Evaluation II

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Summer 2021

Designing Evaluation Experiments Hold-out Sampling k-Fold Cross Validation

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Designing Evaluation Experiments

Hold-out Sampling



(a) A 50:20:30 split

Training	Validation	Test
Set	Set	Set

(b) A 40:20:40 split

Figure: Hold-out sampling can divide the full data into training, validation, and test sets.

Hold-out Sampling

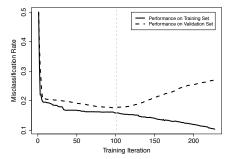


Figure: Using a validation set to avoid overfitting in iterative machine learning algorithms.

Fold	C	Class Accuracy			
1	Target	'lateral' 'frontal'	Predi 'lateral' 43 10	iction 'frontal' 9 38	81%
2		//a.t.a.a.l/		'frontal'	88%
	Target	'lateral' 'frontal'	46 3	9 42	
3				'frontal'	82%
3	Target	'lateral' 'frontal'	51 8	10 31	02 /6
4			Predi	iction 'frontal'	85%
4	Target	'lateral' 'frontal'	51 7	8 34	65%
_			iction 'frontal'		
5	Target	'lateral' 'frontal'	46 7	9	84%
Overall				iction 'frontal'	84%
	Target	'lateral' 'frontal'	237 35	45 183	0470



k-Fold Cross Validation



Figure: The division of data during the *k*-fold cross validation process. Black rectangles indicate test data, and white spaces indicate training data.

Leave-one-out Cross Validation

Fold 1	
Fold 2	
Fold 3	
Fold 4	
Fold 5	
•	•
	•
	•
Fold <i>k-2</i>	
Fold <i>k-1</i>	
Fold k	

Figure: The division of data during the **leave-one-out cross validation** process. Black rectangles indicate instances in the test set, and white spaces indicate training data.

Bootstrapping

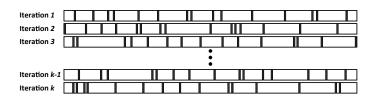


Figure: The division of data during the $\epsilon 0$ bootstrap process. Black rectangles indicate test data, and white spaces indicate training data.

Out-of-time Sampling

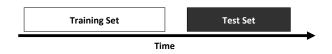


Figure: The out-of-time sampling process.

Performance Measures: Categorical Targets

$$TPR = \frac{TP}{(TP + FN)} \tag{1}$$

$$TNR = \frac{TN}{(TN + FP)}$$
 (2)

$$FPR = \frac{FP}{(TN + FP)}$$
 (3)

$$FNR = \frac{FN}{(TP + FN)} \tag{4}$$

Confusion Matrix-based Performance Measures

Design

TPR
$$=\frac{6}{(6+3)} = 0.667$$

TNR $=\frac{9}{(9+2)} = 0.818$
FPR $=\frac{2}{(9+2)} = 0.182$
FNR $=\frac{3}{(6+3)} = 0.333$

Precision, Recall and F₁ Measure

precision =
$$\frac{TP}{(TP + FP)}$$
 (5)
recall = $\frac{TP}{(TP + FN)}$ (6)

$$recall = \frac{TP}{(TP + FN)} \tag{6}$$

Precision, Recall and F₁ Measure

precision =
$$\frac{6}{(6+2)} = 0.75$$

recall = $\frac{6}{(6+3)} = 0.667$

Precision, Recall and F₁ Measure

$$F_{1}\text{-measure} = 2 \times \frac{(precision \times recall)}{(precision + recall)}$$
 (7)

$$F_{1}\text{-measure} = 2 \times \frac{(precision \times recall)}{(precision + recall)}$$
 (7)

$$\begin{aligned} \text{F}_{1}\text{-measure} &= 2 \times \frac{\left(\frac{6}{(6+2)} \times \frac{6}{(6+3)}\right)}{\left(\frac{6}{(6+2)} + \frac{6}{(6+3)}\right)} \\ &= 0.706 \end{aligned}$$

Table: A confusion matrix for a k-NN model trained on a churn prediction problem.

		Prediction		
		'non-churn'	'churn'	
Target	'non-churn'	90	0	
	'churn'	9	1	

Table: A confusion matrix for a naive Bayes model trained on a churn prediction problem.

