Scikit-SpLearn : a toolbox for the spectral learning of weighted automata compatible with scikit-learn*†

Denis Arrivault[1], Dominique Benielli[1], François Denis[2], et Rémi Eyraud[2]

[1]LabEx Archimède, Aix-Marseille University, France
[2]QARMA team, Laboratoire d'Informatique Fondamentale de Marseille, France

Résumé

Scikit-SpLearn is a Python toolbox for the spectral learning of weighted automata from a set of strings, licensed under Free BSD, and compatible with the well-known scikit-learn toolbox. This paper gives the main formal ideas behind the spectral learning algorithm and details the content of the toolbox. Use cases and an experimental section are also provided.

Mots-clef : Toolbox, Spectral Learning, Weighted Automata

1 Introduction

Grammatical inference is a sub-field of machine learning that mainly focuses on the induction of grammatical models such as, for instance, finite state machines and generative grammars. However, the core of this field may appear distant from mainstream machine learning : the methods, algorithms, approaches, paradigms, and even mathematical tools used are usually not the ones of statistical machine learning.

There exists one important exception to this observation : the recent developments of what is called spectral learning are building a bridge between these two facets of machine learning. Indeed, by allowing the use of linear algebra in the context of finite state machine learning, tools of statistical machine learning are now usable to infer grammatical formalisms.

The initial idea of spectral learning is to describe finite state machines using linear representations : instead of sets of states and transitions, these equivalent models are made of vectors and matrices [BR88]. The class of machines representable with these formalisms is the one of Weighted Automata (WA) [1] [Moh09], sometimes called multiplicity automata [BBB+96], that are a strict generalization of Probabilistic Automata (PA) [Sch61], of Hidden Markov Models (HMM) [DDE05], and of Partially Observable Markov Decision Processes (POMDP) [TJ15] .

The corner stone of the spectral learning approach is the use of what is called the Hankel matrix. In its classical version, this bi-infinite matrix has rows that correspond to prefixes and columns to suffixes : the value of a cell is then the weight of the corresponding sequence in the corresponding WA. Importantly, the rank of this matrix is the number of states of a minimal WA computing the weights : this allows the construction of this automaton from a rank factorization of the matrix [BCLQ14].

Following this result, the behavior of the spectral learning algorithm relies on the construction of a finite sub-block approximation of the Hankel matrix from a sample of sequences. Then, using a Singular Value Decomposition of this empirical Hankel matrix, one can obtain a rank factorization and thus a weighted automaton.

From the seminal work of Hsu et al. [HKZ09] and Bailly et al. [BDR09], important developments have been achieved. For example, Siddiqi et al. [SBG10] obtain theoretical guaranties for low-rank HMM ; A PAC-learning result is provided by Bailly [Bai11] for stochastic weighted automata ; Balle et al. [BCLQ14] extend the algorithm to variants of the Hankel matrix and show their interest for natural language processing ; Extensions to the spectral learning of weighted tree automata have been published by Bailly et al. [BHD10].

In the context of this great research effervescence,

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1. Only WA whose weights are real numbers are considered in this work.

we felt that an important piece was missing which would help the widespread adoption of spectral learning techniques : an easy to use and to install program with broad coverage to convince non-initiated researchers about the interest of this approach. This is the main motivation behind the project of the scikit Spectral Learning (Scikit-SpLearn) Python toolbox [2] that this paper presents. Indeed, this software contains several variants of the spectral learning algorithm, together with optimized data structures (for instance an implementation of weighted automata), and is compatible with the internationally known scikit-learn toolbox [PVG+11].

We notice that a code for 3 methods of moments, including a spectral learning algorithm, is available at https ://github.com/ICML14MoMCompare/spectral-learn. However, this code was designed for a research paper and suffers many limitations, as for instance only a small number of data sets, the one studied in the article, can be used easily.

Section 2 gives formal details about the spectral learning of weighted automata. Section 3 carefully describes the toolbox content and provides use cases. Some experiments showing the potential of Scikit-SpLearn are given in Section 4, while Section 5 concludes by giving ideas for future developments.

2 Spectral learning of weighted automata

2.1 Weighted Automata

A finite set of symbols is called an alphabet. A string over an alphabet Σ is a finite sequence of symbols of Σ. Σ^* is the set of all strings over Σ. The length of a string w is the number of symbols in the string. We let ϵ denote the empty string, that is the string of length 0. For any $w \in \Sigma^*$, let $pref(w) = \{u \in \Sigma^* : \exists v \in \Sigma^*, uv = w\}$ be its set of prefixes, $suff(w) = \{u \in \Sigma^* : \exists v \in \Sigma^*, vu = w\}$ be its set of suffixes, and $fact(w) = \{u \in \Sigma^* : \exists l, r \in \Sigma^*, lur = w\}$ be the set of factors of w (sometime called the set of substrings).

