A PILOT STUDY FOR THE PREDICTION OF LIVER FUNCTION RELATED SCORES USING BREATH BIOMARKERS AND MACHINE LEARNING

Supplementary information

Section1: Clinical score calculation

The formula for the APRI score is [(AST/upper limit of the normal AST range) X 100]/Platelet Count. First, divide AST count by the upper limit of the normal AST range. Most experts say that 40 is a good value to use here. Then multiply that answer by 100 and at last divide that answer by your platelet count. If the score is less than 0.5 it is free from fibrosis and if it is higher than 1.5 then the liver has scaring and leads to cirrhosis[1].
Following table 1 consider five clinical parameters and there is different range according it counts some values finally it gets totaled to deliver the CTP score[2].

Supplementary Table 1. CTP score calculation

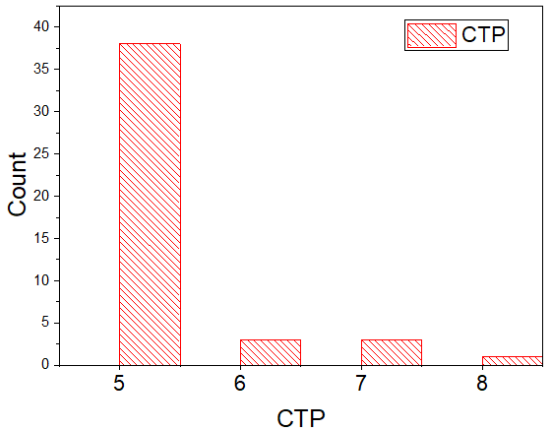
TBIL	<2mg/dL (<34.2 umol/L)	+1
	2-3mg/dL (<34.2-51.3 umol/L)	+2
	>3mg/dL (>51.3 umol/L)	+3
ALB	>3.5g/dL (>35g/L)	+1
	2.8-3.5 g/dL (28-35 g/L)	+2
	<2.8 g/dL (<28 g/L)	+3
INR	<1.7	+1
	1.7-2.2	+2
	>2.2	+3
ASC	Absent	+1
	Slight	+2
	Moderate	+3
HE	No	+1
	Grade 1-2	+2
	Grade 3-4	+3

CTP score is between 5 and 6 treated as class A, between 7 to 9 is class B and above 10 is class C. Class A, B and C has one year of survival 100%, 80% and 45%, respectively.

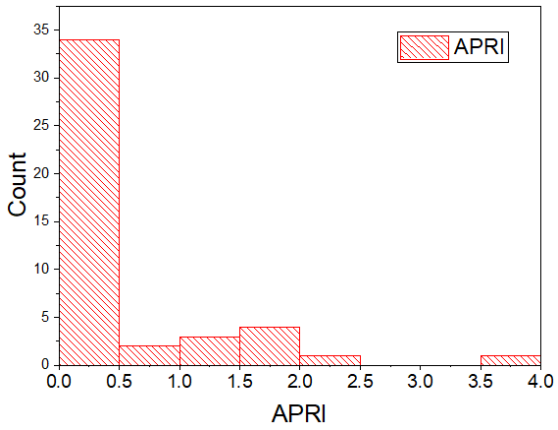
End stage liver health can be judged using MELD score. MELD score calculated counting on TBIL, CRE, INR, Na and dialysis in last two weeks[2]. Renal dysfunction because of kidney failure may disturb the MELD score prediction.

MELD=10* (0.957* ln [Creatinine]) + (0.378* ln [Bilirubin]) + (1.12 ln [INR])) + 6.43
And MELD-Na=MELD + 1.32 x (137 - Na) - [0.033 x MELD*(137 - Na)].
Interpretation of MELD score is less than 9, 1.9% mortality. As the score increase mortality percentage also increases.

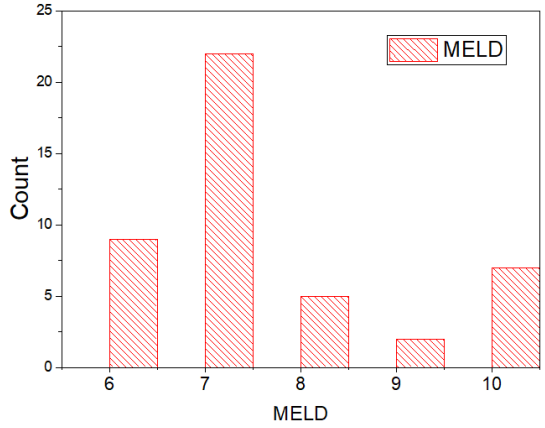
Section2: Clinical score distribution



Supplementary figure 1. Distribution of CTP score among study subjects



Supplementary figure 2. Distribution of APRI score among study subjects



Supplementary figure 3. Distribution of MELD score among study subjects

Section3: Hyperparameters of regression methods

Supplementary table 2. List of major parameters of chosen regression methods

SVR	Parameters	CTP	APRI	MELD
	C	0.01	1	0.01
	Kernel	Linear	Linear	Linear
	Degree	0	0	0
	Score	-0.32	-0.31	-0.88
RFR	**Number of trees**	10	10	100

	Maximum depth	5	3	1
	Maximum features	3	7	7
	Minimum split size	3	5	2
	Score	-0.2	-0.27	-0.89
ETR	**Number of tress**	10	500	500
	Maximum depth	5	10	5
	Maximum features	7	7	5
	Minimum split size	2	3	2
	Score	-0.15	-0.24	-0.85

1. Petersen, J. R. *et al.* Evaluation of the aspartate aminotransferase/platelet ratio index and enhanced liver fibrosis tests to detect significant fibrosis due to chronic hepatitis C. *J. Clin. Gastroenterol.* **48**, 370–376 (2014).

2. Cholongitas, E. *et al.* Systematic review: The model for end-stage liver disease--should it replace Child-Pugh's classification for assessing prognosis in cirrhosis? *Aliment. Pharmacol. Ther.* **22**, 1079–1089 (2005).