

# Supplementary materials

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## 0.1 Table 3-4

Dataset	Thresh.	Acc.	MCC
<b>Optimization set (subset1)</b>	$10^{-4}$	1.0	0.907
	$10^{-5}$	1.0	0.955
	$10^{-6}$	1.0	0.969
	$10^{-7}$	1.0	0.984
	$10^{-8}$	1.0	0.992
	$10^{-9}$	1.0	1.0
	$10^{-10}$	1.0	1.0
	$10^{-11}$	1.0	1.0
<b>Validation set (subset2)</b>	$10^{-9}$	1.0	0.991

Table 1: Performance of the Markovian Model based on a multiple sequence alignment using various threshold, subset 1 as optimization set and subset 2 as validation set

Dataset	Thresh.	Acc.	MCC
<b>Optimization set (subset2)</b>	$10^{-4}$	1.0	0.935
	$10^{-5}$	1.0	0.984
	$10^{-6}$	1.0	0.996
	$10^{-7}$	1.0	0.996
	$10^{-8}$	1.0	0.996
	$10^{-9}$	1.0	0.992
	$10^{-10}$	1.0	0.992
	$10^{-11}$	1.0	0.992
<b>Validation set (subset1)</b>	$10^{-6}$	1.0	0.969

Table 2: Performance of the Markovian Model based on a multiple sequence alignment using various threshold, subset 2 as optimization set and subset 1 as validation set

## 0.2 Table 5-6

Dataset	Thresh.	Acc.	MCC
<b>Optimization set (subset1)</b>	$10^{-4}$	1.0	0.913
	$10^{-5}$	1.0	0.973
	$10^{-6}$	1.0	0.977
	$10^{-7}$	1.0	0.992
	$10^{-8}$	1.0	1.0
	$10^{-9}$	1.0	1.0
	$10^{-10}$	1.0	1.0
	$10^{-11}$	1.0	1.0
<b>Validation set (subset2)</b>	$10^{-8}$	1.0	0.992

Table 3: Performance of the Markovian Model based on a multiple structure alignment using various threshold, subset 1 as optimization set and subset 2 as validation set

Dataset	Thresh.	Acc.	MCC
<b>Optimization set (subset2)</b>	$10^{-4}$	1.0	0.942
	$10^{-5}$	1.0	0.988
	$10^{-6}$	1.0	1.0
	$10^{-7}$	1.0	0.996
	$10^{-8}$	1.0	0.992
	$10^{-9}$	1.0	0.992
	$10^{-10}$	1.0	0.992
	$10^{-11}$	1.0	0.992
<b>Validation set (subset1)</b>	$10^{-6}$	1.0	0.977

Table 4: Performance of the Markovian Model based on a multiple structure alignment using various threshold, subset 2 as optimization set and subset 1 as validation set

