X CAB2C

X Argentinian Conference on Bioinformatics and Computational Biology
November 13, 2019

MicroRNA prediction from genome-wide data with deep learning: a novel approach based on convolutional residual networks

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Research Institute for Signals, Systems and Computational Intelligence

UNL CONICET

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1. Introduction
   - Background
   - Motivation
2. Proposed method
   - Convolutional Neural Networks
   - Proposed architecture
3. Results
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   - Precision-recall curves
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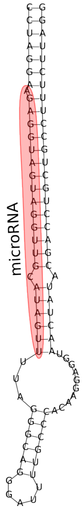

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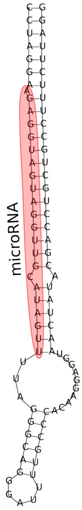

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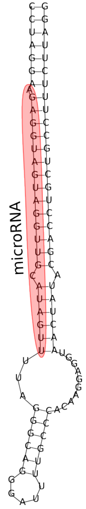

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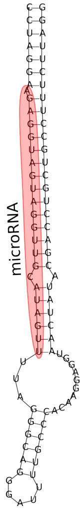

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But, there are some problems with ML methods

- Datasets used are not representative of the wide variety of negative examples.
  $\rightarrow$ Use all hairpins of the genome for validation.

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Can it be done better?

> cel-mir-62

GUGAGUUAGAUCUCAUAUCCUUCCGCAAAAUGGAAAUGAUAUGUAAUCUAGCUUACAG

(((((((((((..((((((.(((((.....)))))..))))))..)))))))))))..

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> Unknown sequence 2

GUGAGUUAGAUCUCAUAUCCUUCCGCAAAAUGGAAAUCCGAUCUAAUCUACCUUACAG

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Matching score: 189 (clustalw2)

> Unknown sequence 2

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Matching score: 249 (clustalw2)

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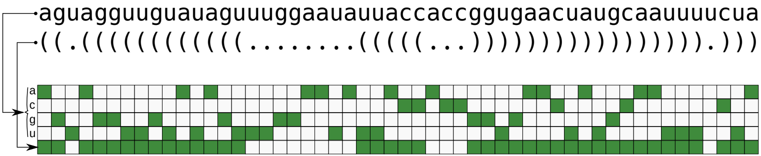
A gentle introduction to Convolutional Neural Networks



Each column represents a nucleotide

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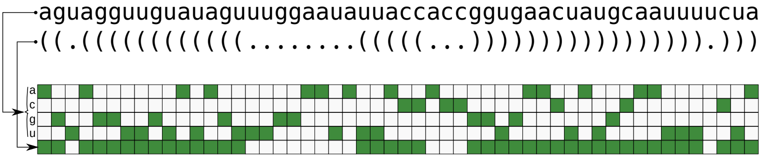

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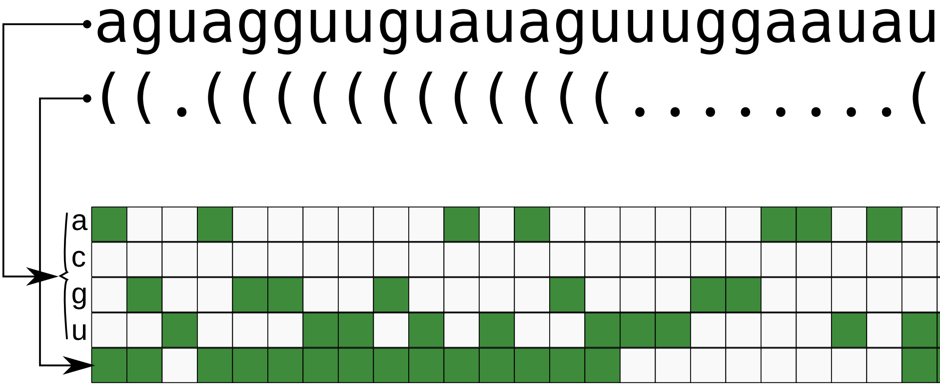

