Additional Material: Fitting the data from embryo implantation prediction: learning from label proportions

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	Variable		Brief description
	Indication	endometriosis, failed intrauterine	Indication of the cycle
		insemination, tubal factor, male,	
		mixed, other, unknown	
	Infert.time	numeric	Time since infertility was detected
	Age	$(0,30],(30,35],(35,\inf)$	Age
	BMI	(0, 20], (20, 25], (25, inf)	Body mass index
	Prev.Pregnancy		Has she ever got pregnant?
	Prev.Abortion	No, Yes	Has she ever aborted?
	Prev.Cycles	0,1,2+	Number of previously undergone ART
			cycles
l e	FSH	$[x \le 10], [10 < x]$	Quantity of follicle-stimulating hormone
Female	AMH	[0, 0.5], (0.5, 1], (1, inf)	Quantity of anti-mullerian hormone
Ę.	antralFol	$[x \le 4], [4 < x]$	Number of antral follicles
1"	E2	$[x \le 3000], [3000 < x]$	Quantity of estradiol
	P4	$[x \le 1.5], [1.5 < x]$	Quantity of progesterone
	lEnd	numeric	Endometrial thickness
Male		A, N, O, OA, OAT	Quality of the semen
Ĭ	REM	[0, 0.5], (0.5, 1], (1, inf)	Total pregressive sperm recovery
	Protocol	PC, PL	Stimulation protocol
ti:	Stimulation		Stimulation treatment
la la		FSHrec+hMG, FSHur,	
1 🖬		FSHur+hMG, hMG	
Stimulation	dEst	numeric	Number of days of stimulation
01	unitFSH	numeric	Units of FSH
	unitLH	[0], (0, 1500], (1500, inf)	Units of LH
embr.	No.Oocytes	numeric	Number of retrieved oocytes
E	No.MII	numeric	Number of mature oocytes (MII state)
		numeric	Number of embryos
F.		[0, 0.5], (0.5, 1]	No.Embryos / No.MII
В	No.Transf.Emb		Number of transferred embryos
Summary	SelectiveTransf	No, Yes	Were transferred embryos selected?
Sc			(No.Embryos > No.Transf.Emb)
	No.Sacs		Number of gestational sacs

Table 1. Features collected for each ART cycle. *No.sacs* is an outcome variable which can only assessed after decisions are taken.

		Variable	Possible values	Brief description			
	e	Vac	No, Yes	Presence of vacuoles			
	إج	SER	No, Yes	Presence of smooth endoplasmic reticulum			
	Oocyte			clusters			
1	ا ۲	PVS	Normal, Augmented	Description of the perivitelline space			
	Ì	PB	Normal, Abnormal	Description of the first polar body			
_		Technique	IVF, ICSI	Fertilization technique			
	+1	PB.1	1, 2, 3+	Number of polar bodies			
	7	Z	Z1, Z2, Z3, Z4	Scott's pronuclear grade [?]			
		nCel.2	{4}, {2;5}, {other}	Number of cells			
	Ì	frag.2	[0, 10], (10, 25], (25, 35],	Percentage of cell fragmentation			
0	30		(35, 100]				
	7	symmet.2	No, Yes	Are the blastomeres symmetric?			
-	7	PZ.2	Normal, Abnormal	Presence of abnormalities in the pellucid zone			
		vac.2	No, Yes	Presence of vacuoles			
		multiNuc.2	No, Yes	Presence of multi-nucleation in a cell			
				$(\text{no.nuclei} \ge 2)$			
		1 0	A, B, C, D	ASEBIR quality grade [?]			
		Implantation	No, Yes	Did it get implanted?			
	1	O T	11 1 1 0 1 1	/ 1 7 7 4 4: 11			

Table 2. Features collected for each oocyte/embryo. *Implantation* variable cannot be always annotated by clinicians.