The following definitions are adapted from Mohri [Moh09] :

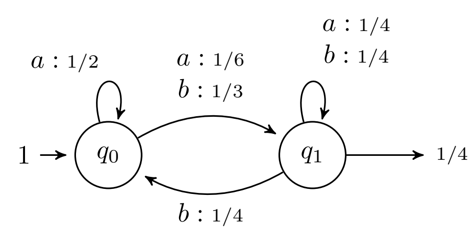
Définition 1 (Weighted automaton) *A weighted automaton (WA) is a tuple $\langle \Sigma, Q, I, F, \mathcal{T}, \lambda, \rho \rangle$ such that : Σ is a finite alphabet ; Q is a finite set of states ; $\mathcal{T} : Q \times \Sigma \times Q \to \mathbb{R}$ is the transition function ; $\lambda : Q \to \mathbb{R}$ is an initial weight function ; $\rho : Q \to \mathbb{R}$ is a final weight function.*

A transition is usually denoted (q_1, σ, p, q_2) instead of $\mathcal{T}(q_1, \sigma, q_2) = p$. We say that two transitions $t_1 = (q_1, \sigma_1, p_1, q_2)$ and $t_2 = (q_3, \sigma_2, p_2, q_4)$ are consecutive if $q_2 = q_3$. A path π is an element of $\mathcal{T}^*$ made of consecutive transitions. We denote by $o[\pi]$ its origin and by $d[\pi]$ its destination. The weight of a path is defined by $\mu(\pi) = \lambda(o[\pi]) \times \omega \times \rho(d[\pi])$ where ω is the multiplication of the weights of the constitutive transitions of π. We say that a path $(q_0, \sigma_1, p_1, q_1) \ldots (q_{n-1}, \sigma_n, p_n, q_n)$ reads a string w if $w = \sigma_1 \ldots \sigma_n$. The weight of a string w is the sum of the weights of the paths that read w.

A series r over an alphabet Σ is a mapping $r : \Sigma^* \to \mathbb{R}$. A series r over Σ^* is *rational* if there exists an integer $k \geq 1$, vectors $I, T \in \mathbb{R}^k$, and matrices $M_\sigma \in \mathbb{R}^{k \times k}$ for every $\sigma \in \Sigma$, such that for all $u = \sigma_1 \sigma_2 \ldots \sigma_m \in \Sigma^*$,

$$r(u) = I M_u T = I M_{\sigma_1} M_{\sigma_2} \ldots M_{\sigma_m} T$$

The triplet $\langle I, (M_\sigma)_{\sigma \in \Sigma}, T \rangle$ is called a *k-dimensional linear representation* of r. The rank of a rational series r is the minimal dimension of a linear representation of r. Linear representations are equivalent to weighted automata where each coordinate corresponds to a state, the vector I provides the initial weights (*i.e.* the values of function λ), the vector T is the terminal weights (*i.e.* the values of function ρ), and each matrix M_σ corresponds to the σ-labeled transition weights ($M_\sigma(q_1, q_2) = p \iff (q_1, \sigma, p, q_2)$ is a transition).



$$I = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad T = \begin{bmatrix} 0 \\ 1/4 \end{bmatrix}$$

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

FIGURE 1 – A weighted automaton and the equivalent linear representation.

In what follows, we will confound the two notions and consider that weighted automata are defined in terms of linear representations.

A particular kind of WA is of main interest in the spectral learning framework : a weighted automata A

2. A previous version of the toolbox, not compatible with scikit-learn, was released as a toolbox for the Sequence PredIction ChallengE (SPiCe), an on-line competition [BEL+16].

is *stochastic* if the series r it computes is a probability distribution over Σ^*, *i.e.* $\forall x \in \Sigma^*, r(x) \geq 0$ and $\sum_{x\in\Sigma^*} r(x) = 1$. These WA enjoy properties that are important for learning. For instance, in addition to the probability of a string $r(x)$, a WA can compute the probability of a string to be a prefix $r_p(x) = r(x\Sigma^*)$, or to be a suffix $r_s(x) = r(\Sigma^* x)$. It can be shown that the rank of the series r, r_p, and r_s are equal [BCLQ14]. Other properties of stochastic WA are of great interest for spectral learning but it is beyond the scope of this paper to describe them all. We refer the Reader to the work of Balle et al. [BCLQ14] for more details.

Finally, stochastic weighted automata are related to other finite state models : they are strictly more expressive than Probabilistic Automata [DEH06] (which are equivalent to discrete Hidden Markov Models [DDE05]) and thus than Deterministic Probabilistic Automata [CO94].

2.2 Hankel matrices

The following definitions are based on the ones of Balle et al.[BCLQ14].

Définition 2 *Let r be a rational series over Σ. The Hankel matrix of r is a bi-infinite matrix $H \in \mathbb{R}^{\Sigma^*\times\Sigma^*}$ whose entries are defined as $H(u, v) = r(uv)$ for any $u, v \in \Sigma^*$. That is, rows are indexed by prefixes and columns by suffixes.*

For obvious reasons, only finite sub-blocks of Hankel matrices are going to be of interest. An easy way to define such sub-blocks is by using a basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$, where $\mathcal{P}, \mathcal{S} \subseteq \Sigma^*$. We write $p = |\mathcal{P}|$ and $s = |\mathcal{S}|$. The sub-block of H defined by $\mathcal{B}$ is the matrix $H_\mathcal{B} \in \mathbb{R}^{p\times s}$ with $H_\mathcal{B}(u, v) = H(u, v)$ for any $u \in \mathcal{P}$ and $v \in \mathcal{S}$. We may just write H if the basis $\mathcal{B}$ is arbitrary or obvious from the context.