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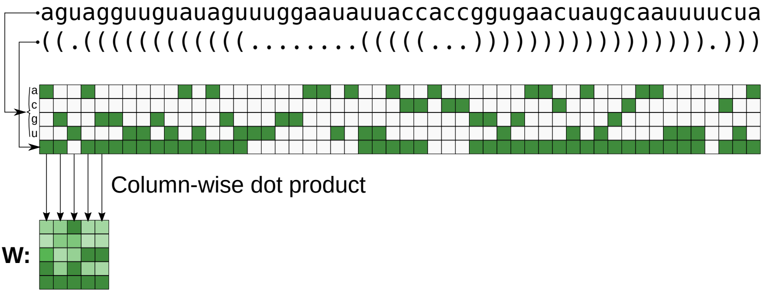

Convolution of the input tensor with the filter **W**

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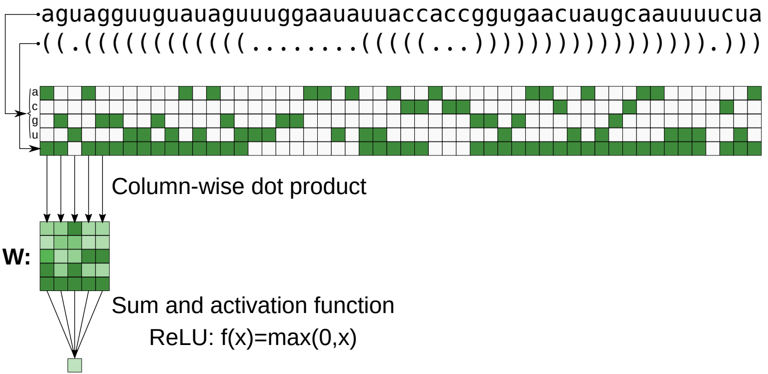

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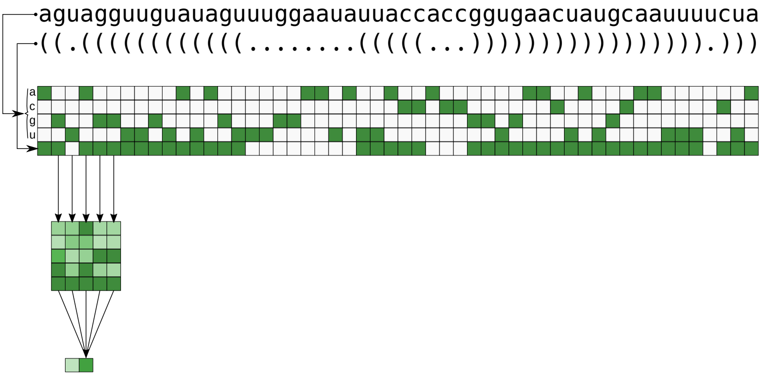

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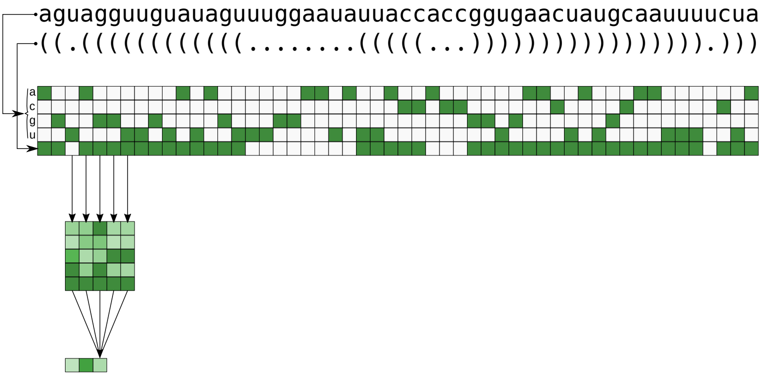

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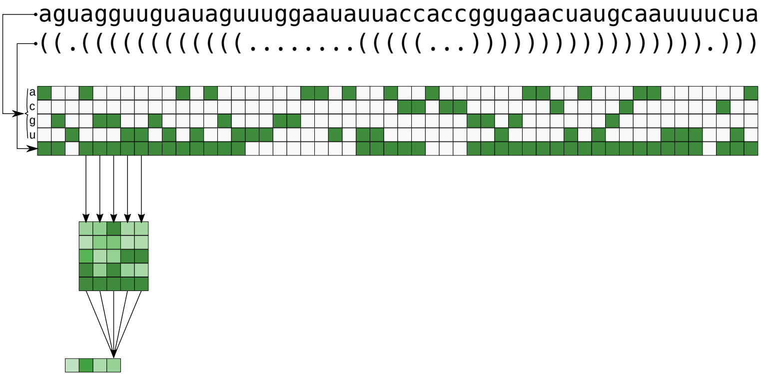