		Prediction			
		'non-churn'	'churn'		
Target	'non-churn'	70	20		
Target	'churn'	2	8		

average class accuracy =
$$\frac{1}{|\textit{levels}(t)|} \sum_{l \in \textit{levels}(t)} \text{recall}_l$$
 (8)

average class accuracy_{HM} =
$$\frac{1}{\frac{1}{|levels(t)|} \sum_{l \in levels(t)} \frac{1}{\text{recall}_{l}}}$$
(9)

Design

$$\frac{1}{\frac{1}{2}\left(\frac{1}{1.0} + \frac{1}{0.1}\right)} = \frac{1}{5.5} = 18.2\%$$

$$\frac{1}{\frac{1}{2}\left(\frac{1}{0.778} + \frac{1}{0.800}\right)} = \frac{1}{1.268} = 78.873\%$$

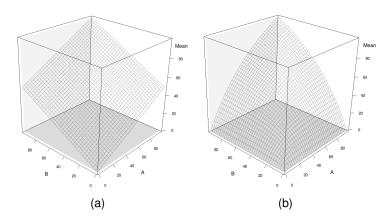


Figure: Surfaces generated by calculating (a) the **arithmetic mean** and (b) the **harmonic mean** of all combinations of features A and B that range from 0 to 100.

Measuring Profit and Loss

- It is not always correct to treat all outcomes equally
- In these cases, it is useful to take into account the cost of the different outcomes when evaluating models

Measuring Profit and Loss

Table: The structure of a **profit matrix**.

		Prediction		
		positive	negative	
Target	positive	TP _{Profit}	FN _{Profit}	
	negative	FP _{Profit}	TN_{Profit}	

Measuring Profit and Loss

Table: The **profit matrix** for the pay-day loan credit scoring problem.

		Predicti	ion
		'good' 'l	bad'
Torgot	'good'	140 –	-140
Target	'bad'	-700	0

Table: (a) The confusion matrix for a k-NN model trained on the pay-day loan credit scoring problem (average class accuracy $_{HM} = 83.824\%$); (b) the confusion matrix for a decision tree model trained on the pay-day loan credit scoring problem (average class accuracy_{HM} = 80.761%).

(a) k-NIN model

	(a) A ININI	Houci		(b) accision tree				
		Predic 'good'				Predic 'good'		
Target	'good'	57	3	Target	'good'	43	17	_
rarget	'bad'	10	30	rarget	'bad'	3	37	

(b) decision tree

Table: (a) Overall profit for the k-NN model using the profit matrix in Table 4 [25] and the confusion matrix in Table 5(a) [26]; (b) overall profit for the decision tree model using the profit matrix in Table 4 [25] and the confusion matrix in Table 5(b) [26].

(a) k-NN model

		Prediction	
		'good' 'bad	ľ
Towast	'good'	7 980 -42	0
Target	'bad'	−7 000	0
	Profit	56	0

(b) decision tree

		Prediction			
		'good'	'bad'		
Tourst	'good'	6 020 -	-2380		
Target	'bad'	-2100	0		
	Profit		1 540		

Performance Measures: Prediction Scores

Example

$$\textit{threshold(score}, 0.5) = \begin{cases} \textit{positive} & \textit{if score} \geq 0.5 \\ \textit{negative} & \textit{otherwise} \end{cases} \tag{10}$$

Table: A sample test set with model predictions and scores (threshold= 0.5.

		Pred-		Out-			Pred-		Out-
ID	Target	iction	Score	come	ID	Target	iction	Score	come
7	ham	ham	0.001	TN	-5	ham	ham	0.302	TN
11	ham	ham	0.003	TN	14	ham	ham	0.348	TN
15	ham	ham	0.059	TN	17	ham	spam	0.657	FP
13	ham	ham	0.064	TN	8	spam	spam	0.676	TP
19	ham	ham	0.094	TN	6	spam	spam	0.719	TP
12	spam	ham	0.160	FN	10	spam	spam	0.781	TP
2	spam	ham	0.184	FN	18	spam	spam	0.833	TP
3	ham	ham	0.226	TN	20	ham	spam	0.877	FP
16	ham	ham	0.246	TN	9	spam	spam	0.960	TP
1	spam	ham	0.293	FN	4	spam	spam	0.963	TP

- We have ordered the examples by score so the threshold is apparent in the predictions.
- Note that, in general, instances that actually should get a
 prediction of 'ham' generally have a low score, and those
 that should get a prediction of 'spam' generally get a high
 score.

- There are a number of performance measures that use this ability of a model to rank instances that should get predictions of one target level higher than the other, to assess how well the model is performing.
- The basis of most of these approaches is measuring how well the distributions of scores produced by the model for different target levels are separated

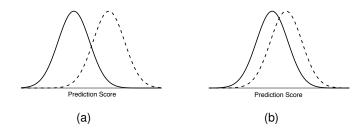


Figure: Prediction score distributions for two different prediction models. The distributions in (a) are much better separated than those in (b).

