

The Composition of Dense Neural Networks and Formal Grammars for Secondary Structure Analysis

Polina Lunina, **Semyon Grigorev**

JetBrains Research, Programming Languages and Tools Lab
Saint Petersburg University

February !!!, 2019

Problem Statement

- Sequences classification
 - ▶ Lexer and parser
 - ▶ Translator
 - ▶ Types mapping
 - ▶ Headers files processing
 - ▶ ...
- Unify kernels on client side
 - ▶ Currently native Brahma.FSharp's kernel and kernel loaded by type provider are different types
- Improve mechanism of kernels composition

Secondary structure!!!

- Key is secondary structure: Infernal, other works
- Problem: high variability.
- Solutions: PCFG, CM

Our receipt: Parsing + DNN

- Idea: not secondary structure modelling, but features extraction!

Our receipt: Parsing + DNN

- Idea description. Figure

Grammar

```
s1: stem<s0>
any_str : any_smb*[2..10]
s0: any_str | any_str stem<s0> s0
any_smb: A | T | C | G
stem1<s>:                \\ stem of height exactly 1
    A s T | G s C | T s A | C s G
stem2<s>:                \\ stem of height exactly 2
    stem1< stem1<s> >
stem<s>:                 \\ stem of height 3 or more
    A stem<s> T
    | T stem<s> A
    | C stem<s> G
    | G stem<s> C
    | stem1< stem2<s> >
```

Grammar

```
s1: stem<s0>
any_str : any_smb*[2..10]
s0: any_str | any_str stem<s0> s0
any_smb: A | T | C | G
stem1<s>:                \\ stem of height exactly 1
    A s T | G s C | T s A | C s G
stem2<s>:                \\ stem of height exactly 2
    stem1< stem1<s> >
stem<s>:                \\ stem of height 3 or more
    A stem<s> T
    | T stem<s> A
    | C stem<s> G
    | G stem<s> C
    | stem1< stem2<s> >
```

Grammar

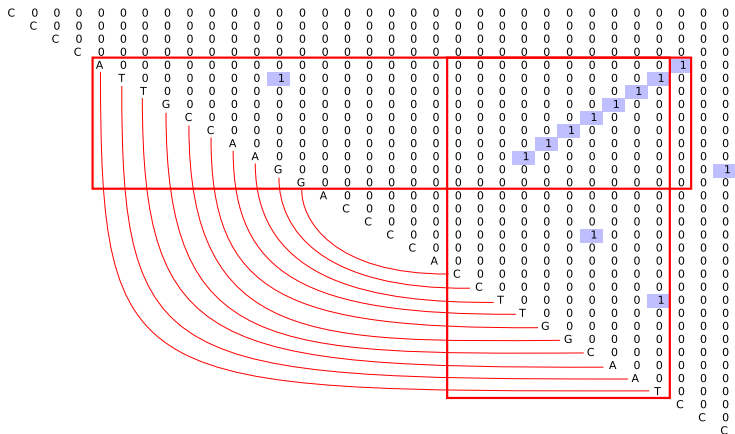
```
s1: stem<s0>
any_str : any_smb*[2..10]
s0: any_str | any_str stem<s0> s0
any_smb: A | T | C | G
stem1<s>:                \\ stem of height exactly 1
    A s T | G s C | T s A | C s G
stem2<s>:                \\ stem of height exactly 2
    stem1< stem1<s> >
stem<s>:                \\ stem of height 3 or more
    A stem<s> T
    | T stem<s> A
    | C stem<s> G
    | G stem<s> C
    | stem1< stem2<s> >
```


Grammar

```
s1: stem<s0>
any_str : any_smb*[2..10]
s0: any_str | any_str stem<s0> s0
any_smb: A | T | C | G
stem1<s>:                \\ stem of height exactly 1
    A s T | G s C | T s A | C s G
stem2<s>:                \\ stem of height exactly 2
    stem1< stem1<s> >
stem<s>:                \\ stem of height 3 or more
    A stem<s> T
    | T stem<s> A
    | C stem<s> G
    | G stem<s> C
    | stem1< stem2<s> >
```

