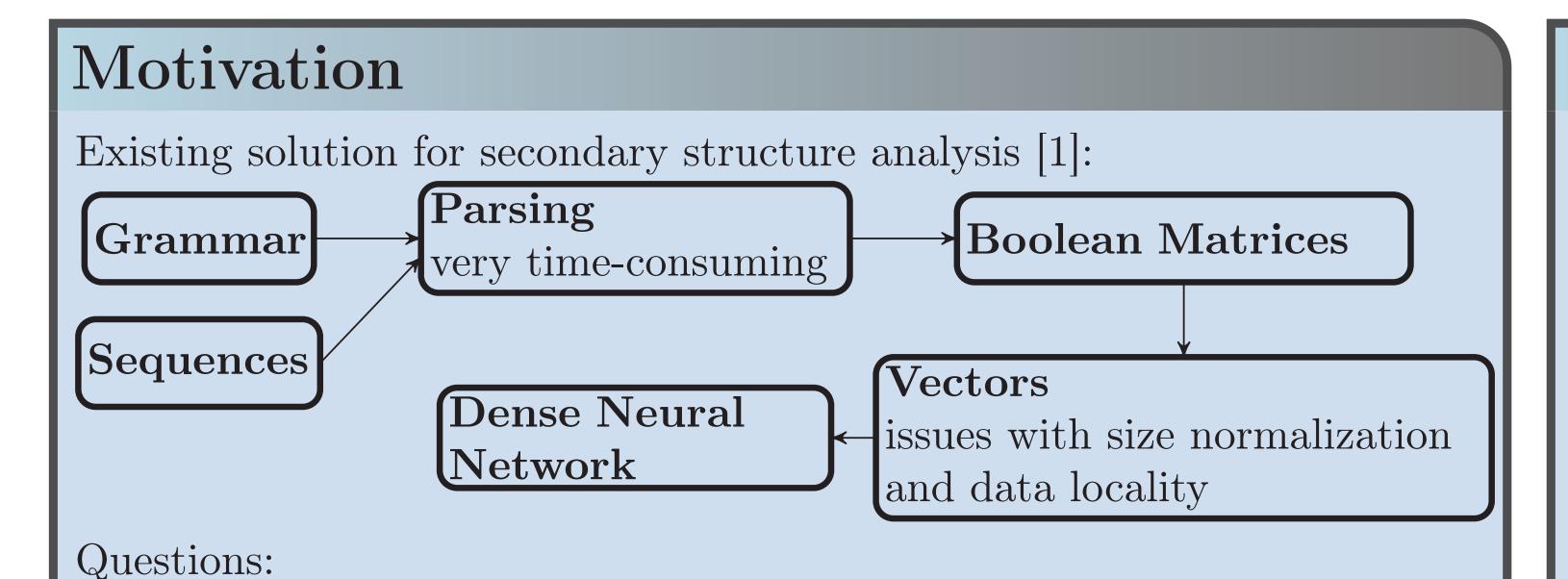


Improved Architecture of Artificial Neural Network for Secondary Structure Analysis

Polina Lunina¹, Semyon Grigorev¹

¹Saint Petersburg State University, JetBrains Reserach, St. Petersburg, Russia E-mail: lunina polina@mail.ru, semyon.grigorev@jetbrains.com





- Is it possible to move parsing to network training step?
- Is it possible to use convolutional neural networks for parsing result processing?

Results: tRNA classification

- 2 classes: eukaryotes and prokaryotes (EP).
- 4 classes: archaea, bacteria, fungi and plants (ABFP).

Classifier	EP		ABFP	
Approach	Vectors	Images	Vectors	Images
Base model accuracy	94.1%	96.2%	86.7%	93.3%
Extended model accuracy	97.5%	97.8%	96.2%	95.7%
Total samples (train:valid:test)	20000:5000:10000		8000:1000:3000	

Sequences from open databases [2, 3].

Parsing elimination

We solve this problem by using two-staged learning.