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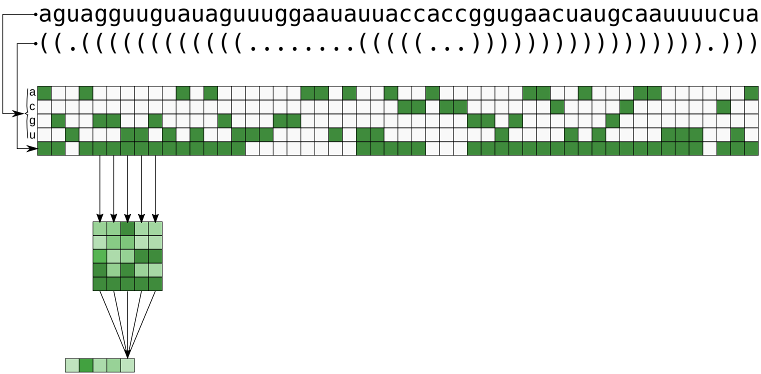

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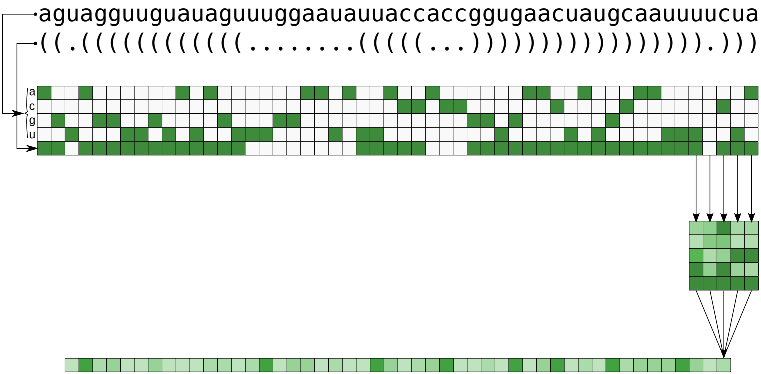

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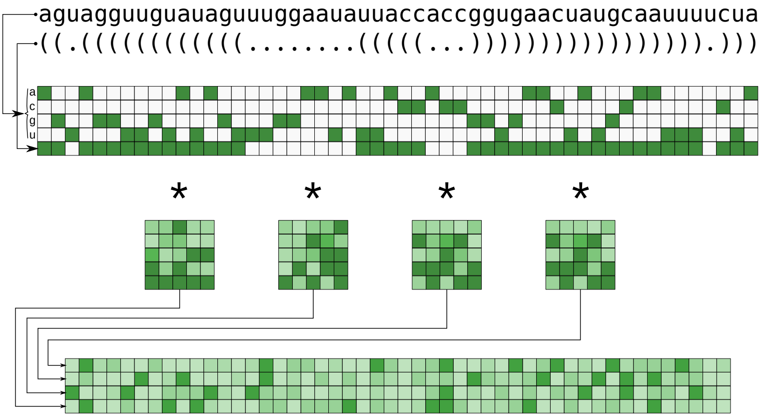

