,2009; Balle et al.,2014]:

- Given H a Hankel matrix of a series r and $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ a *complete prefix-close* basis
- For $\sigma \in \Sigma$, let H_σ the sub-block on the basis $(\mathcal{P}\sigma, \mathcal{S})$
- $H_{\mathcal{B}} = PS$ a rank factorization, *i.e.* $P \in \mathcal{R}^{p \times rank(r)}$ and $S \in \mathcal{R}^{rank(r) \times s}$
- Then $\langle \alpha_0, (M_\sigma)_{\sigma \in \Sigma}, \alpha_\infty \rangle$ is a minimal WA for r with
  - $\alpha_0^\top = h_{\epsilon,\mathcal{S}}^\top S^+$
  - $\alpha_\infty = P^+ h_{\mathcal{P},\epsilon}$
  - $M_\sigma = P^+ H_\sigma S^+$

  where $h_{\mathcal{P},\epsilon} \in \mathbb{R}^{\mathcal{P}}$ denotes the p-dimensional vector with coordinates $h_{\mathcal{P},\epsilon}(u) = r(u)$, and $h_{\epsilon,\mathcal{S}}$ the s-dimensional vector with coordinates $h_{\epsilon,\mathcal{S}}(v) = r(v)$

Hankel matrix variants

- The *prefix Hankel matrix*: $H^p(u, v) = r(uv\Sigma^*) = r_p(uv)$ for any $u, v \in \Sigma^*$. Rows are indexed by prefixes and columns by factors (substrings).
- The *suffix Hankel matrix*: $H^s(u, v) = r(\Sigma^* uv) = r_s(uv)$ for any $u, v \in \Sigma^*$. Rows are indexed by factors and columns by suffixes.
- The *factor Hankel matrix*: $H^f(u, v) = r(\Sigma^* uv\Sigma^*) = r_f(uv)$ for any $u, v \in \Sigma^*$. In this matrix both rows and columns are indexed by factors.

Theorem [Balle et al, 2014; Gybels et al., 2014]:
The ranks of r_p, r_s, and r_f are all equal to the rank of r.

Spectral learning of WA

- Fix a Hankel variant, a basis, and a rank value
- Estimate the corresponding Hankel sub-block(s) using the training data (positive examples only)
- Compute the truncated singular value decomposition (SVD) (gives you a rank factorization)
- Generate the corresponding WA

Some theoretical results

[Hsu et al., 2009] With high probability:

$$||H_{\mathcal{B}} - \hat{H}_{\mathcal{B}}||_F \leq \mathcal{O}(\frac{1}{\sqrt{m}})$$

where m is the number of examples and $\hat{H}_{\mathcal{B}}$ the *empirical Hankel sub-block*.

[Bailly et al., 2009] $\hat{H}_{\mathcal{B}}$ is of full rank with probability one.

[Balle & Mohri, 2018] The Rademacher complexity of the class of WA with n states is bounded.

Extension

- Spectral Learning of Weighted Tree Automata: [Bailly et al., 2010; Rabusseau et al., 2015]
- Spectral Learning of Graph Weighted Models: [Rabusseau, 2018]
- Multitask Spectral Learning of Weighted Automata [Rabusseau et al., 2017]
- A priori basis selection [Quattoni et al., 2017]
- Nonlinear Weighted Finite Automata [Li et al., 2017]

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Spectral Learning of Weighted Automata (WA)

Scikit SpLearn toolbox

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Toolbox environment

- Scikit-Learn: a toolbox with main machine learning algorithms, widely used.

- Written in Python 3.5 (compatible 2.7)
- Easy installation:

  `pip install scikit-splearn`
- Sources easily downloadable (Free BSD license): `https://pypi.python.org/pypi/scikit-splearn`
- Detailed documentation and more: `http://pageperso.lis-lab.fr/~remi.eyraud/scikit-splearn/`

Content

4 classes:

- Automaton: a linear representation of WA, including useful methods (e.g. numerically stable PA minimization)
- Datasets.base: to load samples
- Hankel: for Hankel matrices, with a bunch of tools
- Spectral: main class, with functions `fit`, `predict`, `score` and many other

Load data

Function `load_data_sample` loads from a file with usual GI format and returns a sample in Scikit-Learn format.

```
>>> from splearn.datasets.base import load_data_sample
>>> train = load_data_sample("3.pautomac.train")
>>> train.nbEx
20000
>>> train.nbL
4
```