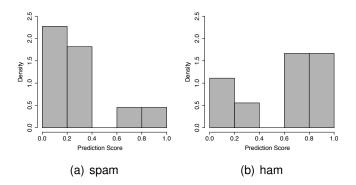


Figure: Prediction score distributions for the (a) 'spam' and (b) 'ham' target levels based on the data in Table 7 [30].

- The receiver operating characteristic index (ROC index), which is based on the receiver operating characteristic curve (ROC curve), is a widely used performance measure that is calculated using prediction scores.
- TPR and TNR are intrinsically tied to the threshold used to convert prediction scores into target levels.
- This threshold can be changed, however, which leads to different predictions and a different confusion matrix.

Table: Confusion matrices for the set of predictions shown in Table 7 [30] using (a) a prediction score threshold of 0.75 and (b) a prediction score threshold of 0.25.

(a) Threshold: 0.75

		Prediction			
		'spam'	'ham'		
Torget	'spam'	4	4		
Target	'ham'	2	10		

(b) Threshold: 0.25

		Prediction	
		'spam'	'ham'
Target	'spam'	7	2
	'ham'	4	7

	·		Pred.	Pred.	Pred.	Pred.	Pred.
ID Target Score		(0.10)	(0.25)	(0.50)	(0.75)	(0.90)	
7 ham 0.001		ham	ham	ham	ham	ham	
11 ham 0.003		ham	ham	ham	ham	ham	
15 ham 0.059		ham	ham	ham	ham	ham	
13 ham 0.064		ham	ham	ham	ham	ham	
19	ham	0.094	ham	ham	ham	ham	ham
12	spam	0.160	spam	ham	ham	ham	ham
2	spam	0.184	spam	ham	ham	ham	ham
3	ham	0.226	spam	ham	ham	ham	ham
16	ham	0.246	spam	ham	ham	ham	ham
1	spam	0.293	spam	spam	ham	ham	ham
5	ham	0.302	spam	spam	ham	ham	ham
14	ham	0.348	spam	spam	ham	ham	ham
17	ham	0.657	spam	spam	spam	ham	ham
8	spam	0.676	spam	spam	spam	ham	ham
6	spam	0.719	spam	spam	spam	ham	ham
10	spam	0.781	spam	spam	spam	spam	ham
18	spam	0.833	spam	spam	spam	spam	ham
20	ham	0.877	spam	spam	spam	spam	ham
9	spam	0.960	spam	spam	spam	spam	spam
4	spam	0.963	spam	spam	spam	spam	spam
Misclassification Rate			0.300	0.300	0.250	0.300	0.350
		e Rate (TPR)	1.000	0.778	0.667	0.444	0.222
	•	ve rate (TNR)	0.455	0.636	0.818	0.909	1.000
		e Rate (FPR)	0.545	0.364	0.182	0.091	0.000
Fals	se Negativ	e Rate (FNR)	0.000	0.222	0.333	0.556	0.778

Receiver Operating Characteristic Curves

- Note: as the threshold increases TPR decreases and TNR increases (and vice versa).
- Capturing this tradeoff is the basis of the ROC curve.

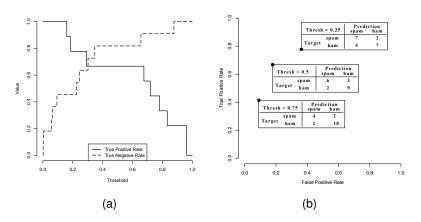


Figure: (a) The changing values of TPR and TNR for the test data shown in Table 36 [37] as the threshold is altered; (b) points in ROC space for thresholds of 0.25, 0.5, and 0.75.

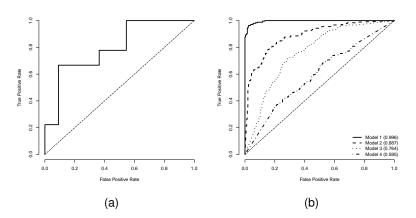


Figure: (a) A complete ROC curve for the email classification example; (b) a selection of ROC curves for different models trained on the same prediction task.

- We can also calculate a single performance measure from an ROC curve
- The ROC Index measures the area underneath an ROC curve.

ROC index =

$$\sum_{i=2}^{|\mathbf{T}|} \frac{(FPR(\mathbf{T}[i]) - FPR(\mathbf{T}[i-1])) \times (TPR(\mathbf{T}[i]) + TPR(\mathbf{T}[i-1]))}{2}$$
(11)

(11)

Receiver Operating Characteristic Curves

Design

The Gini coefficient is a linear rescaling of the ROC index

Gini coefficient =
$$(2 \times ROC \text{ index}) - 1$$
 (12)

Kolmogorov-Smirnov Statistic

 The Kolmogorov-Smirnov statistic (K-S statistic) is another performance measure that captures the separation between the distribution of prediction scores for the different target levels in a classification problem.