Infert.time	Indication	Age	BMI	Prev.Pregnancy	Prev.Abortion	FSH	Prev.Cycles
(-inf, 3]:380	unknown : 35	(-inf, 30]: 81	(-inf, 20]:111	No :463	No :507	(-inf, 10]:655	0:306
(3, 4]:179	endometriosis: 20	· ·	(20, 25]:397	Yes:233	Yes:189	(10, inf]: 41	
(4,inf]:137	failed i.i. :170	(35,inf]:291	(25,inf]:188			·	2+:165
	male :342	·					
	mixed : 57						
	other : 21						
	tubal factor : 51						
AMH	antralFol	E2	P4	1End	Qua.Semen	REM	Protocol
(-inf,0.5]: 59	(-inf, 4]: 84	(-inf,3000]:516	(-inf,1.5]:643	(-inf, 9.4]:232	A :191	(-inf,0.5]:198	PC:613
(0.5,1.0]: 76	(4,inf]:612	(3000, inf]:180	(1.5,inf]: 53	(9.4,11.0]:290	N :210	(0.5,1.0]: 57	PL: 83
(1.0,inf]:561				(11.0, inf]:174	0:9	(1.0, inf]:441	
					OA : 94		
					OAT:192		
Stimulation	dEst	unitFSH	unitLH	No.Oocytes	No.MII	No.Embryos	transSelect
FSH+Lhrec : 94	(-inf, 10]:419	(-inf,2400]:243	(-inf, 0]:303	(-inf, 6]:232	(-inf, 5]:256	(-inf, 4]:329	No :154
FSHrec :263	(10, 11]:201	(2400,3300]:260	(0,1500]:252	(6, 10]:256	(5, 9]:258	(4, 6]:147	Yes:542
FSHrec+hMG:155	(11,inf]: 76	(3300, inf]:193	(1500, inf]:141	(10,inf]:208	(9,inf]:182	(6,inf]:220	
FSHur : 33							
FSHur+hMG :121							
hMG : 30							
FertilityRate	No.Transf.Emb	Technique	Vac	SER	PVS	PB	PB.1
(-inf, 50]:127	1: 40	IVF :128	No :692	No :680	Augmented: 11	Abnormal: 21	1: 1
(50,inf]:569	2:428	ICSI:568	Yes: 4	Yes: 16	Normal:685	Normal :675	2:695
	3:228						
Z	nCel.2	frag.2	symmet.2	PZ.2	vac.2	multiNuc.2	quality.2
Z1:472	A: 62	(-inf, 10]:481	No :279	Abnormal: 1	No :687	No :684	A:284
Z2: 23	B:149	(10, 25]:141	Yes:417	Normal :695	Yes: 9	Yes: 12	B:134
Z3:140	C:485	(25, 35]: 43					C:228
Z4: 61		(35,inf]: 31					D: 50
Implantation							

No :447 Yes: 72 ? :177

Table 3. List of variables in the table of embryos and values. *CP.1*, *PZ.2*, *Vac* and *multiNuc.2* were not considered in the experiments because of lack of balance in the values and/or no correlation.

Technique	Vac	SER	PVS	PB	PB.1	Z	nCel.2	frag.2
IVF :128	No :692	No :680	Augmented: 11	Abnormal: 21	1: 1	Z1:472	A: 62	(-inf, 10]:481
ICSI:568	Yes: 4	Yes: 16	Normal:685	Normal :675	2:695	Z2: 23	B:149	(10, 25]:141
						Z3:140	C:485	(25, 35]: 43
						Z4: 61		(35,inf]: 31
PZ.2	symmet.2	vac.2	multiNuc.2	quality.2	Implantation			
Abnormal: 1	No :279	No :687	No :684	A:284	No :447			
Normal :695	Yes:417	Yes: 9	Yes: 12	B:134	Yes: 72			
				C:228	? :177			
				D: 50				

Table 4. List of variables in the table of embryos and values. *CP.1*, *PZ.2*, *Vac* and *multiNuc.2* were not considered in the experiments because of lack of balance in the values and/or no correlation.