Splearn-array

Inherit from python `numpy` `ndarray` object

```
>>> train.data
SplearnArray([[ 3.,  0.,  3., ..., -1., -1., -1.],
              [ 3.,  3., -1., ..., -1., -1., -1.],
              [ 3.,  2.,  0., ..., -1., -1., -1.],
              ...,
              [ 3.,  1.,  3., ..., -1., -1., -1.],
              [ 3.,  3., -1., ..., -1., -1., -1.],
              [ 3.,  1.,  3., ..., -1., -1., -1.]])
```

Contains also the dictionaries `train.data.sample`, `train.data.pref`, `train.data.suff`, and `train.data.fact` (empty at that moment).

Estimator: Spectral

- Inherit from BaseEstimator (sklearn.base)
- parameters:
  - `rank`: the value for the rank factorization
  - `version`: the variant of Hankel matrix to use
  - `sparse`: if `True`, uses a sparse representation for the Hankel matrix
  - `partial`: if `True`, computes only a specified sub-block of the Hankel matrix
  - `lrows` and `lcolumns`: if `partial` is `True`, either integers corresponding to the max length of elements to consider, or list of strings to use for the Hankel matrix
  - `smooth_method`: `'none'` or `'trigram'` (so far)
  - `full_svd_calculation`: random or full SVD computation
  - `mode_quiet`

Estimator: Spectral

Usage:

```
>>> from splearn.spectral import Spectral
>>> est = Spectral()
>>> est.get_params()
{'rank': 5, 'version': 'classic', 'lrows': 7,
    'lcolumns': 7, 'partial': True, 'sparse': True,
    'full_svd_calculation': False,
    'smooth_method': 'none', 'mode_quiet': False}
>>> est.set_params(lrows=5, lcolumns=5,
                   smooth_method='trigram',
                   version='factor')
Spectral(full_svd_calculation=False, lcolumns=5,
    lrows=5, mode_quiet=False, partial=True, rank=5,
    smooth_method='trigram', sparse=True,
    version='factor')
```

Estimator: Spectral

Main methods:

- **fit**(self, X, y=None)
- **predict**(self, X)
- **predict_proba**(self,X)
- **loss**(self, X, y=None)
- **score**(self, X, y=None, scoring="perplexity")
- **nb_trigram**(self)

SpLearn use case

```
>>> est.fit(train.data)
Start Hankel matrix computation
End of Hankel matrix computation
Start Building Automaton from Hankel matrix
End of Automaton computation
Spectral(full_svd_calculation=False, lcolumns=5, lrows=5,
     mode_quiet=False,partial=True, rank=5,
     smooth_method='trigram', sparse=True, version='factor
>>> test = load_data_sample("3.pautomac.test")
>>> est.predict(test.data)
array([3.23849562e-02, 1.24285813e-04, ...
...])
>>> est.nb_trigram()
80
```

SpLearn use case (cont'd)

```
>>> #Create y vector for supervised evaluation
>>> targets = open("3.pautomac_solution.txt", "r")
>>> targets.readline()   #get rid of nb lines
>>> target_proba = [float(line[:-1]) for line in targets]
>>>
>>> # Compute the means of squared differences
>>> est.loss(test.data, y=target_proba)
2.162725190444073e-05
>>> # Compute the perplexity
>>> est.score(test.data, y=target_proba)
71.49521987246547
```

SpLearn and Scikit methods

- Cross-validation

```
>>> from sklearn.model_selection import cross_val_score
>>> est.set_params(mode_quiet=True)
>>> scores = cross_val_score(est, train.data, cv=5)
>>> scores
array([-10.11871728, -10.44673223, -10.36855581,
   -10.39396116, -10.34336961])
>>> scores = cross_val_score(est, test.data,
                             target_proba, cv=5)
>>> scores
array([31.52112125, 80.45998967, 87.53014326,
       73.43037055, 73.30544451])
```