 To calculate the K-S statistic, we first determine the cumulative probability distributions of the prediction scores for the positive and negative target levels:

$$CP(positive, ps) = \frac{\text{num positive test instances with score} \le ps}{\text{num positive test instances}}$$
 (13)

$$CP(\textit{negative}, ps) = \frac{\text{num negative test instances with score} \le ps}{\text{num negative test instances}}$$
 (14)

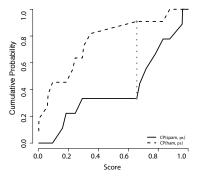


Figure: The K-S chart for the email classification predictions shown in Table 7 [30].

Kolmogorov-Smirnov Statistic

Design

 The K-S statistic is calculated by determining the maximum difference between the cumulative probability distributions for the positive and negative target levels.

$$K-S = \max_{ps} (CP(positive, ps) - CP(negative, ps))$$
 (15)

		Positive	Negative	Positive	Negative	
		('spam')	('ham')	('spam')	('ham')	
	Prediction	Cumulative	Cumulative	Cumulative	Cumulative	
ID	Score	Count	Count	Probability	Probability	Distance
7	0.001	0	1	0.000	0.091	0.091
11	0.003	0	2	0.000	0.182	0.182
15	0.059	0	3	0.000	0.273	0.273
13	0.064	0	4	0.000	0.364	0.364
19	0.094	0	5	0.000	0.455	0.455
12	0.160	1	5	0.111	0.455	0.343
2	0.184	2	5	0.222	0.455	0.232
3	0.226	2	6	0.222	0.545	0.323
16	0.246	2	7	0.222	0.636	0.414
1	0.293	3	7	0.333	0.636	0.303
5	0.302	3	8	0.333	0.727	0.394
14	0.348	3	9	0.333	0.818	0.485
17	0.657	3	10	0.333	0.909	0.576*
8	0.676	4	10	0.444	0.909	0.465
6	0.719	5	10	0.556	0.909	0.354
10	0.781	6	10	0.667	0.909	0.242
18	0.833	7	10	0.778	0.909	0.131
20	0.877	7	11	0.778	1.000	0.222
9	0.960	8	11	0.889	1.000	0.111

11

1.000

1.000

0.000

0.963

4

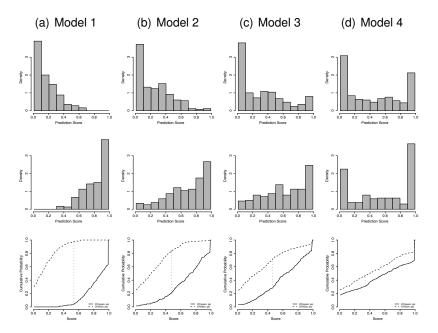


Figure: A series of charts for different model performance on the

Table: The test set with model predictions and scores from Table 7 [30] extended to include deciles.