In the context of learning weighted automata, the focus is on a particular kind of bases. They are called *closed bases* : a basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ is prefix-closed [3] if there exists a basis $\mathcal{B}' = (\mathcal{P}', \mathcal{S})$ such that $\mathcal{P} = \mathcal{P}'\Sigma'$, where $\Sigma' = \Sigma \cup \{\epsilon\}$. A prefix-closed basis can be partitioned into $|\Sigma| + 1$ blocks of the same size (a given string may belong to several blocks) : given a Hankel matrix H and a prefix-closed basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ with $\mathcal{P} = \mathcal{P}'\Sigma'$, we have, for a particular ordering of the elements of $\mathcal{P}$:

$$H_\mathcal{B}^\top = [H_\epsilon^\top | H_{\sigma_1}^\top | H_{\sigma_2}^\top | \ldots | H_{\sigma_{|\Sigma|}}^\top]$$

where H_σ are sub-blocks defined over the basis $(\mathcal{P}'\sigma, \mathcal{S})$ such that $H_\sigma(u, v) = H(u\sigma, v)$. The notation uses here means that $H_\mathcal{B}^\top$ can be restricted to each of the other sub-blocks.

The rank of a rational series r is equal to the rank of its Hankel matrix H which is thus the number of states of a minimal weighted automaton that represents r. The rank of a sub-block cannot exceed the rank of H and we are interested by full rank sub-blocks : a basis $\mathcal{B}$ is *complete* if $H_\mathcal{B}$ has full rank, that is $rank(H_\mathcal{B}) = rank(H)$.

We will consider different variants of the classical Hankel matrix H of an absolutely convergent series r, i.e. $\sum_w |r(w)|$ converges :

- H^p is the *prefix Hankel matrix*, where $H^p(u, v) = r(uv\Sigma^*) = \sum_w r(uvw)$ for any $u, v \in \Sigma^*$. In this case rows are indexed by prefixes and columns by factors.
- H^s is the *suffix Hankel matrix*, where $H^s(u, v) = r(\Sigma^* uv) = \sum_w r(wuv)$ for any $u, v \in \Sigma^*$. In this matrix rows are indexed by factors and columns by suffixes.
- H^f is the *factor Hankel matrix*, where $H^f(u, v) = \sum_{w_1,w_2} r(w_1uvw_2)$ [4] for any $u, v \in \Sigma^*$. In this matrix both rows and columns are indexed by factors.

2.3 Hankel matrices and WA

We consider a rational series r, H its Hankel matrix, and $A = \langle I, (M_\sigma)_{\sigma\in\Sigma}, T\rangle$ a minimal WA computing r. We suppose that A has n states.

We first notice that A induces a *rank factorization* of H : we have $H = PS$, where $P \in \mathbb{R}^{\Sigma^*\times n}$ is such that its u^{th} row equals $I^\top M_u$, and similarly $S \in \mathbb{R}^{n\times\Sigma^*}$ is such that its v^{th} column is $M_v T$. Similarly, given a sub-block $H_\mathcal{B}$ of H defined by the basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ we have $H_\mathcal{B} = P_\mathcal{B} S_\mathcal{B}$ where $P_\mathcal{B} \in \mathbb{R}^{P\times n}$ and $S_\mathcal{B} \in \mathbb{R}^{n\times S}$ are restrictions of P and S on $\mathcal{P}$ and $\mathcal{S}$, respectively. Besides, if $\mathcal{B}$ is complete then $H_\mathcal{B} = P_\mathcal{B} S_\mathcal{B}$ is a rank factorization.

Moreover, the converse occurs : given a sub-block $H_\mathcal{B}$ of H defined by the complete basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$, one can compute a minimal WA for the corresponding rational series r using a rank factorization PS of $H_\mathcal{B}$. Let H_σ be the sub-block of the prefix closure of $H_\mathcal{B}$ corresponding to the basis $(\mathcal{P}\sigma, \mathcal{S})$, and let $h_{\mathcal{P},\epsilon} \in \mathbb{R}^\mathcal{P}$ 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

3. Similar notions of closure can be designed for suffix and factor.

4. Note that even if r is a rational stochastic language, the series $w \to r(\Sigma^* w \Sigma *)$, i.e. the probability that w appears as a factor of a string drawn at random, may be not rational [DGH16].

$h_{\epsilon,\mathcal{S}}(v) = r(v)$. Then the WA $A = \langle I, (M_\sigma)_{\sigma\in\Sigma}, T\rangle$, with $I^\top = h_{\epsilon,\mathcal{S}}^\top S^+$, $T = P^+ h_{\mathcal{P},\epsilon}$, and $M_\sigma = P^+ H_\sigma S^+$, is minimal for r [BCLQ14]. As usual, N^+ denotes the Moore-Penrose pseudo-inverse of a matrix N.

2.4 Learning weighted automata using spectral learning

The core idea of the spectral learning of weighted automata is to use a rank factorization of a complete sub-block of the Hankel matrix of a target series to induce a weighted automaton.