SpLearn and Scikit methods

- Gridsearch

```
>>> from sklearn.model_selection import GridSearchCV
>>> param = {'version': ['suffix','prefix'],
             'lcolumns': [5, 6, 7], 'lrows': [5, 6, 7]}
>>> grid = GridSearchCV(est, param)
>>> grid.fit(train.data)
GridSearchCV(cv=None, error_score='raise',
       estimator=Spectral(...),
       fit_params=None, iid=True, n_jobs=1,
       param_grid={'version': ['suffix', 'prefix'],
          'lcolumns': [5, 6, 7], 'lrows': [5, 6, 7]},
       pre_dispatch='2*n_jobs', refit=True,
       return_train_score='warn', scoring=None,
       verbose=0)
>>> grid.best_params_
{'lcolumns': 5, 'lrows': 7, 'version': 'prefix'}
```

- And all other (not contractual...) Scikit-learn methods

More than a learning toolbox

- Lots of tools to play with weighted automata:
  - A numerically stable and parametrized minimization algorithm
  - Possibilities of saving or downloading an automaton
  - Visualization methods
  - Prefix/Suffix/Factor/Next symbol transformation
  - Test for absolute convergence
  - ...
- Data treatments
- Results analysis

New in version 1.2: modularity for learning

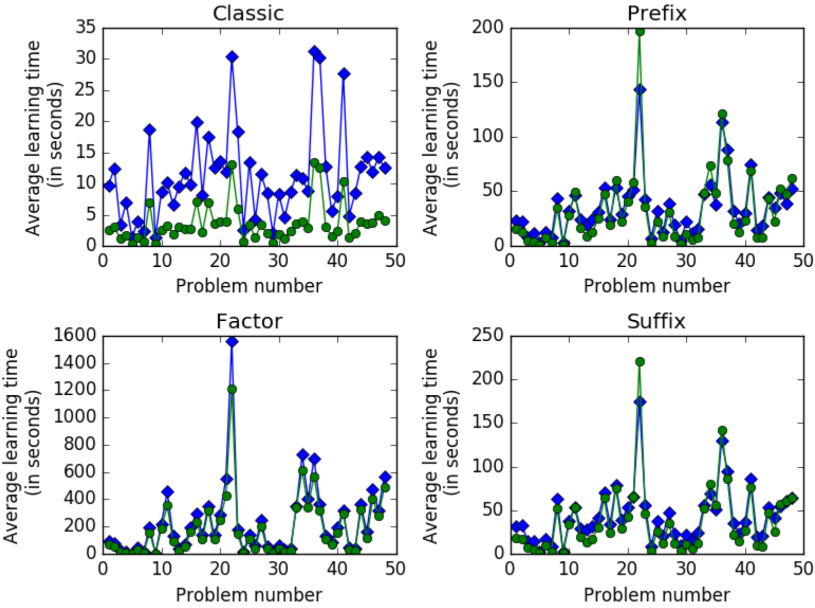
- Decomposition of the spectral learning algorithm:
  - `polulate_dictionnaries(Spectral.self, X)`: creates the needed dictionaries (prefixes/suffixes/factors of needed sizes)
  - `Hankel(sample_instance,` *`+ parameters of fit`*`)`: creates the needed blocks of Hankel
  - `to_automaton(Hankel.self, rank, mode_quiet)`: creates the WA from the Hankel blocks.
- Different uses: for instance, to evaluate a black-box

Outline

Conclusion

- Tested (unitary, 95% coverage)
- Used on all 48 PAutomaC data (results in the article)
    - `rank` between 2 and 40
    - `lrows` and `lcolumns` between 2 and 6
    - for all 4 Hankel matrix variants
    - a total of 28 000+ runs

Time comparison between sp2learn and splearn



Future developments

- Data generation tools
- Basis selection function(s)
- Other scoring functions (WER, KL, NDCG ...)
- Real smoothing methods (Baum-Welch?)
- Other Method of Moments algorithms
- Moving to tree automata

Any comment (and help) welcomed!

Some advertisement to finish: 2 upcoming events

- LearnAut 2018:
  - mid-FLoC workshop
  - July 13th, Oxford, UK
  - Early registration deadline: June 6th
  - Nice program, including 4 invited talks:
    - Doina Precup (McGill University & DeepMind, Canada)
    - Alexander Clark (King's College London, UK)
    - Kousha Etessami (University of Edinburg, UK)
    - George Argyros (Columbia University, USA)
  - `https://learnaut2018.wordpress.com/`
- ICGI 2018
  - 14th International Conference in Grammatical Inference
  - September 5-7 2018, Wrocław, Poland
  - submission deadline: June 15
  - preliminary works also welcomed
  - `http://icgi2018.pwr.edu.pl/`