1st 9 spam spam 0.960 TP 2nd 18 spam spam 0.963 TP 2nd 18 spam spam 0.833 TP 20 ham spam 0.877 FP 3rd 6 spam spam 0.719 TP 10 spam spam 0.781 TP 4th 17 ham spam 0.657 FP 8 spam spam 0.676 TP 5th 5 ham ham 0.302 TN 14 ham ham 0.348 TN	Decile	ID	Target	Prediction	Score	Outcome
4 spam spam 0.963 TP 2nd 18 spam spam 0.833 TP 20 ham spam 0.877 FP 3rd 6 spam spam 0.719 TP 10 spam spam 0.781 TP 4th 17 ham spam 0.657 FP 8 spam spam 0.676 TP 5th 5 ham ham 0.302 TN 14 ham ham 0.348 TN 6th 16 ham ham 0.246 TN 7th 2 spam ham 0.184 FN 7th 2 spam ham 0.184 FN 8th 19 ham ham 0.094 TN 9th 15 ham ham 0.059 TN 13 ham ham 0.064 TN 10th 7 ham ham 0.001 TN		9	spam	spam	0.960	TP
2nd 20 ham spam 0.877 FP 3rd 6 spam spam 0.719 TP 10 spam spam 0.781 TP 4th 17 ham spam 0.657 FP 8 spam spam 0.676 TP 5th 5 ham ham 0.302 TN 14 ham ham 0.348 TN 6th 16 ham ham 0.246 TN 1 spam ham 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.226 TN 8th 19 ham ham 0.094 TN 9th 15 ham ham 0.060 FN 13 ham ham 0.064 TN 10th 7 ham ham 0.001 TN	1	4	spam	spam	0.963	TP
20 ham spam 0.877 FP 3rd 6 spam spam 0.719 TP 10 spam spam 0.781 TP 4th 17 ham spam 0.657 FP 8 spam spam 0.676 TP 5th 5 ham ham 0.302 TN 14 ham ham 0.348 TN 6th 16 ham ham 0.246 TN 7th 2 spam ham 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.226 TN 8th 19 ham ham 0.094 TN 9th 15 ham ham 0.059 TN 13 ham ham 0.064 TN 10th 7 ham ham 0.001 TN		<u></u> 18	spam	spam	0.833	TP
10 spam spam 0.781 TP	2	20	ham	spam	0.877	FP
10 spam spam 0.781 IP 4th 17 ham spam 0.657 FP 8 spam spam 0.676 TP 5th 5 ham ham 0.302 TN 14 ham ham 0.348 TN 6th 16 ham ham 0.246 TN 1 spam ham 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.094 TN 8th 19 ham ham 0.160 FN 9th 15 ham ham 0.059 TN 13 ham ham 0.064 TN 10th 7 ham ham 0.001 TN	2rd	6_	spam	spam	0.719	TP
4th 8 spam spam 0.676 TP 5th 5 ham ham 0.302 TN 14 ham ham 0.348 TN 6th 16 ham ham 0.246 TN 1 spam ham 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.226 TN 8th 19 ham ham 0.094 TN 12 spam ham 0.160 FN	3	10	spam	spam	0.781	TP
8 spam spam 0.676 IP 5 ham ham 0.302 TN 14 ham ham 0.348 TN	-	17	ham	spam	0.657	FP
5th 14 ham ham 0.348 TN 6th 16 ham ham 0.246 TN 1 spam ham 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.226 TN 8th 19 ham ham 0.094 TN 12 spam ham 0.160 FN 15 ham ham 0.059 TN 10th 7 ham ham 0.064 TN 10th 7 ham ham 0.001 TN	4	8	spam	spam	0.676	TP
14		5_	ham	ham -	0.302	ĪN
6th 1 spam ham 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.226 TN 8th 19 ham ham 0.094 TN 12 spam ham 0.160 FN	3	14	ham	ham	0.348	TN
1 spam nam 0.293 FN 7th 2 spam ham 0.184 FN 3 ham ham 0.226 TN 8th 19 ham ham 0.094 TN 12 spam ham 0.160 FN - 9th 15 ham ham 0.059 TN - 13 ham ham 0.064 TN 10th 7 ham ham 0.001 TN	eth	16	ham	ham	0.246	TN
3 ham ham 0.226 TN 8 th 19 ham ham 0.094 TN 12 spam ham 0.160 FN 15 ham ham 0.059 TN 13 ham ham 0.064 TN 10 th 7 ham ham 0.001	0	1	spam	ham	0.293	FN
3 ham ham 0.226 IN 8th 19 ham ham 0.094 TN 12 spam ham 0.160 FN 9th 15 ham ham 0.059 TN 13 ham ham 0.064 TN 10th 7 ham ham 0.001 TN	 7th	2_	spam	ham	0.184	FN
8"' 12 spam ham 0.160 FN 9 th 15 ham ham 0.059 TN - 13 ham ham 0.064 TN - 10 th 7 ham ham 0.001 TN	7	3	ham	ham	0.226	TN
12 spam nam 0.160 FN - 9 th 15 ham ham 0.059 TN - 13 ham ham 0.064 TN - 10 th 7 ham ham 0.001		19	ham	ham	0.094	TN
13 ham ham 0.064 TN ham 0.001 TN	0	12	spam	ham	0.160	FN
- 13 nam nam 0.064 IN - 10 th 7 ham ham 0.001 TN	oth	<u></u>	ham	ham -	0.059	<u>T</u> N
104	9	13	ham	ham	0.064	TN
11 ham ham 0.003 TN	10th	7	ham	ham -	0.001	TN
	10	11	ham	ham	0.003	TN

Measuring Gain and Lift

$$Gain(dec) = \frac{\text{num positive test instances in decile } dec}{\text{num positive test instances}}$$
 (16)

Table: Tabulating the workings required to calculate **gain**, cumulative gain, lift, and cumulative lift for the data given in Table 7 [30].