Of course, in a learning context, one does not have access to the Hankel matrix : all that is available is a (multi-)set of strings $LS = \{x^1, \dots, x^m\}$, usually called a learning sample. The learning process thus relies on *the empirical Hankel matrix* given by $\hat{H}_\mathcal{B}(u,v) = \hat{\mathbb{P}}_{LS}(u,v)$ where $\mathcal{B}$ is a given basis and $\hat{\mathbb{P}}_{LS}$ is the observed frequency of strings inside LS. Hsu et al. [HKZ09] proves that with high probability we have $||H_\mathcal{B} - \hat{H}_\mathcal{B}||_F \leq \mathcal{O}(\frac{1}{\sqrt{m}})$ (see Denis et al. [DGH16] for other concentration bounds).

In the learning framework we are considering, we suppose that there exists an unknown rational series r of rank n and we want to infer a WA for r. We are assuming that we know a complete basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ and have access to a learning sample LS. Obviously, we can compute sub-blocks H_σ for $\sigma \in \Sigma'$, $h_{\mathcal{P},\epsilon}$, and $h_{\epsilon,\mathcal{S}}$ from LS. Thus, the only thing needed is a rank factorization of $\hat{H}_\mathcal{B} = H_\epsilon$. We are going to use the compact Singular Value Decomposition (SVD).

The SVD of a $p \times s$ matrix H_ϵ of rank n is $H_\epsilon = U\Lambda V^\top$ where $U \in \mathbb{R}^{p\times n}$ and $V \in \mathbb{R}^{s\times n}$ are orthogonal matrices, and $\Lambda \in \mathbb{R}^{n\times n}$ is a diagonal matrix containing the singular values of H_ϵ. An important property is that $H_\epsilon = (U\Lambda)V^\top$ is a rank factorization. As V is orthogonal, we have $V^\top V = I$ and thus $V^+ = V^\top$. Using previously described results (see Section 2.3), this allows the inference of a WA $A = \langle I, (M_\sigma)_{\sigma\in\Sigma}, T\rangle$ such that :

$$I^\top = h_{\epsilon,\mathcal{S}}^\top V$$

$$T = (H_\epsilon V)^+ h_{\mathcal{P},\epsilon}$$

$$M_\sigma = (H_\epsilon V)^+ H_\sigma V$$

These equations are what is called the spectral learning algorithm. The Reader interested in more details about spectral learning is referred to the work of Balle et al. [BCLQ14].

3 Toolbox description

The Scikit-SpLearn toolbox is made of 5 Python classes and implements several variants of the spectral learning algorithm. A detailed documentation and a technical manual are available on-line at http ://pageperso.lif.univ-mrs.fr/∼remi.eyraud/scikit-splearn/, it enjoys an easy installation process and is extremely tunable due to the wide range of parameters allowed. An earlier version [ABDE16], not compatible with scikit-learn, was released in the context of the SPiCe competition [BEL+16].

3.1 The different classes

The corner stone of the toolbox is the `Automaton` class. It implements weighted automata as linear representations and offers valuable methods, such as computing the weight of a string or the sum of the weights of all strings, testing absolute convergence, etc. Two particular methods are worth being detailed. The first one consists in a numerically robust and stable minimization following the work of Kieffer et al. [KW14]. The second is a transformation method that constructs a WA from a given one computing $r(\cdot)$ such that the new WA computes the prefix weights $r_p(\cdot)$, the suffix ones $r_s(\cdot)$, or the factor ones $r_f(\cdot)$. Moreover, the reverse conversion is also doable with this method.

The second and third classes, `datasets/base.py` and `datasets/data_sample.py`, are used to parse a learning sample in the now standard PAutomaC format [VEdlH14] and to create an array representing these data, following the requirements of scikit-learn. This object type is called `Splearn_array` and is made of the needed array and of several dictionaries that are used to represent the data in a form more efficient for the learning algorithm : they are the dictionaries of prefixes, suffixes, or factors, needed to build the Hankel matrix from a sample.

The class named `Hankel` is a private class that creates a Hankel matrix from a `Splearn_array` instance containing all needed dictionaries.

Finally, the class `Spectral` is the core of the toolbox : the main methods required by scikit-learn are implemented within this class that we detail below.

3.2 Installing Scikit-SpLearn

The installation of the toolbox is made easy by the use of `pip` : one just has to execute `pip install scikit-splearn` in a terminal.

If needed, the package can be downloaded at https ://pypi.python.org/pypi/scikit-splearn.
A technical documentation is available at https ://pythonhosted.org/scikit-splearn/.

3.3 Using Scikit-SpLearn

Loading data

Function `load_data_sample` loads and returns a sample in scikit-learn format.

```
>>> from splearn.datasets.base
...    import load_data_sample
>>> train = load_data_sample("1.pautomac.train")
>>> train.nbEx
20000
>>> train.nbL
4
>>> train.data
Splearn_array([[ 5.,  4.,  1., ..., -1., -1., -1.],
       [ 4.,  4.,  7., ..., -1., -1., -1.],
       [ 2.,  4.,  4., ..., -1., -1., -1.],
       ...,
       [ 4.,  1.,  3., ..., -1., -1., -1.],
       [ 0.,  6.,  5., ..., -1., -1., -1.],
       [ 4.,  0., -1., ..., -1., -1., -1.]])
>>> train.data.sample, train.data.pref,
...    train.data.suff, train.data.fact
({}, {}, {}, {})
```