NB		TAN					2DB		
Accuracy Recall Precision F1 PPR	Accuracy Recal		F1	PPR	Accuracy	Recall	Precision	F1	PPR
$0.86 \pm 0.00 0.00 \pm 0.0$									
$0.86 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00$									
$0.86 \pm 0.00 0.03 \pm 0.00 0.29 \pm 0.00 0.05 \pm 0.00 0.01 \pm 0.00 $									
$0.86 \pm 0.00 0.03 \pm 0.00 0.29 \pm 0.00 0.05 \pm 0.00 0.01 \pm 0.00 $									
$0.86 \pm 0.00 0.03 \pm 0.00 0.29 \pm 0.00 0.05 \pm 0.00 0.01 \pm 0.00 $									
$0.86 \pm 0.00 0.03 \pm 0.00 0.40 \pm 0.00 0.05 \pm 0.00 0.01 \pm 0.00 $									
$0.85 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.01 \pm 0.00 $									
$0.85 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.01 \pm 0.00 $									
$0.85 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.01 \pm 0.00 $									
$0.86 \pm 0.00 0.00 \pm 0.0$									
$0.86 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 0.00 \pm 0.00 $	$ 0.86 \pm 0.00 0.00 \pm 0$	$.00 0.00 \pm 0.00$	0.00 ± 0.00	0.00 ± 0.00	0.86 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
$0.79 \pm 0.00 0.19 \pm 0.00 0.21 \pm 0.00 0.20 \pm 0.00 0.13 \pm 0.0$	$0.79 \pm 0.00 0.11 \pm 0$	$.02 \mid 0.15 \pm 0.02$	0.12 ± 0.02	0.10 ± 0.00	0.76 ± 0.00	0.18 ± 0.00	0.16 ± 0.00	0.17 ± 0.00	0.15 ± 0.00
0.79 ± 0.00 0.19 ± 0.00 0.21 ± 0.00 0.20 ± 0.00 0.13 ± 0.00									
$0.72 \pm 0.00 0.42 \pm 0.00 0.23 \pm 0.00 0.29 \pm 0.00 0.25 \pm 0.0$									
$ 0.72 \pm 0.00 $ $ 0.42 \pm 0.00 $ $ 0.23 \pm 0.00 $ $ 0.29 \pm 0.00 $ $ 0.25 \pm 0.00 $									
$ 0.73 \pm 0.00 $ $ 0.42 \pm 0.00 $ $ 0.23 \pm 0.00 $ $ 0.30 \pm 0.00 $ $ 0.25 \pm 0.00 $									
$ 0.73 \pm 0.00 $ $ 0.42 \pm 0.00 $ $ 0.23 \pm 0.00 $ $ 0.30 \pm 0.00 $ $ 0.25 \pm 0.00 $									
$ 0.74 \pm 0.00 $ $ 0.44 \pm 0.00 $ $ 0.25 \pm 0.00 $ $ 0.32 \pm 0.00 $ $ 0.25 \pm 0.00 $									
$ 0.74 \pm 0.00 $ $ 0.44 \pm 0.00 $ $ 0.25 \pm 0.00 $ $ 0.32 \pm 0.00 $ $ 0.25 \pm 0.00 $									
$ 0.74 \pm 0.00 $ $ 0.44 \pm 0.00 $ $ 0.25 \pm 0.00 $ $ 0.32 \pm 0.00 $ $ 0.24 \pm 0.00 $									
$ 0.75 \pm 0.00 $ $ 0.44 \pm 0.00 $ $ 0.26 \pm 0.00 $ $ 0.33 \pm 0.00 $ $ 0.24 \pm 0.00 $									
0.74 ± 0.00 0.44 ± 0.00 0.26 ± 0.00 0.32 ± 0.00 0.24 ± 0.00									
0.76 ± 0.00 0.42 ± 0.00 0.27 ± 0.00 0.33 ± 0.00 0.21 ± 0.00									
0.76 ± 0.00 0.44 ± 0.00 0.27 ± 0.00 0.34 ± 0.00 0.23 ± 0.00									
0.76 ± 0.00 0.49 ± 0.00 0.29 ± 0.00 0.36 ± 0.00 0.23 ± 0.00									
0.77 ± 0.00 0.47 ± 0.00 0.29 ± 0.00 0.36 ± 0.00 0.23 ± 0.00									
0.76 ± 0.00 0.42 ± 0.00 0.26 ± 0.00 0.32 ± 0.00 0.22 ± 0.00									
0.76 ± 0.00 0.42 ± 0.00 0.26 ± 0.00 0.32 ± 0.00 0.22 ± 0.00									
$\begin{vmatrix} 0.75 \pm 0.00 & 0.42 \pm 0.00 & 0.26 \pm 0.00 & 0.32 \pm 0.00 & 0.22 \pm 0.00 \\ 0.76 \pm 0.00 & 0.46 \pm 0.00 & 0.28 \pm 0.00 & 0.35 \pm 0.00 & 0.23 \pm 0.00 \end{vmatrix}$									
$0.76 \pm 0.00 0.46 \pm 0.00 0.28 \pm 0.00 0.35 \pm 0.00 0.23 \pm 0.00 0.76 \pm 0.00 0.44 \pm 0.00 0.28 \pm 0.00 0.34 \pm 0.00 0.22 \pm 0.00 0.20 $									
$0.76 \pm 0.00 0.44 \pm 0.00 0.28 \pm 0.00 0.34 \pm 0.00 0.22 \pm 0.00 0.77 \pm 0.00 0.40 \pm 0.00 0.28 \pm 0.00 0.33 \pm 0.00 0.20 \pm 0.00 0.20 $									
$0.77 \pm 0.00 0.40 \pm 0.00 0.28 \pm 0.00 0.33 \pm 0.00 0.20 \pm 0.00 0.78 \pm 0.00 0.40 \pm 0.00 0.28 \pm 0.00 0.33 \pm 0.00 0.20 \pm 0.00 $									
$0.78 \pm 0.00 0.40 \pm 0.00 0.28 \pm 0.00 0.33 \pm 0.00 0.20 \pm 0.00 0.78 \pm 0.00 0.29 \pm 0.00 0.26 \pm 0.00 0.27 \pm 0.00 0.16 \pm 0.00 0.20 $									
$0.78 \pm 0.00 0.29 \pm 0.00 0.26 \pm 0.00 0.27 \pm 0.00 0.16 \pm 0.00 0.80 \pm 0.00 0.38 \pm 0.00 0.31 \pm 0.00 0.34 \pm 0.00 0.17 \pm 0.00 0.18 \pm 0.00 0.19 \pm 0.00 $									
0.80 ± 0.00 0.38 ± 0.00 0.31 ± 0.00 0.34 ± 0.00 0.17 ± 0.00 0.79 ± 0.00 0.29 ± 0.00 0.27 ± 0.00 0.28 ± 0.00 0.15 ± 0.00									
$0.79 \pm 0.00 0.29 \pm 0.00 0.27 \pm 0.00 0.28 \pm 0.00 0.15 \pm 0.00 0.80 \pm 0.00 0.32 \pm 0.00 0.29 \pm 0.00 0.30 \pm 0.00 0.15 \pm 0.00 0.10 $									
[0.00 ± 0.00 0.02 ± 0.00 0.23 ± 0.00 0.30 ± 0.00 0.13 ± 0.00	110.00 ± 0.00 0.22 ± 0	.01 0.20 ± 0.01	10.23 ± 0.01	0.12 ± 0.00	U.0.11 ± 0.00	0.14 _ 0.00	0.10 ± 0.00	0.14 1 0.00	0.13 ± 0.00