Each filter generates a row in the output tensor

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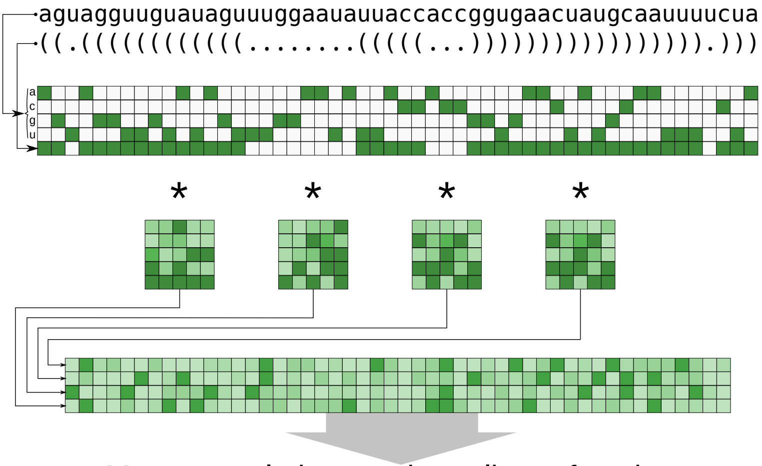
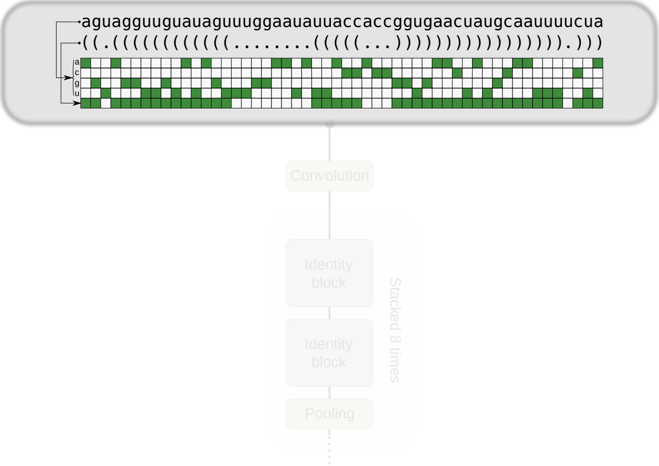


More convolutions and non-linear functions

Proposed architecture: mirDNN



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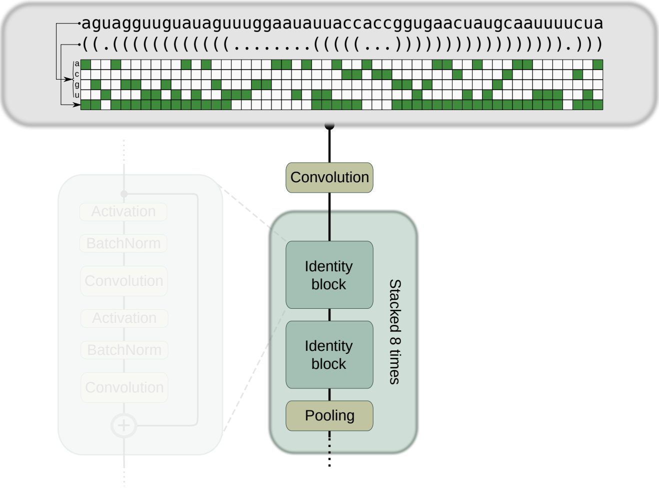

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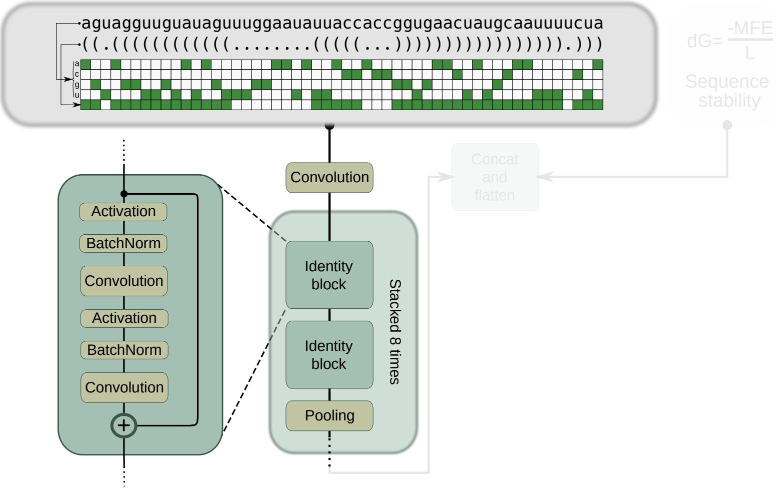