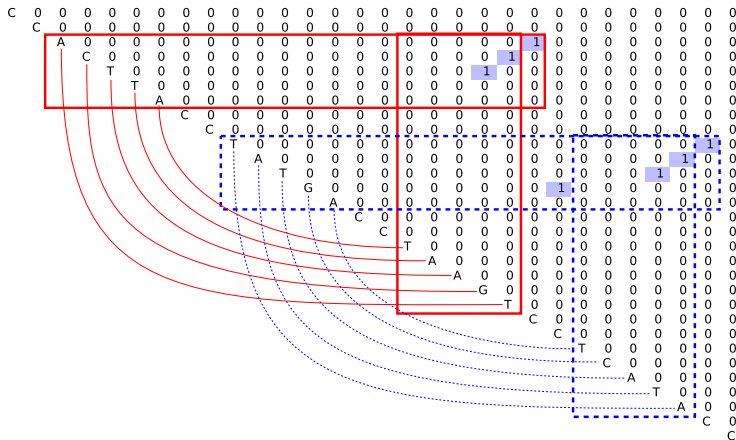
Example 1: Stem

$\omega_1 = \text{CCCCATTGCCAAGGACCCACCTTGGCAATCCC}$



Example 2: Pseudoknot

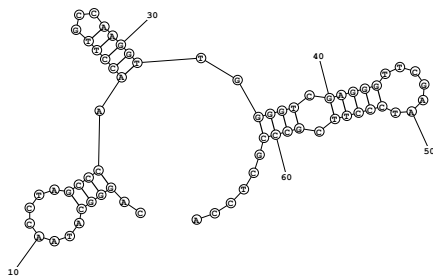
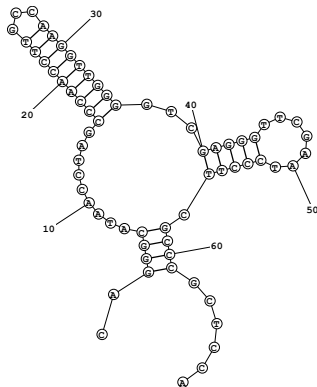
$\omega_2 = \text{C C A C T T A C C T A T G A C C T A A G T C C T C A T A C C}$