	Positive	Negative		0		0
	('spam')	('ham')		Cum.		Cum.
Decile	Count	Count	Gain	Gain	Lift	Lift
1 st	2	0	0.222	0.222	2.222	2.222
2 nd	1	1	0.111	0.333	1.111	1.667
3 rd	2	0	0.222	0.556	2.222	1.852
4 th	1	1	0.111	0.667	1.111	1.667
5 th	0	2	0.000	0.667	0.000	1.333
6 th	1	1	0.111	0.778	1.111	1.296
7 th	1	1	0.111	0.889	1.111	1.270
8 th	1	1	0.111	1.000	1.111	1.250
9 th	0	2	0.000	1.000	0.000	1.111
10 th	0	2	0.000	1.000	0.000	1.000

Measuring Gain and Lift

Cumulative gain(
$$dec$$
) = $\frac{\text{num positive test instances in all deciles up to } dec}{\text{num positive test instances}}$
(17)

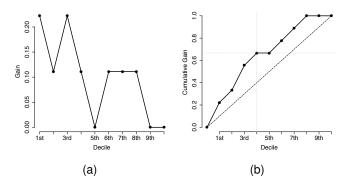


Figure: The (a) gain and (b) cumulative gain at each decile for the email predictions given in Table 7 [30].

Measuring Gain and Lift

$$Lift(dec) = \frac{\% \text{ of positive test instances in decile } dec}{\% \text{ of positive test instances}}$$
 (18)

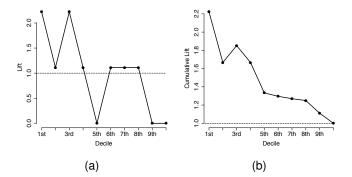
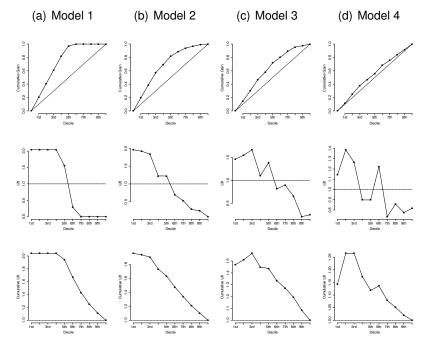


Figure: The (a) lift and (b) cumulative lift at each decile for the email predictions given in Table 7 [30].

Measuring Gain and Lift

Cumulative lift(
$$dec$$
) = $\frac{\% \text{ of positive instances in all deciles up to } dec}{\% \text{ of positive test instances}}$

(19)



Performance Measures: Multinomial Targets

Table: The structure of a confusion matrix for a multinomial prediction problem with *I* target levels.

			Prediction					
		level1	level1 level2 level3 ··· levell					
	level1	-	-	-		-	-	
	level2	-	-	-		-	-	
Target	level3	-	-	-		-	-	
	:				٠		:	
	levell	-	-	-		-	-	
	Precision	-	-	-		-		

precision(I) =
$$\frac{TP(I)}{TP(I) + FP(I)}$$

$$recall(I) = \frac{TP(I)}{TP(I) + FN(I)}$$
(20)

$$recall(I) = \frac{IP(I)}{TP(I) + FN(I)}$$
 (21)

Table: A sample test set with model predictions for a bacterial species identification problem.

ID	Target	Prediction	ID	Target	Prediction
1	durionis	fructosus	16	ficulneus	ficulneus
2	ficulneus	fructosus	17	ficulneus	ficulneus
3	fructosus	fructosus	18	fructosus	fructosus
4	ficulneus	ficulneus	19	durionis	durionis
5	durionis	durionis	20	fructosus	fructosus
6	pseudo.	pseudo.	21	fructosus	fructosus
7	durionis	fructosus	22	durionis	durionis
8	ficulneus	ficulneus	23	fructosus	fructosus
9	pseudo.	pseudo.	24	pseudo.	fructosus
10	pseudo.	fructosus	25	durionis	durionis
11	fructosus	fructosus	26	pseudo.	pseudo.
12	ficulneus	ficulneus	27	fructosus	fructosus
13	durionis	durionis	28	ficulneus	ficulneus
14	fructosus	fructosus	29	fructosus	fructosus
15	fructosus	ficulneus	30	fructosus	fructosus

Table: A confusion matrix for a model trained on the bacterial species identification problem.