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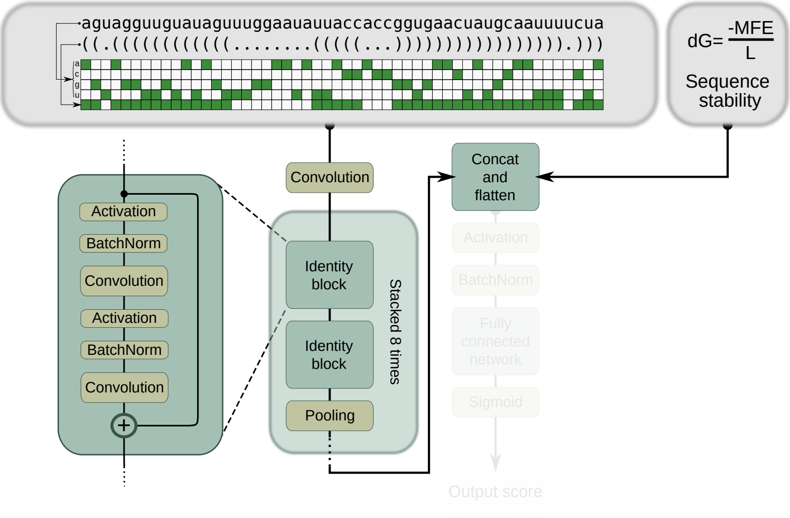

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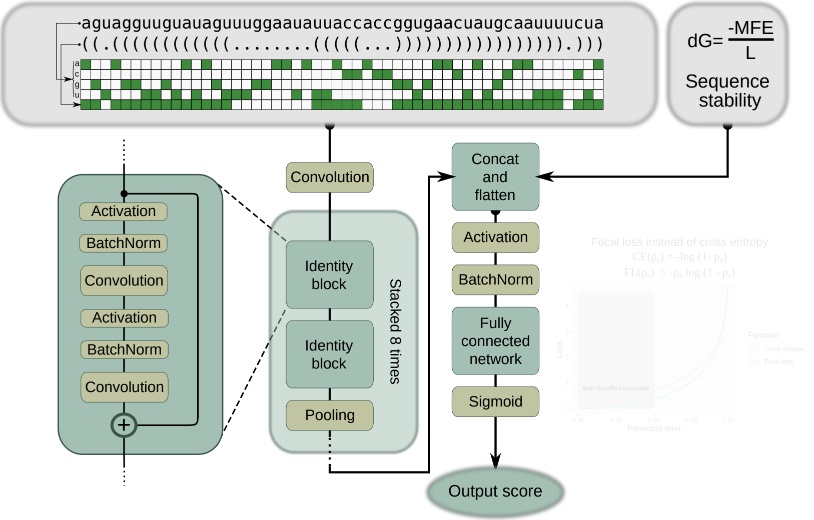

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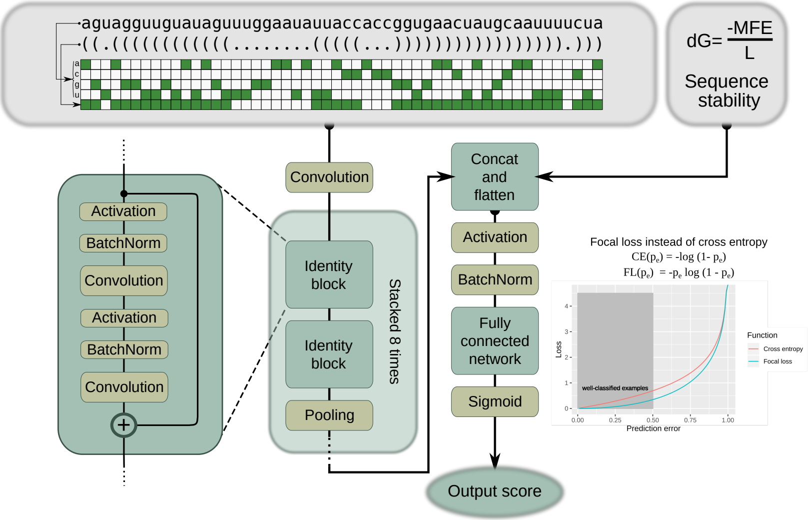

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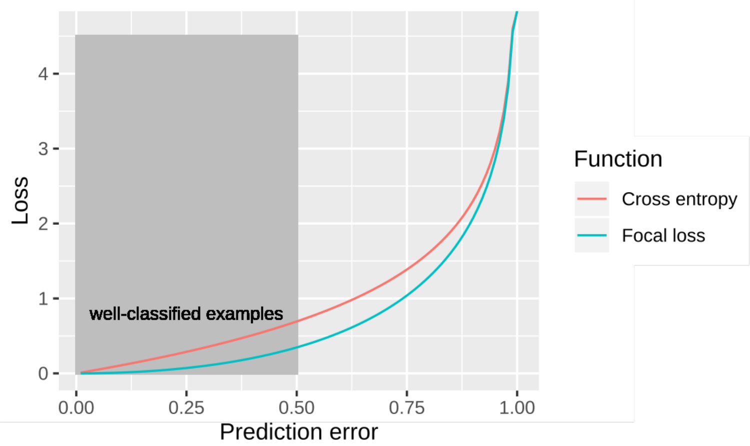
Focal loss instead of cross entropy