### 0.3 ROC curves

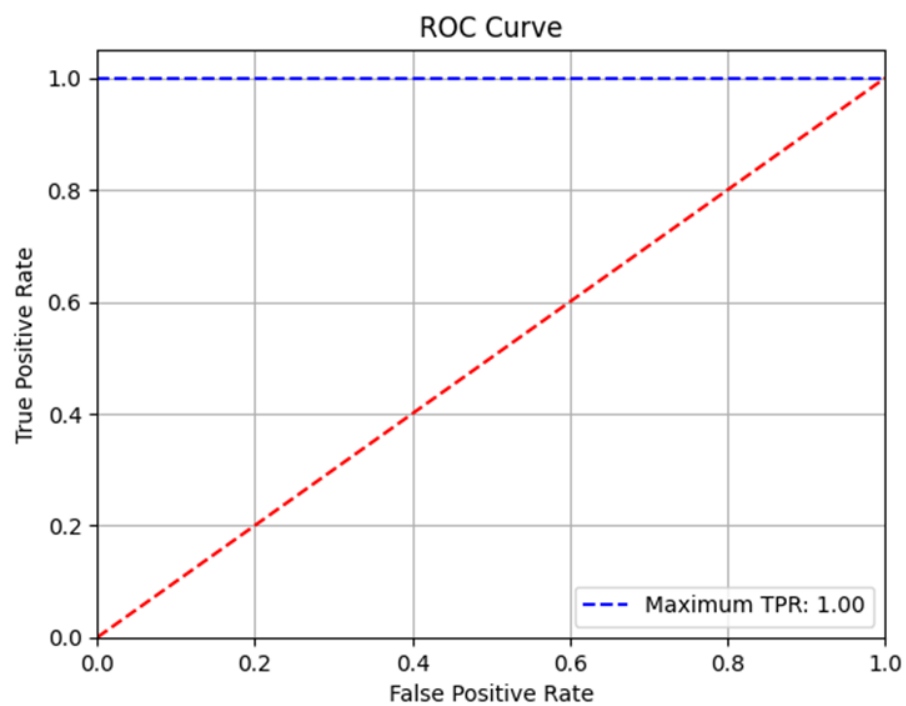


Figure 1: ROC curve obtained from the first cross-validation phase in the multiple sequence alignment model.

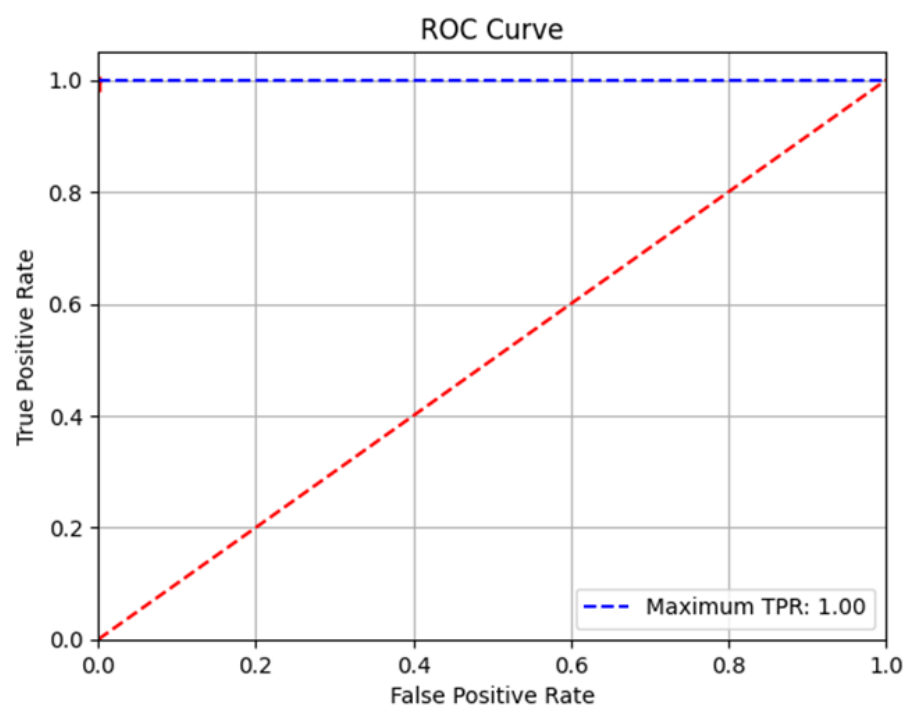


Figure 2: ROC curve obtained from the second cross-validation phase in the multiple sequence alignment model

