Fundamentals of Machine Learning for Predictive Data Analytics

Chapter 8: Evaluation
Sections 8.4, 8.5

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Designing Evaluation Experiments

Design   Cat. Targets   Pred. Scores   Multinomial Cont. Targets Deployment   Sum.

Hold-out Sampling

(a) A 50:20:30 split

(b) A 40:20:40 split

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

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.

Hold-out Sampling
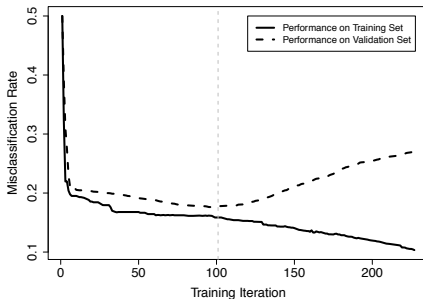
Figure: Using a validation set to avoid overfitting in iterative machine learning algorithms.

Fold	Confusion Matrix				Class Accuracy
			Prediction		
			'lateral'	*'frontal'*	
1	Target	*'lateral'*	43	9	81%
		'frontal'	10	38	
			Prediction		
			'lateral'	*'frontal'*	
2	Target	*'lateral'*	46	9	88%
		'frontal'	3	42	
			Prediction		
			'lateral'	*'frontal'*	
3	Target	*'lateral'*	51	10	82%
		'frontal'	8	31	
			Prediction		
			'lateral'	*'frontal'*	
4	Target	*'lateral'*	51	8	85%
		'frontal'	7	34	
			Prediction		
			'lateral'	*'frontal'*	
5	Target	*'lateral'*	46	9	84%
		'frontal'	7	38	
			Prediction		
			'lateral'	*'frontal'*	
Overall	Target	*'lateral'*	237	45	84%
		'frontal'	35	183	

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.

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.
○○○○●○○ ○○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○○○○○○ ○○○ ○○○○○○○○○○○○

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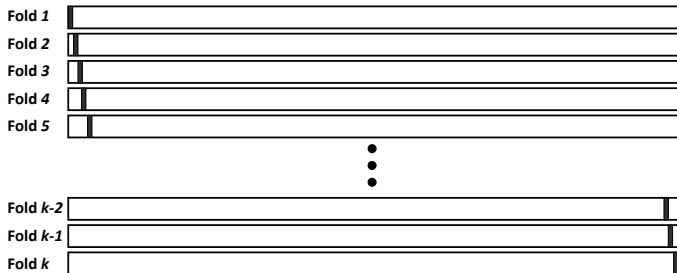
Figure: The division of data during the **leave-one-out cross validation** process. Black rectangles indicate instances in the test set, and white spaces indicate training data.

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.
○○○○○●○ ○○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○○○○○○ ○○○ ○○○○○○○○○○○
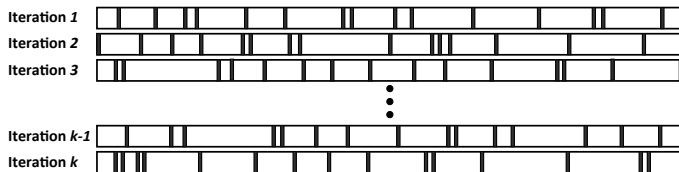
Bootstrapping

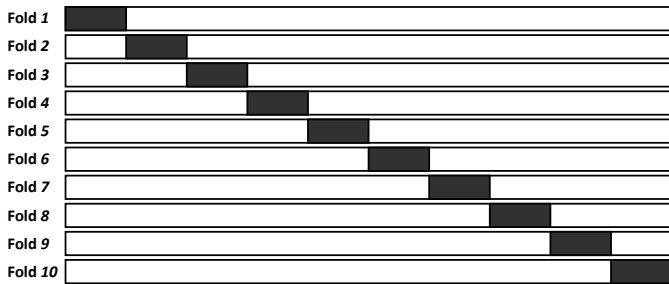**Figure:** The division of data during the $\epsilon 0$ bootstrap process. Black rectangles indicate test data, and white spaces indicate training data.

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.
○○○○○○● ○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○○○○○○○ ○○○ ○○○○○○○○○○○○

Out-of-time Sampling
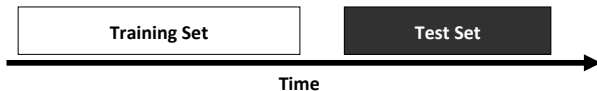
Figure: The **out-of-time sampling** process.

Performance Measures: Categorical Targets

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.
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Confusion Matrix-based Performance Measures

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

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

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

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

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.