Example 3: real tRNA

$\omega_3 = \text{CAGGGCATAACCTAGCCCAACCTTGCCAAGG}$
 $\text{TTGGGGTCGAGGGTTCGAATCCCTTCGCCCCTCCA}^1$

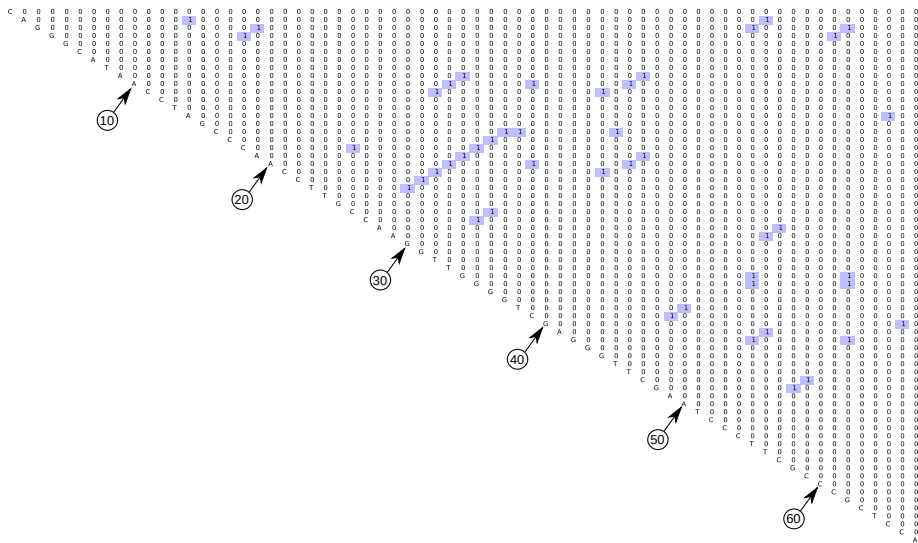
Predicted secondary structures²



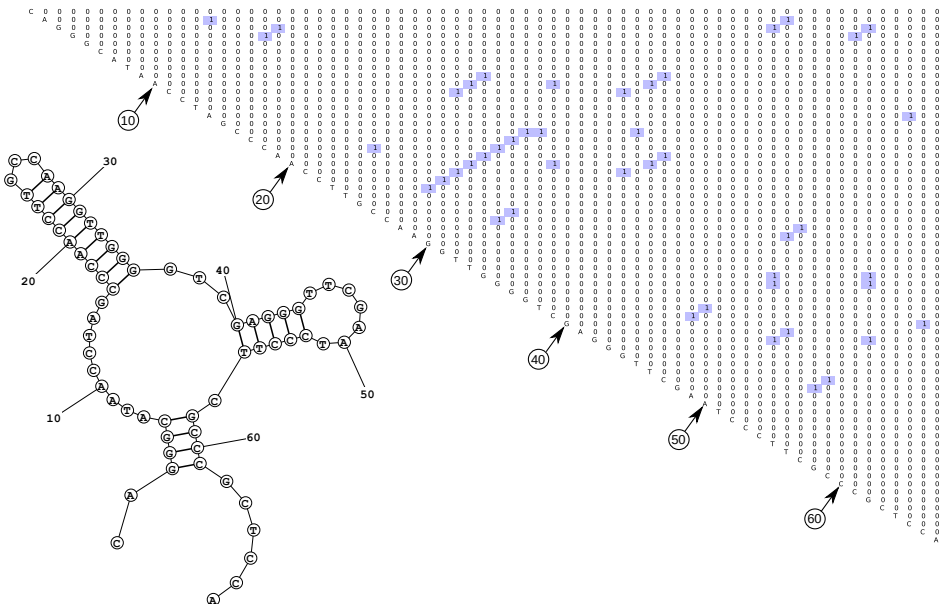
¹ Novosphingobium aromaticivorans from GtRNAdb.

² Results are given by using the Fold Web Server with default settings.