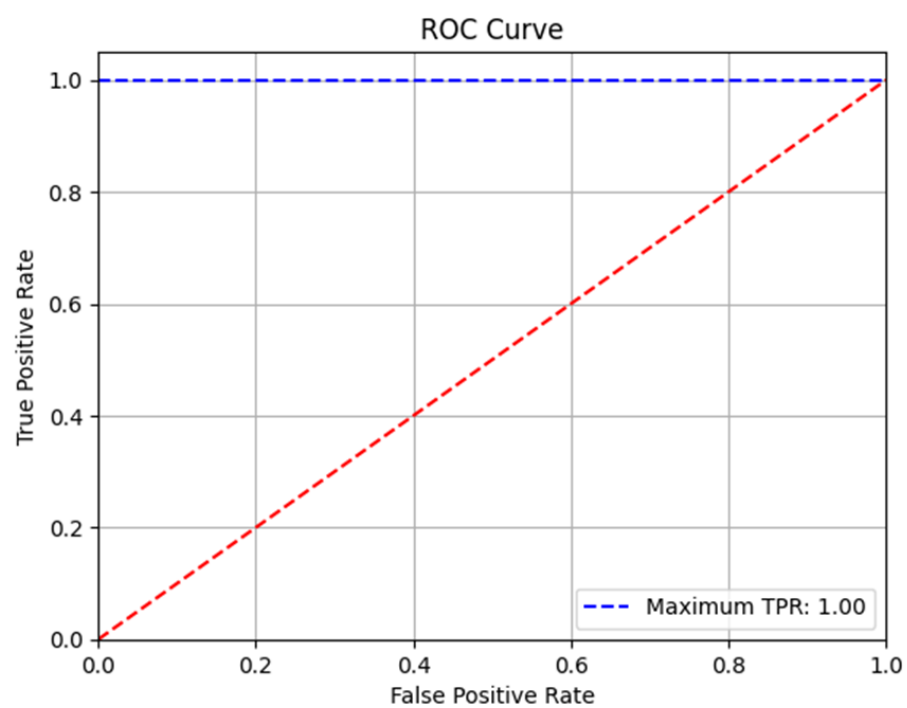


Figure 3: ROC curve obtained from the first cross-validation phase in the multiple structure alignment model.

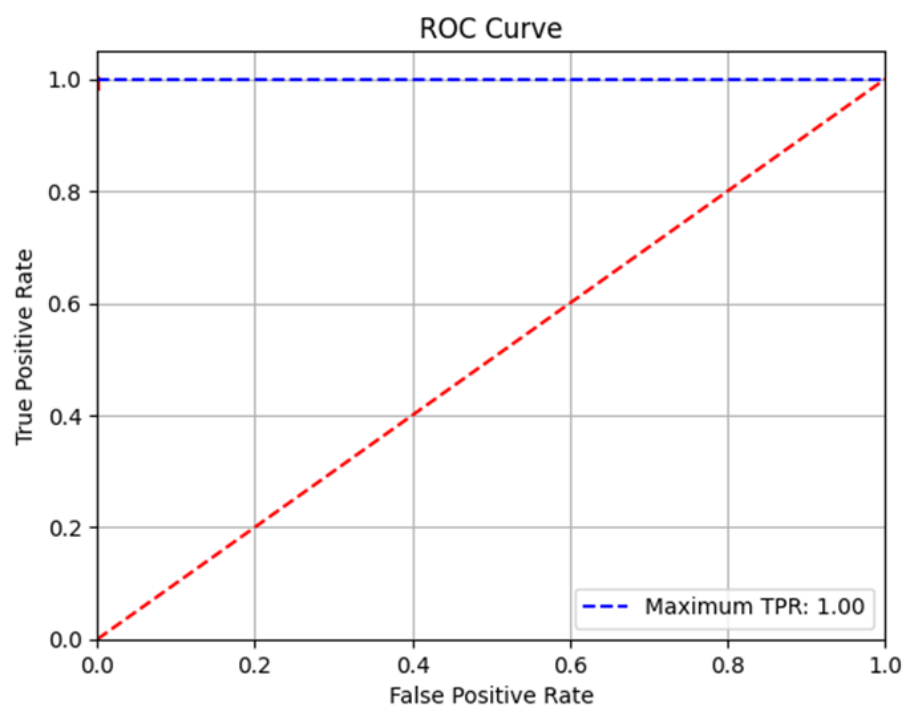


Figure 4: ROC curve obtained from the second cross-validation phase in the multiple structure alignment model.