$$CE(p_e) = -\log(1 - p_e)$$

$$FL(p_e) = -p_e \log(1 - p_e)$$



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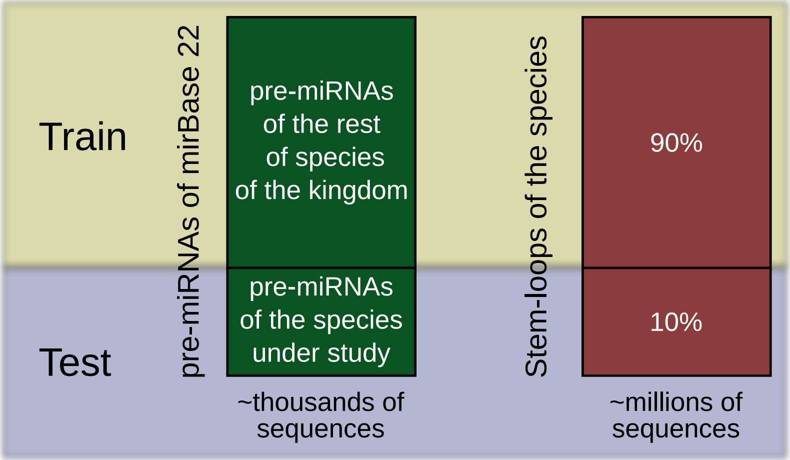
Experimental setup

Validation on a *leave-species-out* scheme



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- Two machine learning methods and one sequence alignment method were used for comparison.

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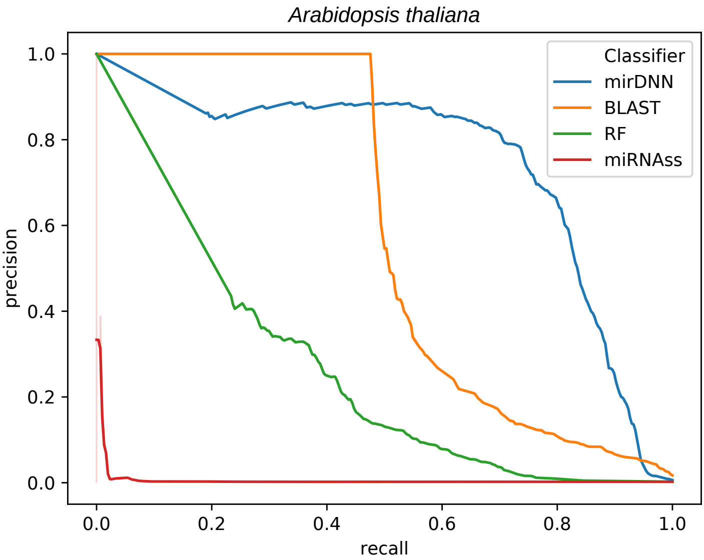
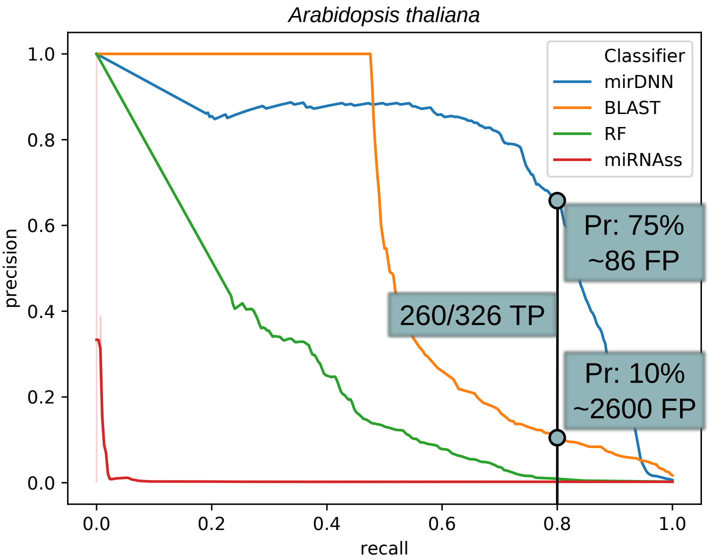
Precision-recall curves