The Spectral estimator

As required, the class `Spectral` inherits from `BaseEstimator` of `sklearn.base`. At the initialization of an instance of the class, these parameters can be specified :

- `rank` is the estimated value for the rank factorization.
- `version` indicates which variant of the Hankel matrix is going to be used (possible values are `classic` for $\hat{H}$, `prefix` for $\hat{H}^p$, `suffix` for $\hat{H}^s$, and `factor` for $\hat{H}^f$).
- `partial` indicates whether all the elements have to be taken into account in the Hankel matrix.
- `lrows` and `lcolumns` can either be lists of strings that form the basis $\mathcal{B}$ of the sub-block that is going to be considered, or integers corresponding to the maximal length of elements of the basis. In the latter case, all elements present in the sample whose length are smaller than the given values are in the basis. This ensures the basis to be complete if enough data is available. These parameters have to be set only when `partial` is activated.
- `smooth_method` can be `'none'` (by default) or `'trigram'` if one wants to replace possible negative weights given by the learned WA by corresponding 3-gram values.
- `mode_quiet` is a boolean indicating whether a run will indicate the different steps followed successively.

Here is a use case for initializing a Spectral estimator

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

The main public methods of the toolbox are implemented in this `Spectral` class :

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

These functions enjoy the exact same arguments than their scikit-learn analogues : **fit** takes a `Splearn_array` as input, populates the dictionaries needed by the set variant of the algorithm, creates the corresponding Hankel matrix, and generates the weighted automaton accordingly ; **predict** and **predict_proba** compute the weights of the strings passed as input (a `Splearn_array`) ; **loss** takes an `Splearn_array` and computes the Log-likelihood or the quadratic difference if target probabilities are given (the lesser the better) ; **score** is giving the inverse of **loss** in default mode (the greater the better) but can also compute the perplexity [CT91] if used with the target probability of each strings.

A possible use case following the previous example can be :

```
>>> est.fit(train.data)
Spectral(lcolumns=5, lrows=5, partial=True, rank=5,
     smooth_method='trigram', sparse=True,
     version='factor', mode_quiet=True)
>>> test = load_data_sample("1.pautomac.test")
>>> est.predict(test.data)
array([  3.23849562e-02,   1.24285813e-04, ...
...])
>>> est.loss(test.data), est.score(test.data)
(23.234189560218198, -23.234189560218198)
>>> est.nb_trigram()
61
>>> targets = open("1.pautomac_solution.txt", "r")
>>> target_proba = [float(r[:-1]) for r in targets]
>>> est.loss(test.data, y=target_proba)
```

```
2.6569772687614514e-05
>>> est.score(test.data, y=target_proba)
46.56212657907001
```

Importantly, Scikit-SpLearn is compatible with scikit-learn, which implies for instance that the evaluating estimator performance functions can be used with Scikit-SpLearn :

```
>>> from sklearn import cross_validation as c_v
>>> c_v.cross_val_score(est, train.data, cv = 5)
array([-17.74749858, -17.63678657, -17.60412108,
      -17.43726243, -17.73316833])
>>> c_v.cross_val_score(est, test.data,
                        target_proba,
                        cv = 5)
array([ 16.48311708,  56.46485233,  111.20384957,
     89.13625474,   28.84640423])

>>> from sklearn import grid_search as g_s
>>> param = {'version': ['suffix','prefix'],
            'lcolumns': [5, 6, 7],
            'lrows': [5, 6, 7]}
>>> grid = g_s.GridSearchCV(est, param, cv = 5)
>>> grid.fit(train.data)
>>> grid.best_params_
{'version': 'prefix', 'lcolumns': 5, 'lrows': 6}
>>> grid.best_score_
-17.636386233284796
```

4 Experiments

We tested the Scikit-SpLearn toolbox on the 48 synthetic problems of the PAutomaC competition [VEdlH14]. These data sets correspond to randomly generated sets of strings from randomly generated probabilistic finite states machines : Hidden Markov Models (HMM), Probabilistic Automata (PA), and Deterministic Probabilistic Automata (DPA). Several sparsity parameters were used to generate various machines for each models.

4.1 Settings

For each problem, PAutomaC provides a training sample (11 with 100 000 strings, the rest with 20 000 strings), a test set of 1 000 strings, the finite state machine used to generate the data, and the probability in this target machine of each string in the test set.

We ran the toolbox on the 48 data sets using the 4 different variants of the (sparse) Hankel matrix. On each problem and for each version, we made the maximal size of elements used for the matrix range from 2 to 6 (these are parameters `lrows` and `lcolumns` of the toolbox). For each of these values, all ranks between 2 and 40 were tried. This represents 28 032 runs of the toolbox, to which we have to subtract 631 runs that correspond to rank values too large comparing to the size of the Hankel matrix. All these computations were done on a cluster and each process was allowed 20Go of RAM and 4 hours computation on equivalent CPUs.

We evaluated the quality of the learning using perplexity, following what was done for the competition. Given a test set TS, it is given by the formula :

$$perplexity(C, TS) = 2^{-(\sum_{x \in TS} \mathbb{P}_T(x) * log(\mathbb{P}_C(x)))}$$

where $\mathbb{P}_T(x)$ is the true probability of x in the target model and $\mathbb{P}_C(x)$ is the candidate probability, that is the one given by the learned WA. Both probabilities have to be normalized to sum to 1 on strings of TS.