			Prediction					
		'durionis'	Recall					
	'durionis'	5	0	2	0	0.714		
Torget	'ficulneus'	0	6	1	0	0.857		
Target	'fructosus'	0	1	10	0	0.909		
	'pseudo.'	0	0	2	3	0.600		
	Precision	1.000	0.857	0.667	1.000			

• The average class accuracy_{HM} for this problem is:

$$\frac{1}{\frac{1}{4}\left(\frac{1}{0.714} + \frac{1}{0.857} + \frac{1}{0.909} + \frac{1}{0.600}\right)} = \frac{1}{1.333} = 75.000\%$$

Performance Measures: Continuous Targets

sum of squared errors =
$$\frac{1}{2} \sum_{i=1}^{n} (t_i - \mathbb{M}(\mathbf{d}_i))^2$$
 (22)

root mean squared error =
$$\sqrt{\frac{\sum_{i=1}^{n}(t_i - \mathbb{M}(\mathbf{d}_i))^2}{n}}$$
 (24)

mean absolute error
$$= \frac{\displaystyle\sum_{i=1} abs(t_i - \mathbb{M}(\mathbf{d}_i))}{n}$$
 (25)

		Linear Reg	ression	k-NN	1
ID	Target	Prediction	Error	Prediction	Error
1	10.502	10.730	0.228	12.240	1.738
2	18.990	17.578	-1.412	21.000	2.010
3	20.000	21.760	1.760	16.973	-3.027
4	6.883	7.001	0.118	7.543	0.660
5	5.351	5.244	-0.107	8.383	3.032
6	11.120	10.842	-0.278	10.228	-0.892
7	11.420	10.913	-0.507	12.921	1.500
8	4.836	7.401	2.565	7.588	2.752
9	8.177	8.227	0.050	9.277	1.100
10	19.009	16.667	-2.341	21.000	1.991
11	13.282	14.424	1.142	15.496	2.214
12	8.689	9.874	1.185	5.724	-2.965
13	18.050	19.503	1.453	16.449	-1.601
14	5.388	7.020	1.632	6.640	1.252
15	10.646	10.358	-0.288	5.840	-4.805
16	19.612	16.219	-3.393	18.965	-0.646
17	10.576	10.680	0.104	8.941	-1.634
18	12.934	14.337	1.403	12.484	-0.451
19	10.492	10.366	-0.126	13.021	2.529
20	13.439	14.035	0.596	10.920	-2.519
21	9.849	9.821	-0.029	9.920	0.071
22	18.045	16.639	-1.406	18.526	0.482
23	6.413	7.225	0.813	7.719	1.307
24	9.522	9.565	0.043	8.934	-0.588
25	12.083	13.048	0.965	11.241	-0.842
26	10.104	10.085	-0.020	10.010	-0.095
27	8.924	9.048	0.124	8.157	-0.767
28	10.636	10.876	0.239	13.409	2.773
29	5.457	4.080	-1.376	9.684	4.228
30	3.538	7.090	3.551	5.553	2.014
	MSE		1.905		4.394
	RMSE		1.380		2.096
	MAE		0.975		1.750
	R ²		0.889		0.776

Domain Independent Measures of Error

$$R^2 = 1 - \frac{\text{sum of squared errors}}{\text{total sum of squares}}$$
 (26)

total sum of squares =
$$\frac{1}{2} \sum_{i=1}^{n} (t_i - \overline{t})^2$$
 (27)

Evaluating Models after Deployment

To monitor the on-going performance of a model, we need a signal that indicates that something has changed. There are three sources from which we can extract such a signal:

- The performance of the model measured using appropriate performance measures
- The distributions of the outputs of a model
- The distributions of the descriptive features in query instances presented to the model

- The simplest way to get a signal that concept drift has occurred is to repeatedly evaluate models with the same performance measures used to evaluate them before deployment.
- We can calculate performance measures for a deployed model and compare these to the performance achieved in evaluations before the model was deployed.
- If the performance changes significantly, this is a strong indication that concept drift has occurred and that the model has gone stale.

Monitoring Changes in Performance Measures

 Although monitoring changes in the performance of a model is the easiest way to tell whether it has gone stale, this method makes the rather large assumption that the correct target feature value for a query instance will be made available shortly after the query has been presented to a deployed model.