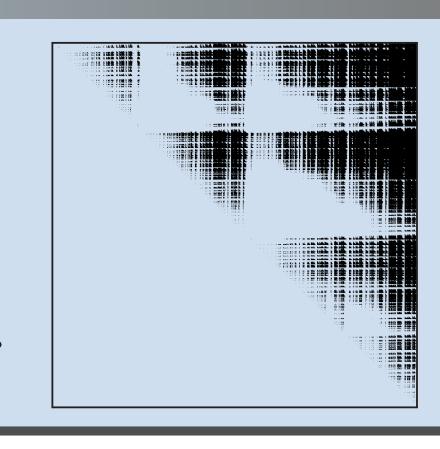
- 1. Train a network which takes parsed data as an input (base model).
- 2. Extend the trained network with a number of layers that convert the nucleotide sequence into a parsing result (extended model).

Parsing is required only for the network training.

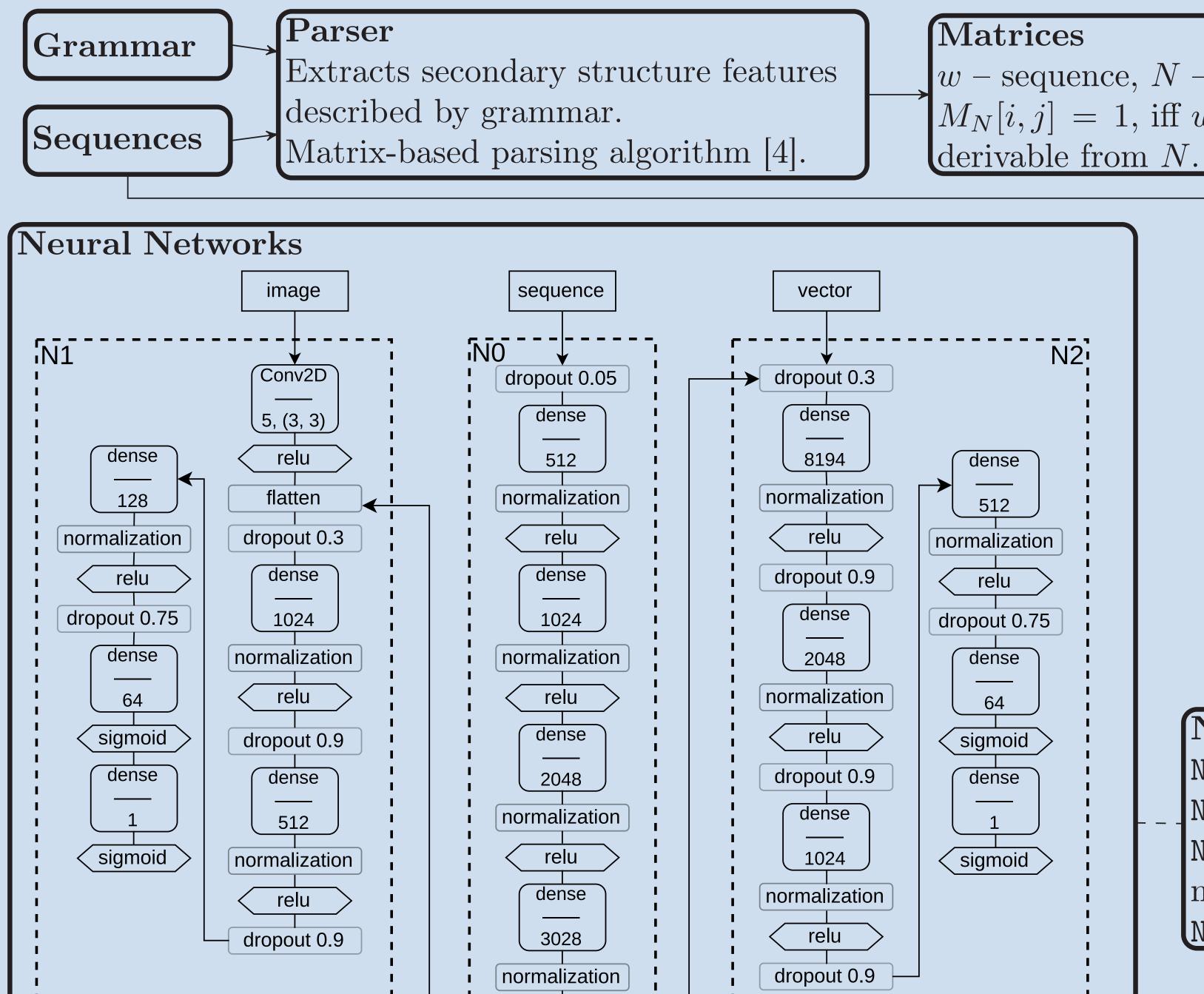
Convolutional networks

Matrices can be treated as bitmaps.

- Images can be easily resized.
- Data locality is preserved.
- We can use convolutional networks.



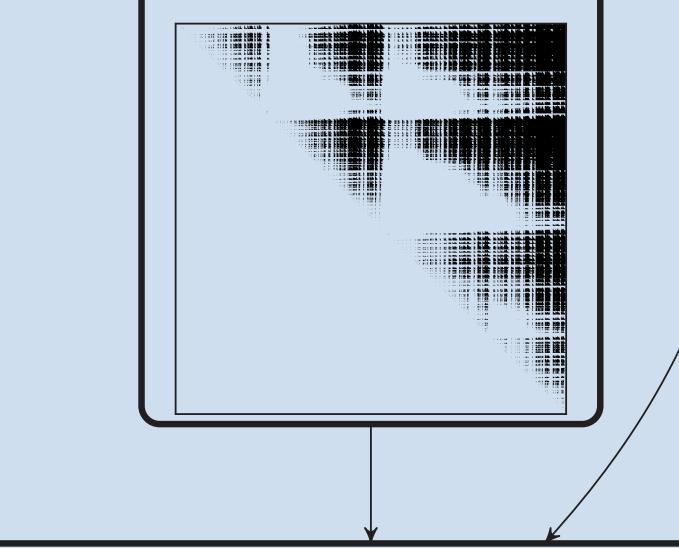
Solution Overview



w – sequence, N – nonterminal $M_N[i,j] = 1$, iff w[i,j-1] is

Vectors

Drop out the bottom left triangle. Vectorize matrix row by row. Length normalization is requried.



Neural Networks

- N1 images classification.
- N2 vectorized data classification.

Images

NO – the extension block which converts the nucleotide sequence into a set of features for N1 or N2.



Future Research

- 16s rRNA processing and chimeric sequences filtration.
- Proteomic sequences processing, proteins functions prediction.
- Generative networks for sequences secondary structure prediction.

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Information

Trained models and other materials are published at GitHub: https://github.com/LuninaPolina/SecondaryStructureAnalyzer.

References

- [1] Semyon Grigorev. and Polina Lunina. The composition of dense neural networks and formal grammars for secondary structure analysis. In *Proceedings* of the 12th International Joint Conference on Biomedical Engineering Systems and Technologies - Volume 3: BIOINFORMATICS,, pages 234–241. INSTICC, SciTePress, 2019.
- [2] Genomic tRNA Database. Web page. URL: http://gtrnadb.ucsc.edu/. Last accessed 05.06.2019.
- [3] tRNADB-CE. Web page. URL: http://trna.ie.niigata-u.ac.jp/ cgi-bin/trnadb/index.cgi. Last accessed 05.06.2019.
- [4] Rustam Azimov and Semyon Grigorev. Context-free path querying by matrix multiplication. In Proceedings of the 1st ACM SIGMOD Joint International Workshop on Graph Data Management Experiences & Systems (GRADES) and Network Data Analytics (NDA), page 5. ACM, 2018.