Precision-recall curves



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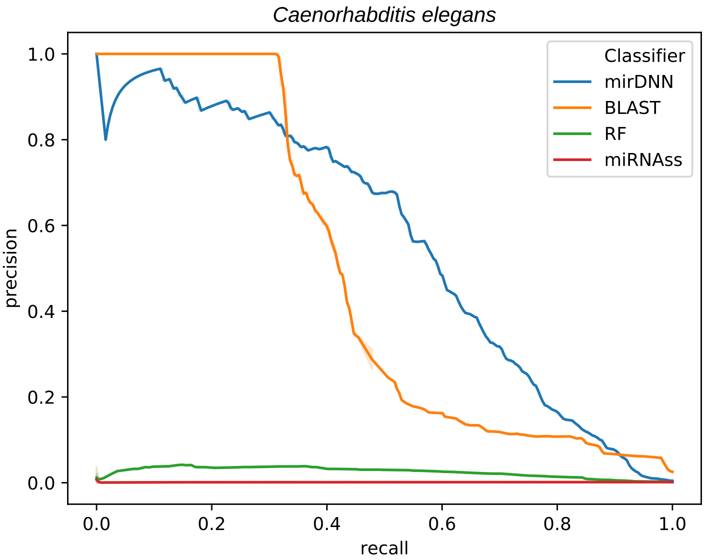

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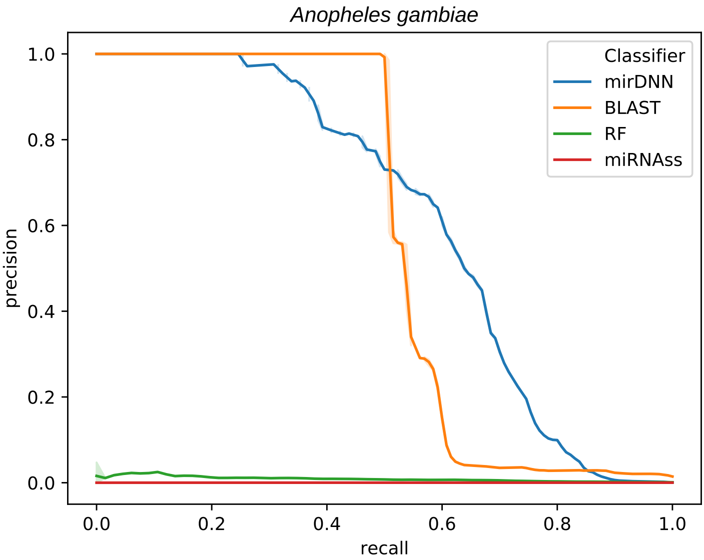
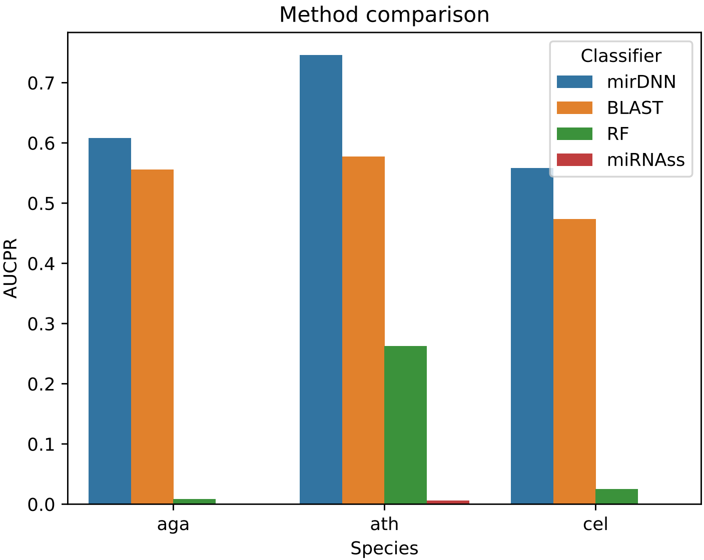


Area under the curves



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