Finally, the main problem of spectral learning of weighted automata is that some strings can have negative weights, if not enough data is available. This is the reason of the possible training of a trigram at the same time of the construction of the WA. We thus used this possibility and carefully kept track of this behavior that we detail the result in the next section.

4.2 Results

We want first to notice that the aim of these experiments was to show the global behavior of the toolbox on a broad and vast class of problems. Indeed, spectral learning algorithms are usually used as a first step of a learning process, usually followed by a smoothing phase that tunes the weights of the model without modifying its structure (Gybels et al. [GDH14] use for instance a Baum-Welch approach for that second step). We did not work on that since the aim was to show the potentiality of the toolbox.

However, the results of the best run on each problem, given in Table 1 (in Annex), show that even without a smoothing phase the toolbox can obtain perplexity scores close to the optimal ones. This would not have permitted the winning of the competition, but it is good enough to be noticed. On can notice that these results are slightly different than the ones published for the first version of the toolbox, Sp2Learn [ABDE16] : in addition to small variations due to numerical instability, a bug in the prefix and suffix variants was fixed which allows these variants to obtain better scores.

The runs realized using the toolbox also allow to evaluate the impact of the value given to the rank parameter. Figure 2 shows the evolution of perplexity on the problems whose target machines are Probabilistic Automata (top) and Deterministic Probabilistic Automata (bottom). This curves were obtained using the classic version of the Hankel matrix for DPA and the factor variant for PA. In both cases, values of `lrows` and `lcolumns` were set to 5.

These results show that in a first phase the perplexity can oscillate when the rank increases. However, in a second phase, the perplexity seems to decrease to a minimal value and then stay stable. This second step is likely to be reached when the value of the rank parameter is equal to the rank of the target machine. At that moment, inferred singular values correspond to the target ones and adding other values later has no impact. Indeed, if the empirical Hankel matrix was the target one, these values would be null. But even if it is not the case, which is likely in this experimental context, the results show that their values are small enough to not degrade the quality of the learning.

Figure 3 shows the average percentage on all problems of the 3-gram uses to find the probability of a test string. Remember that this happens for strings on which the learned automata returns a non-positive weight. These percentages are given for each possible rank parameter. Each curve corresponds to a given value of the size parameter, that is the maximal length of elements taken into account to build the Hankel matrix.

Globally, the use of 3-gram is quite rare, as less than 1.3% of strings requires its use. On the one hand, models built on large Hankel matrices tend to need less uses of 3-gram. On the other hand, models made using a large rank seem to require slightly more uses of 3-gram. This might be due to the overfitting that may occur when the rank parameter is set higher than the actual rank. Notice that no result is possible with large ranks for Hankel matrices made of too few rows and columns : as the dimensions of the matrix are smaller than the asked rank, a SVD cannot be computed.

Finally, Figure 4 shows the learning time of the toolbox on the PAutomaC problems. Each point corresponds to the average computation time of all runs using a given version of the Hankel matrix, in seconds. Clearly, the classic version is the fastest while the factor one is the slowest, suffix and prefix ones are standing in a middle ground. This is expected since the factor version is the less sparse of the Hankel matrix variants. Another not really surprising observation is that the behavior of the prefix and suffix versions are extremely close.

Globally, these values show that the running time of the toolbox is reasonable, even for the slowest variant : on all but one problem the factor version took less than an hour and a half on average.

5 Future developments

The version of the Scikit-SpLearn presented here is 1.1. We are currently working on extending the functionalities of the toolbox, by adding new features for instance related to :

- The word error rate (WER) is a widely used measure for the learning quality.
- Saving and loading WA has to be done efficiently.
- Large automata require sparse representation.
- Basis selection is a topical issue in spectral learning.

We are also planning to develop new useful methods, starting with a Baum-Welch one, that would complete the learning process by allowing a real smoothing phase after the spectral learning one. We might also turn our attention to closely related and promising new algorithms, like the one of Glaude et al. [GP16].

Finally, we are also considering the development of a similar tool for structured inputs, such that tree and graph, as spectral methods have been proposed in this context.

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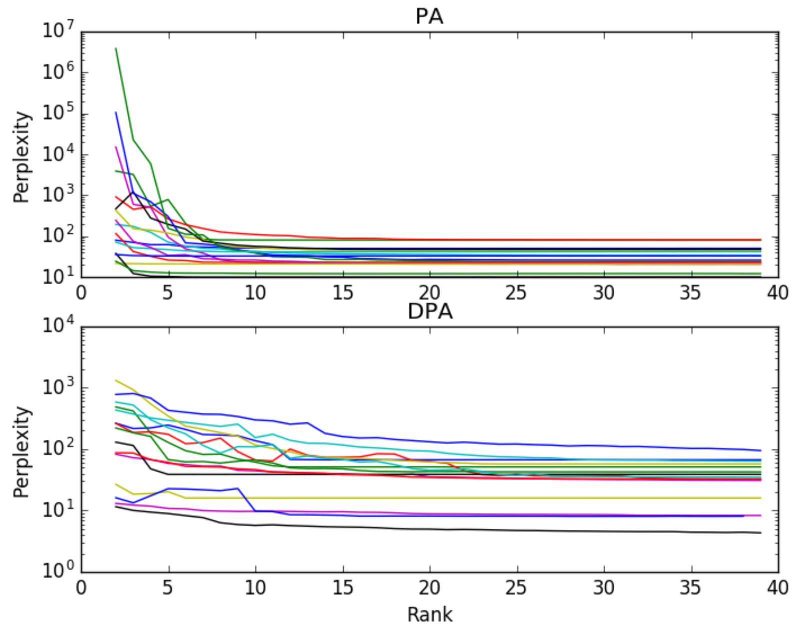

FIGURE 2 – Perplexity evolution with the rank on problems whose targets are Probabilistic Automata (top) and Deterministic Probabilistic Automata (bottom). Each line corresponds to one PAutomaC problem.