Table 5. Results for NB, TAN and 2DB classifiers learnt in the proposed learning from label proportions paradigm. Accuracy, recall, precision, F1 and predicted positive rate (PPR) metrics are used. The horizontal division of the table separates the experiments performed with two datasets: upper rows, where only the embryo features are used as predictive variables and, lower rows, where the cycle features are also used. Specifically, each row collects experiments performed using a different subset of variables: backward/forward CFS and selection of the s most relevant variables ($s \in \{10, \ldots, 2\}$ for the first dataset and $s \in \{36, \ldots, 13\}$ for the second one).

NB				TAN				2DB						
Accuracy	Recall	Precision	F1	PPR	Accuracy	Recall	Precision	F1	PPR	Accuracy	Recall	Precision	F1	PPR
	0.00 ± 0.00													
0.86 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.85 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.85 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.01 ± 0.00
	0.00 ± 0.00									0.86 ± 0.00				
	0.00 ± 0.00									0.86 ± 0.00				
	0.00 ± 0.00									0.86 ± 0.00				
	0.00 ± 0.00									0.86 ± 0.00				
	0.00 ± 0.00													
	0.00 ± 0.00													
	0.00 ± 0.00													
	0.00 ± 0.00													
0.86 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.86 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	$ 0.00 \pm 0.00 $	$ 0.86 \pm 0.00 $	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00
0.81 ± 0.00	0.17 ± 0.00	0.24 ± 0.00	0.20 ± 0.00	0.10 ± 0.00	0.82 ± 0.00	0.10 ± 0.02	0.20 ± 0.03	0.13 ± 0.02	0.07 ± 0.00	0.81 ± 0.00	0.08 ± 0.00	0.15 ± 0.00	0.11 ± 0.00	0.08 ± 0.00
0.81 ± 0.00	0.17 ± 0.00	0.24 ± 0.00	0.20 ± 0.00	0.10 ± 0.00	0.82 ± 0.00	0.09 ± 0.01	0.18 ± 0.02	0.12 ± 0.02	0.07 ± 0.00	0.80 ± 0.00	0.06 ± 0.00	0.10 ± 0.00	0.07 ± 0.00	0.08 ± 0.00
0.85 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.01 ± 0.00	0.86 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.86 ± 0.00	0.01 ± 0.00	0.25 ± 0.00	0.03 ± 0.00	0.01 ± 0.00
	0.00 ± 0.00													
	0.00 ± 0.00													
	0.01 ± 0.00													
	0.01 ± 0.00													
	0.03 ± 0.00													
	0.04 ± 0.00													
	0.03 ± 0.00									$ 0.86 \pm 0.00 $				
	0.04 ± 0.00													
	0.03 ± 0.00													
	0.04 ± 0.00													
	0.04 ± 0.00													
	0.04 ± 0.00													
	0.03 ± 0.00									0.86 ± 0.00				
	0.03 ± 0.00													
	0.03 ± 0.00													
	0.03 ± 0.00													
	0.04 ± 0.00									0.86 ± 0.00				
	0.03 ± 0.00													
	0.03 ± 0.00													
	0.03 ± 0.00													
	0.03 ± 0.00													
	0.03 ± 0.00													
0.84 ± 0.00	0.03 ± 0.00	0.13 ± 0.00	0.05 ± 0.00	0.03 ± 0.00	10.86 ± 0.00	0.04 ± 0.00	0.44 ± 0.05	0.08 ± 0.00	$[0.01 \pm 0.00]$	$[0.86 \pm 0.00]$	U.UI ± 0.00	1.00 ± 0.00	$[0.03 \pm 0.00]$	0.00 ± 0.00

