Improved Architecture of Artificial Neural Network for Secondary Structure Analysis

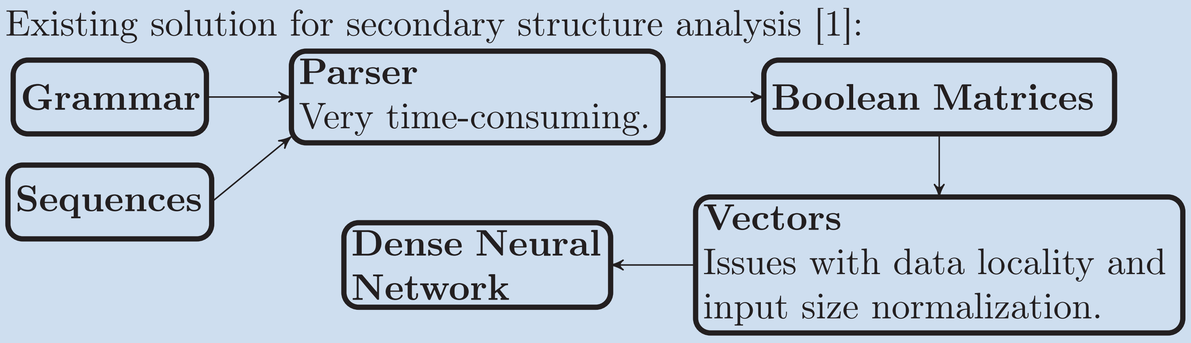
Polina Lunina[1], Semyon Grigorev[1]

[1] *Saint Petersburg State University, JetBrains Reserach, St. Petersburg, Russia*

E-mail: *lunina_polina@mail.ru, semyon.grigorev@jetbrains.com*

Motivation

Existing solution for secondary structure analysis [1]:



Questions:

- **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.

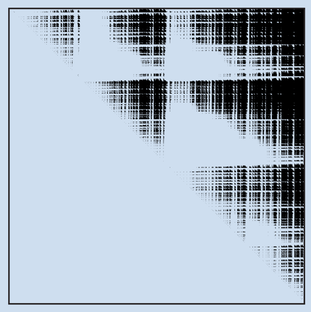
1. Train a network which takes parsed data as an input (**base model**).
2. Extend the trained network with a number of layers that convert the nucleotide sequence into a parsing result (**extended model**).

Parsing is required only for network training.

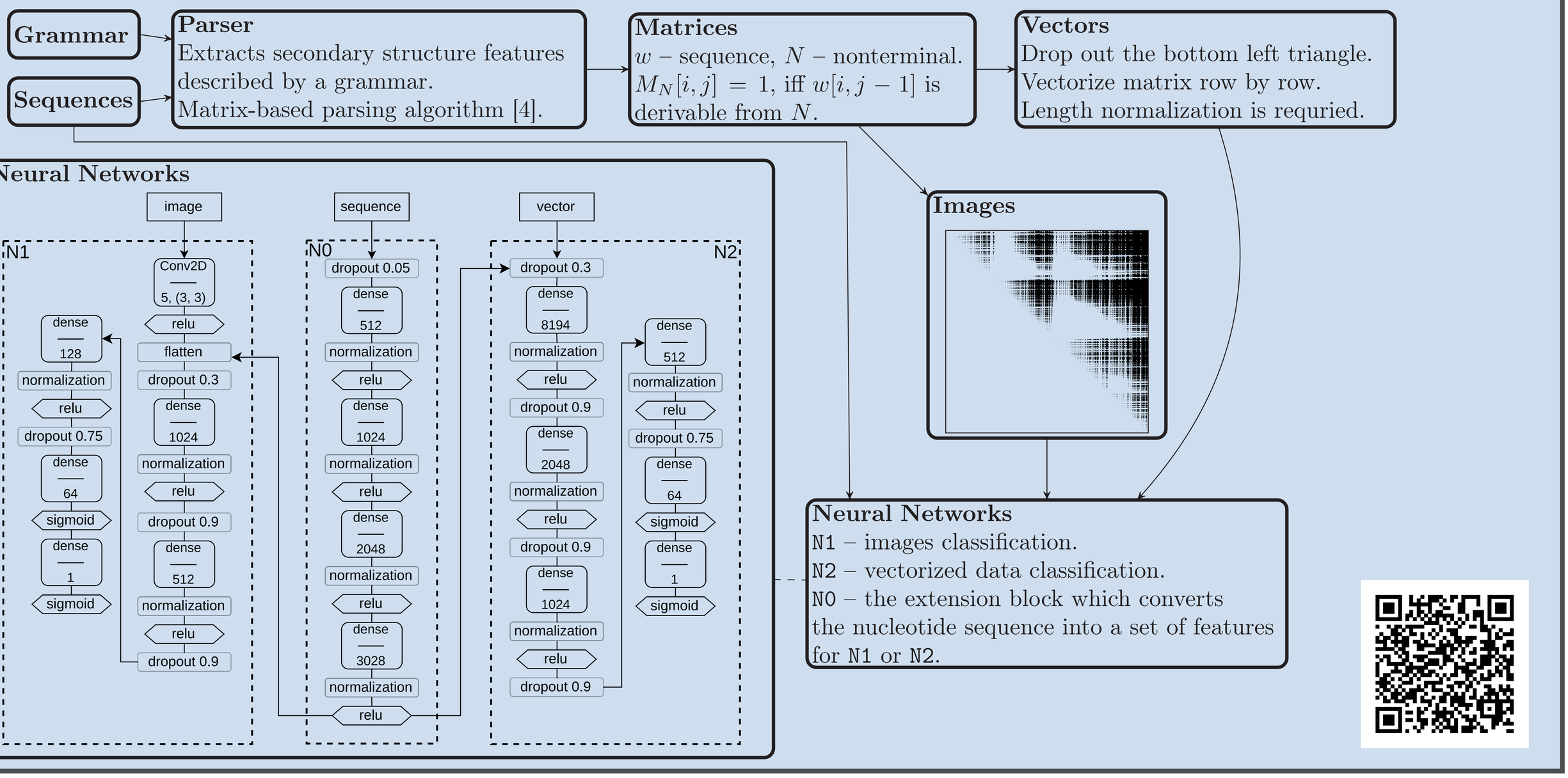
Convolutional Networks

Matrices can be treated as bitmaps.

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



Solution Overview



Future Research

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

Acknowledgments

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Information

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

References

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[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.