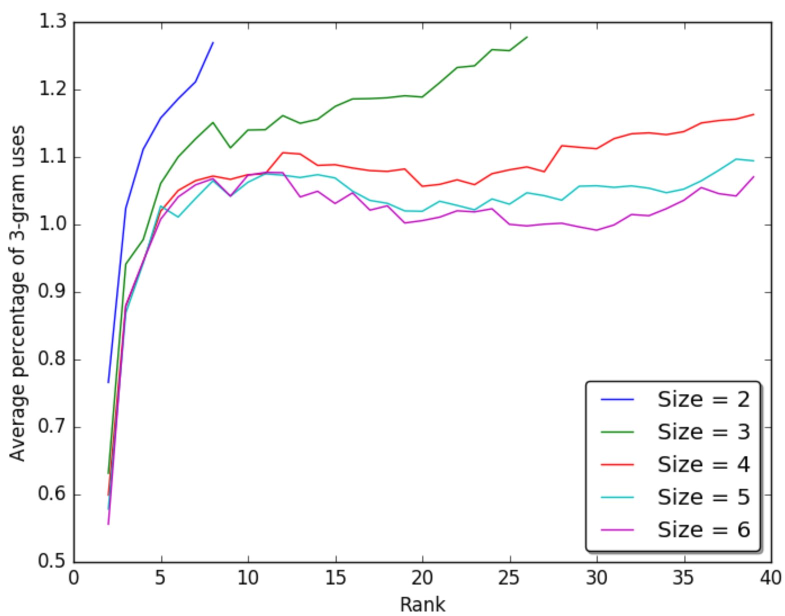

FIGURE 3 – Average percentage of 3-gram uses to find the probability of a test string for different values of the rank parameter (recall that the toolbox uses the trigram iff a test string is given a non-positive value by the learned WA). Each curve corresponds to a value of the maximal length of elements of the Hankel matrix.