 An alternative to using changing model performance is to use changes in the distribution of model outputs as a signal for concept drift.

$$\text{stability index} = \sum_{l \in \textit{levels}(t)} \left(\left(\frac{|\mathcal{A}_{t=l}|}{|\mathcal{A}|} - \frac{|\mathcal{B}_{t=l}|}{|\mathcal{B}|} \right) \times \textit{log}_e \left(\frac{|\mathcal{A}_{t=l}|}{|\mathcal{A}|} / \frac{|\mathcal{B}_{t=l}|}{|\mathcal{B}|} \right) \right) \text{ (28)}$$

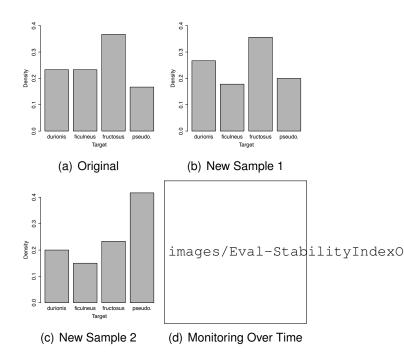
In general,

- stability index < 0.1, then the distribution of the newly collected test set is broadly similar to the distribution in the original test set.
- stability index is between 0.1 and 0.25, then some change has occurred and further investigation may be useful.
- stability index > 0.25 suggests that a significant change has occurred and corrective action is required.

Table: Calculating the **stability index** for the bacterial species identification problem given new test data for two periods after model deployment. The frequency and percentage of each target level are shown for the original test set and for two samples collected after deployment. The column marked SI_t shows the different parts of the stability index sum based on Equation (28)^[72].

	Orig	jinal	Ne	New Sample 1			New Sample 2		
Target	Count	%	Count	%	SI_t	Count	%	SI_t	
'durionis'	7	0.233	12	0.267	0.004	12	0.200	0.005	
'ficulneus'	7	0.233	8	0.178	0.015	9	0.150	0.037	
'fructosus'	11	0.367	16	0.356	0.000	14	0.233	0.060	
'pseudo.'	5	0.167	9	0.200	0.006	25	0.417	0.229	
Sum	30		45		0.026	60		0.331	

stability index
$$= \left(\frac{7}{30} - \frac{12}{45}\right) \times log_{e}\left(\frac{7}{30} / \frac{12}{45}\right) \\ + \left(\frac{7}{30} - \frac{8}{45}\right) \times log_{e}\left(\frac{7}{30} / \frac{8}{45}\right) \\ + \left(\frac{11}{30} - \frac{16}{45}\right) \times log_{e}\left(\frac{11}{30} / \frac{16}{45}\right) \\ + \left(\frac{5}{30} - \frac{9}{45}\right) \times log_{e}\left(\frac{5}{30} / \frac{9}{45}\right) \\ = 0.026$$



- In the same way we can compare the distributions of model outputs between the time that the model was built and after deployment, we can also make the same type of comparison for the distributions of the descriptive features used by the model.
- We can use any appropriate measure that captures the difference between two different distributions for this, including the stability index, the χ^2 statistic, and the K-S statistic.

- There is, however, a challenge here, as usually, there are a large number of descriptive features for which measures need to be calculated and tracked.
- Furthermore, it is unlikely that a change in the distribution of just one descriptive feature in a multi-feature model will have a large impact on model performance.
- For this reason, unless a model uses a very small number of descriptive features (generally fewer than 10), we do not recommend this approach.

Comparative Experiments Using a Control Group

 We use control groups not to evaluate the predictive power of the models themselves, but rather to evaluate how good they are at helping with the business problem when they are deployed.

Table: The number of customers who left the mobile phone network operator each week during the comparative experiment from both the control group (random selection) and the treatment group (model selection).

	Control Group	Treatment Group
Week	(Random Selection)	(Model Selection)
1	21	23
2	18	15
3	28	18
4	19	20
5	18	15
6	17	17
7	23	18
8	24	20
9	19	18
10	20	19
11	18	13
12	21	16
Mean	20.500	17.667
Std. Dev.	3.177	2.708

Comparative Experiments Using a Control Group

 These figures show that, on average, fewer customers churn when the churn prediction model is used to select which customers to call.

Summary

Designing Evaluation Experiments Hold-out Sampling k-Fold Cross Validation

- I eave-one-out Cross Validation
- Bootstrapping
- Out-of-time Sampling
- **Performance Measures: Categorical Targets**
 - Confusion Matrix-based Performance Measures Precision, Recall and F₁ Measure
 - Average Class Accuracy
 - Measuring Profit and Loss
 - Performance Measures: Prediction Scores
 - Receiver Operating Characteristic Curves Kolmogorov-Smirnov Statistic

 - Measuring Gain and Lift
 - **Performance Measures: Multinomial Targets**
 - **Performance Measures: Continuous Targets**
 - Basic Measures of Error
 - Domain Independent Measures of Error
- **Evaluating Models after Deployment**
 - Monitoring Changes in Performance Measures Monitoring Model Output Distributions
 - Monitoring Descriptive Feature Distribution Changes
- Comparative Experiments Using a Control Group
- Summary