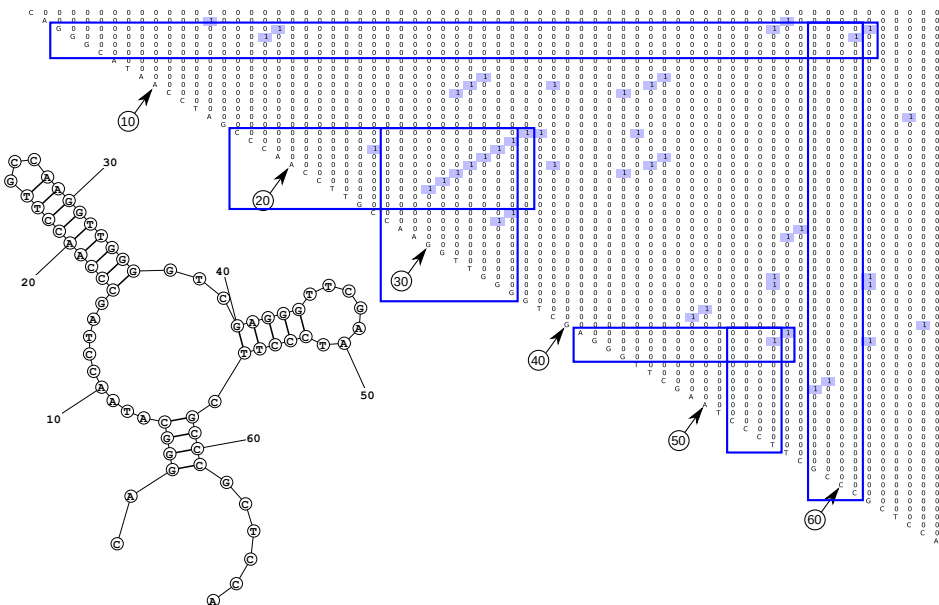
Example 3: real tRNA



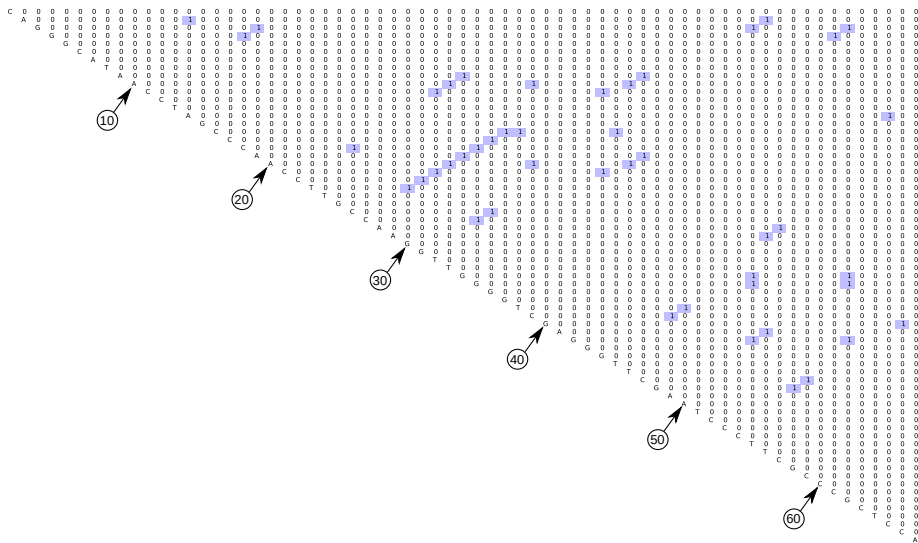
Example 3: real tRNA



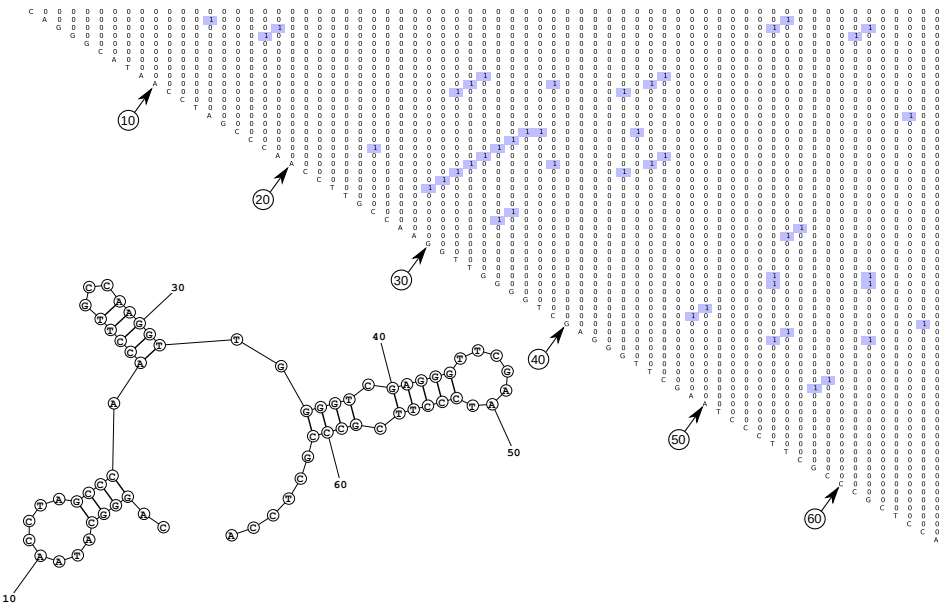
Example 3: real tRNA



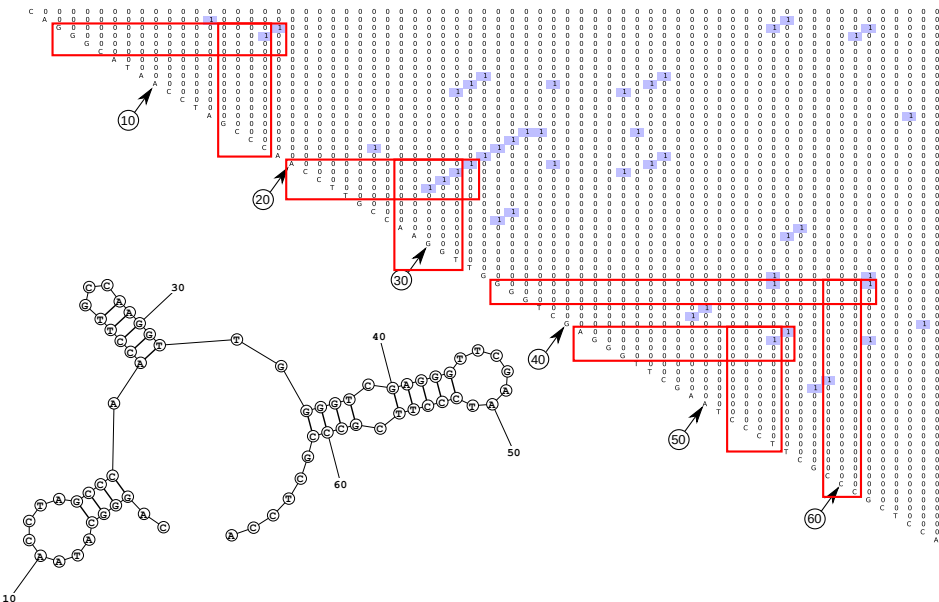
Example 3: real tRNA



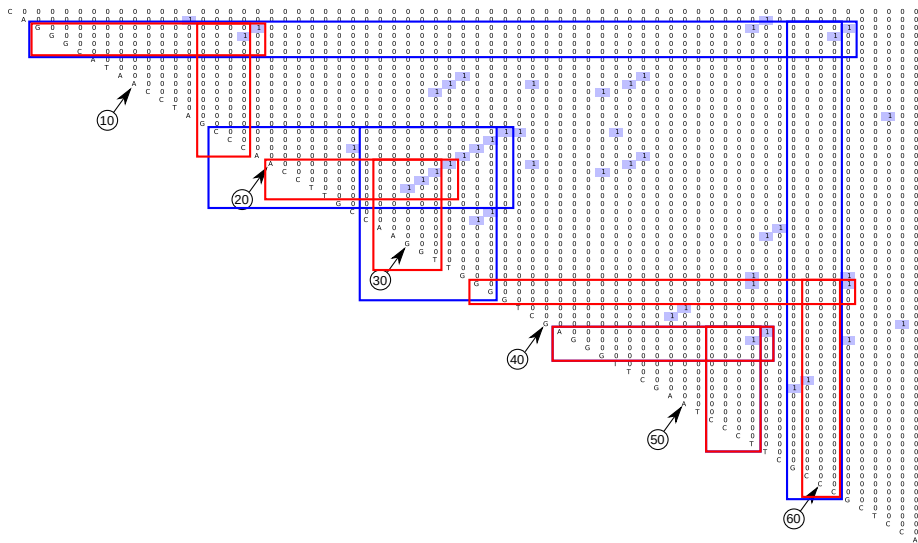
Example 3: real tRNA



Example 3: real tRNA



Example 3: real tRNA



- Compile-time metaprogramming for types creation
 - ▶ Type provider is a **function which constructs type**

- Compile-time metaprogramming for types creation
 - ▶ Type provider is a **function which constructs type**

- Compile-time metaprogramming for types creation
 - ▶ Type provider is a **function which constructs type**

- F# OpenCL C type provider
 - ▶ Type-safe integration of existing OpenCL C code in F# applications
 - ▶ Proof of concept
- Source code on GitHub:
<https://github.com/YaccConstructor/Brahma.FSharp>
- Package on NuGet:
<https://www.nuget.org/packages/Brahma.FSharp/>

- Semyon Grigorev:
 - ▶ s.v.grigoriev@spbu.ru
 - ▶ Semen.Grigorev@jetbrains.com
- Polind Lunina: lunina_polina@mail.ru

Thanks!