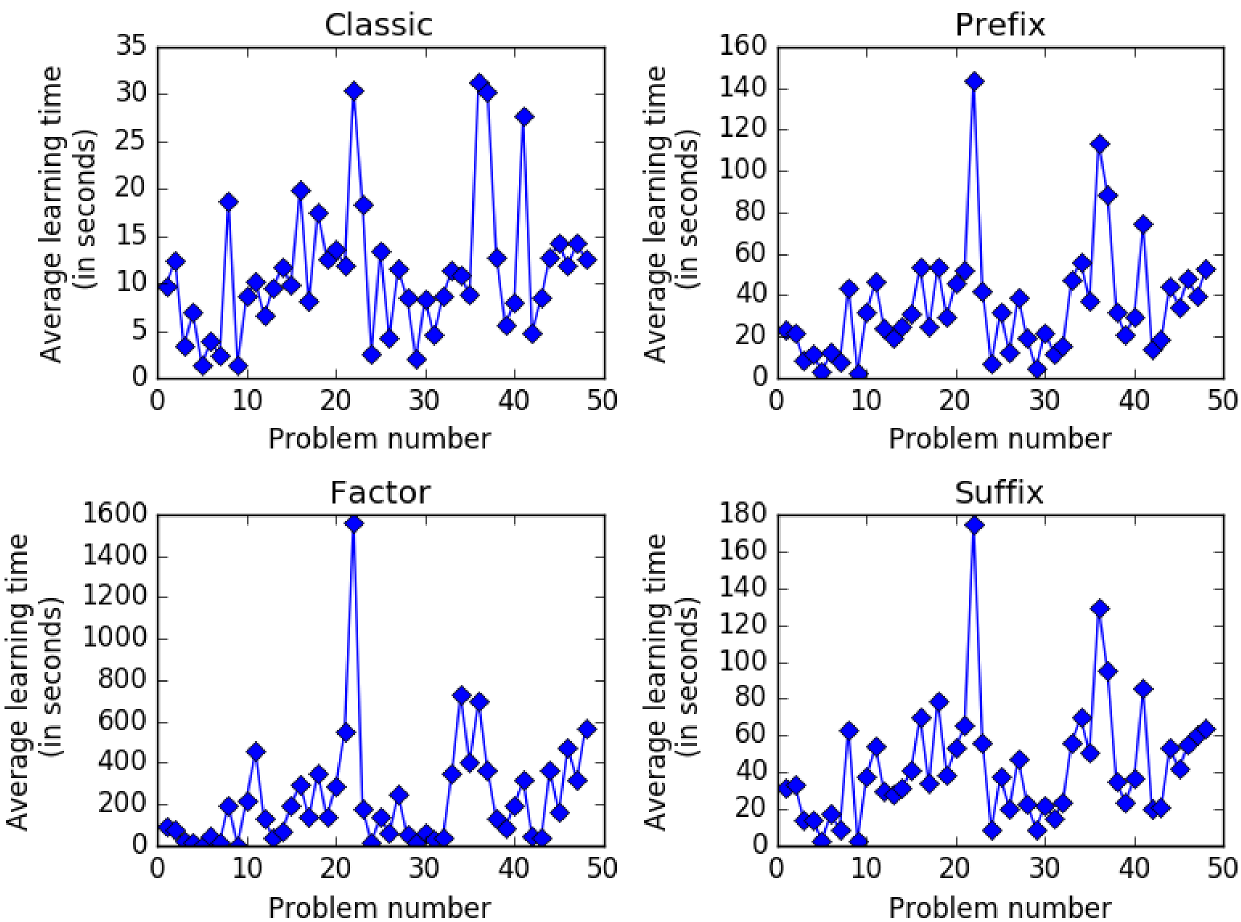

Figure 4 – Average learning time using the 4 variants of the Hankel matrix on the 48 PAutomaC problems.

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Annex

Problem	Solution	Perplexity	Version	Rank	Size	Time
1	29.8978935527	30.35328728565	prefix	28	4	21.962499618
2	168.330805339	168.4673752604	factor	15	3	15.100593090
3	49.956082986	50.269575814	factor	29	4	14.346353054
4	80.8184226132	80.8557036916	factor	11	6	25.159743785
5	33.2352988504	33.2390299542	factor	9	6	2.881478309
6	66.9849579244	67.0522875724	factor	18	6	80.410785913
7	51.2242694583	51.25427076320	factor	12	6	15.491625308
8	81.3750634047	81.6466693978	prefix	39	5	52.629290580
9	20.8395901703	20.88940878005	suffix	37	6	4.552366971
10	33.3030058501	33.9923200515	prefix	39	4	23.416321277
11	31.8113642161	32.2787311808	prefix	39	4	40.661879301
12	21.655287002	21.6701763964	factor	17	5	107.045837163
13	62.8058396015	63.0469463441	classic	39	6	12.809386730
14	116.791881846	116.854374304	factor	7	6	81.706163167
15	44.2420495474	44.3619658374	factor	30	4	96.449448347
16	30.7110624887	30.8283743812	suffix	39	4	71.006728172
17	47.3112160937	47.4862031764	factor	34	4	106.1073915958
18	57.3288608287	57.3331676751	factor	24	5	502.628341436
19	17.8768660563	17.8977286931	suffix	38	5	45.64588999
20	90.9717263176	91.5984831220	factor	8	3	51.1152677536
21	30.518860165	32.0848345134	factor	34	4	360.031714916
22	25.9815361778	26.1185635312	prefix	39	4	105.035097122
23	18.4081615041	18.4317395731	factor	32	5	195.581628561
24	38.7287795405	38.7612120718	suffix	5	6	7.558403968
25	65.7350539501	66.2100554723	factor	23	3	41.1119375228
26	80.7427626831	84.9098521854	classic	39	6	8.6590876579
27	42.427078513	42.6146872776	factor	39	4	189.5968606472
28	52.7435104626	53.0743176494	factor	15	3	8.025611162
29	24.0308339109	24.0839444188	factor	32	5	23.253844738
30	22.925985377	22.9812364259	prefix	9	4	12.742619514
31	41.2136431636	41.4112998547	prefix	12	4	3.970597028
32	32.6134162732	32.6653401781	suffix	36	5	36.127122402
33	31.8650289444	31.9139710172	factor	21	3	56.314493656
34	19.9546848395	20.6207933155	prefix	39	4	72.525197982
35	33.776935538	34.36699781590	prefix	38	4	29.463451862
36	37.985692906	38.11214269249	prefix	33	4	103.591979742
37	20.9797622037	21.0128130185	prefix	18	5	87.288584232
38	21.4457989928	21.5044915638	prefix	5	5	27.591302633
39	10.0020442634	10.0029964620	factor	6	6	106.781083345
40	8.2009545433	8.272854543950	prefix	39	4	37.725449562
41	13.9124713717	13.9374526945	prefix	19	3	22.395074129
42	16.0037636643	16.0087620126	factor	7	3	4.7250144481
43	32.6370243149	32.7816644461	prefix	14	6	33.980755567
44	11.7089059654	11.8216887335	prefix	26	4	37.873082637
45	24.0422109361	24.0468384914	factor	3	3	26.547557353
46	11.9819819343	12.0311419863	factor	38	4	362.170280933
47	4.1189756456	4.176171871767	classic	39	6	30.760368108
48	8.0362199917	8.053478190210	factor	33	5	1054.364390373

Table 1 – Best results on the PAutomaC data. Solution corresponds to the minimal perplexity (the one of the target machine) ; Perplexity is the perplexity obtained by the best run of the toolbox ; Version indicates which version of the Hankel matrix was used ; Rank gives the value of parameter rank for that run ; Size is the maximal length of elements considered for the Hankel matrix ; Time is the computation time of the run (in seconds). Problems marked with a star are the ones whose training set contains 100 000 strings (*vs* 20 000).