Confusion Matrix-based Performance Measures

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

$$\text{TNR} = \frac{9}{(9+2)} = 0.818$$

$$\text{FPR} = \frac{2}{(9+2)} = 0.182$$

$$\text{FNR} = \frac{3}{(6+3)} = 0.333$$

Design | Cat. Targets | Pred. Scores | Multinomial | Cont. Targets | Deployment | Sum.
○○○○○○○ | ○○●○○○○○○○○○○○○○ | ○○○○○○○○○○○○○○○○○○○○○○○ | | ○○○ | ○○○○○○○○○○○○ |

Precision, Recall and F$_1$ Measure

$$\text{precision} = \frac{TP}{(TP + FP)} \qquad (5)$$

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

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.
○○○○○○○ ○○○●○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○○○○○○○ ○○○ ○○○○○○○○○○○○

Precision, Recall and F_1 Measure

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

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

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.

Precision, Recall and F_1 Measure

$$F_1\text{-measure} = 2 \times \frac{(\text{precision} \times \text{recall})}{(\text{precision} + \text{recall})} \qquad (7)$$

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.
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Precision, Recall and F_1 Measure

$$F_1\text{-measure} = 2 \times \frac{(\text{precision} \times \text{recall})}{(\text{precision} + \text{recall})} \tag{7}$$

$$F_1\text{-measure} = 2 \times \frac{\left(\frac{6}{(6+2)} \times \frac{6}{(6+3)}\right)}{\left(\frac{6}{(6+2)} + \frac{6}{(6+3)}\right)}$$
$$= 0.706$$

Design | Cat. Targets | Pred. Scores | Multinomial | Cont. Targets | Deployment | Sum.
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Average Class Accuracy

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
	'churn'	2	8

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.

Average Class Accuracy

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

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.

Average Class Accuracy

$$\text{average class accuracy}_{HM} = \cfrac{1}{\cfrac{1}{|levels(t)|} \displaystyle\sum_{l \in levels(t)} \cfrac{1}{\text{recall}_l}} \quad (9)$$

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.
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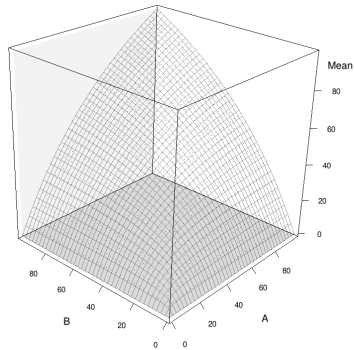
Average Class Accuracy

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

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

Design	Cat. Targets	Pred. Scores	Multinomial	Cont. Targets	Deployment	Sum.
○○○○○○○	○○○○○○○○○●○○○○○	○○○○○○○○○○○○○○○○○○○○○○○○○○○		○○○	○○○○○○○○○○○○	

Average Class Accuracy
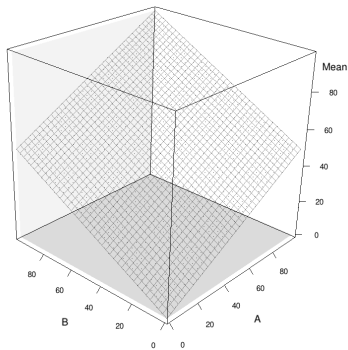
(a)   (b)

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.

Design	Cat. Targets	Pred. Scores	Multinomial	Cont. Targets	Deployment	Sum.
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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

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.
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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}

Design | Cat. Targets | Pred. Scores | Multinomial | Cont. Targets | Deployment | Sum.

Measuring Profit and Loss

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

		Prediction	
		'good'	*'bad'*
Target	*'good'*	140	−140
	'bad'	−700	0

| Design | Cat. Targets | Pred. Scores | Multinomial | Cont. Targets | Deployment | Sum. |

Measuring Profit and Loss

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*-NN model				(b) decision tree		
		Prediction				**Prediction**	
		'good'	*'bad'*			*'good'*	*'bad'*
Target	*'good'*	57	3	**Target**	*'good'*	43	17
	'bad'	10	30		*'bad'*	3	37

Design Cat. Targets Pred. Scores Multinomial Cont. Targets Deployment Sum.

Measuring Profit and Loss

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'*
Target	*'good'*	7 980	−420
	'bad'	−7 000	0
Profit			**560**

(b) decision tree

		Prediction	
		'good'	*'bad'*
Target	*'good'*	6 020	−2 380
	'bad'	−2 100	0
Profit			**1 540**

Performance Measures:
Prediction Scores

- All our classification prediction models return a score which is then thresholded.