Table 6. Results for NB, TAN and 2DB classifiers learnt in the standard supervised classification paradigm. Accuracy, recall, precision, F1 and predicted positive rate (PPR) metrics are used. The horizontal division of the table separates the experiments performed with two datasets: upper rows, where only the embryo features are used as predictive variables and, lower rows, where the cycle features are also used. Specifically, each row collects experiments performed using a different subset of variables: backward/forward CFS and selection of the s most relevant variables ($s \in \{10, \ldots, 2\}$ for the first dataset and $s \in \{36, \ldots, 13\}$ for the second one).

	LLP		Classical supervision				
NB	TAN	2DB	NB	TAN	2DB		
Implantation	Implantation	Implantation	Implantation	Implantation	Implantation		
Infert.time	Infert.time	Infert.time	Infert.time	Infert.time	Infert.time		
Indication	Indication	Indication	Indication	Indication	Indication		
BMI	$_{\mathrm{BMI}}$	BMI	BMI	$_{\mathrm{BMI}}$	$_{\mathrm{BMI}}$		
Prev.Pregnancy	Prev.Pregnancy	Prev.Pregnancy	Prev.Abortion	Prev.Abortion	Prev.Abortion		
Prev.Abortion	Prev. Abortion	Prev.Abortion	FSH	FSH	FSH		
FSH	FSH	FSH	Prev.Cycles	Prev.Cycles	Prev.Cycles		
Prev.Cycles	Prev.Cycles	Prev.Cycles	AMH	AMH	AMH		
AMH	AMH	AMH	E2	E2	E2		
E2	E2	E2	unitFSH	unitFSH	unitFSH		
lEnd	lEnd	lEnd	unitLH	unitLH	unitLH		
Protocol	Protocol	Protocol	No.Transf.Emb	No. Transf. Emb	No. Transf. Emb		
Stimulation	Stimulation	Stimulation	SER	SER	SER		
unitFSH	unitFSH	unitFSH	PVS	PVS	PVS		
unitLH	unitLH	unitLH	nCel.2	nCel.2	nCel.2		
No.Oocytes	transSelect	No.Oocytes	frag.2	frag.2	frag.2		
transSelect	No.Embryos	transSelect					
No.Embryos	No. Transf. Emb	No.Embryos					
FertilityRate	Technique	No.Transf.Emb					
No.Transf.Emb	PB	Technique					
Technique	nCel.2	PB					
SER	frag.2	nCel.2					
PB	quality.2	frag.2					
nCel.2		quality.2					
frag.2							
quality.2							

 $\textbf{Table 7.} \ \text{Cycle+embryonic variables selected for the FSS technique in the experiments of Table 3 (paper). }$

	LLP		Cla	assical supervis	ion
NB	TAN	2DB	NB	TAN	2DB
Implantation	Implantation	Implantation	Implantation	Implantation	Implantation
Technique	Technique	Technique	SER	SER	SER
SER	SER	SER	PVS	PVS	PVS
PB	PVS	PB	PB	PB	PB
nCel.2	PB	${f Z}$	nCel.2	nCel.2	nCel.2
frag.2	${f Z}$	nCel.2	frag.2	frag.2	frag.2
symmet.2	nCel.2	frag.2	vac.2	vac.2	vac.2
quality.2	frag.2	symmet.2			
	symmet.2	quality.2			
	quality.2				

Table 8. Embryonic variables selected for the FSS technique in the experiments of Table 3 (paper).