Example

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

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

ID	Target	Prediction	Score	Outcome	ID	Target	Prediction	Score	Outcome
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
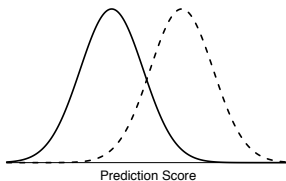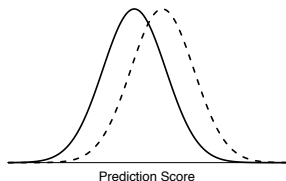
Figure: Prediction score distributions for two different prediction models. The distributions in (a) are much better separated than those in (b).
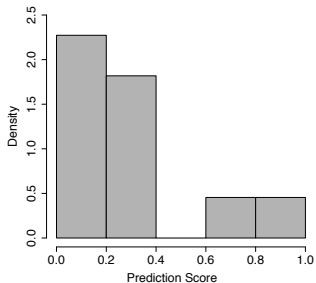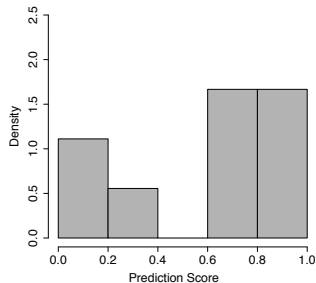
(a) spam   (b) ham

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

Design Cat. Targets **Pred. Scores** Multinomial Cont. Targets Deployment Sum.
○○○○○○○ ○○○○○○○○○○○○○○○○○ ●○○○○○○○○○○○○○○○○○○○○○○○○○○ ○○○ ○○○○○○○○○○○○

Receiver Operating Characteristic Curves

- 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.

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○ ○●○○○○○○○○○○○○○○○○○○○○○○○○○○○○○   ○○○   ○○○○○○○○○○○○

Receiver Operating Characteristic Curves

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'*
Target	*'spam'*	4	4
	'ham'	2	10

(b) Threshold: 0.25

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

ID	Target	Score	Pred. (0.10)	Pred. (0.25)	Pred. (0.50)	Pred. (0.75)	Pred. (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
True Positive Rate (TPR)			1.000	0.778	0.667	0.444	0.222
True Negative rate (TNR)			0.455	0.636	0.818	0.909	1.000
False Positive Rate (FPR)			0.545	0.364	0.182	0.091	0.000
False Negative Rate (FNR)			0.000	0.222	0.333	0.556	0.778

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.

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.

Design Cat. Targets **Pred. Scores** Multinomial Cont. Targets Deployment Sum.
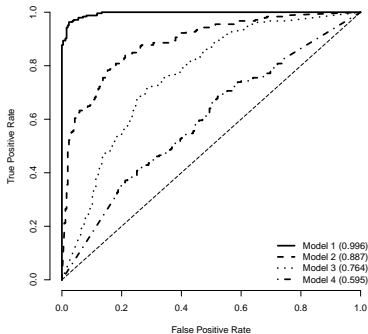○○○○○○○ ○○○○○○○○○○○○○○○○ ○○○○●○○○○○○○○○○○○○○○○○○○○ ○○○ ○○○○○○○○○○○○

Receiver Operating Characteristic Curves
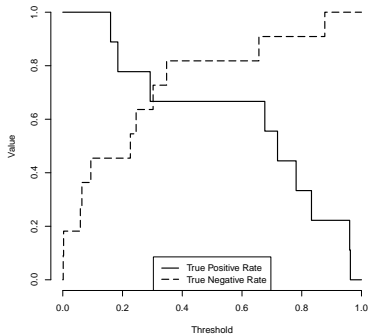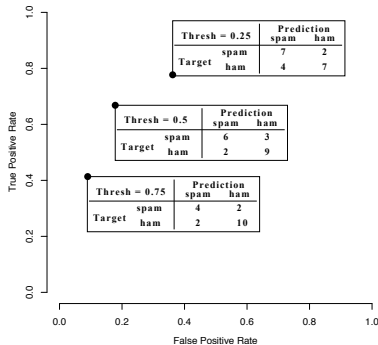
(a)   (b)

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.

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○○   ○○○○○●○○○○○○○○○○○○○○○○○○○○○   ○○○   ○○○○○○○○○○○○

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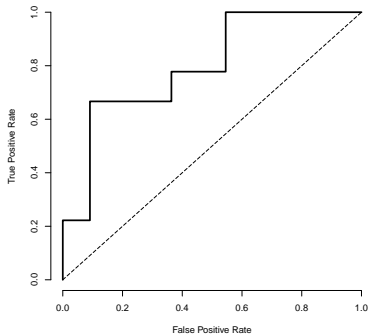
Figure: (a) A complete ROC curve for the email classification example; (b) a selection of ROC curves for different models trained on the same prediction task.

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○ ○○○○○○●○○○○○○○○○○○○○○○   ○○○   ○○○○○○○○○○○○

Receiver Operating Characteristic Curves

- 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)

Design Cat. Targets **Pred. Scores** Multinomial Cont. Targets Deployment Sum.
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Receiver Operating Characteristic Curves

- The **Gini coefficient** is a linear rescaling of the ROC index

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

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○○ ○○○○○○○○●○○○○○○○○○○○○○   ○○○   ○○○○○○○○○○○○

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.

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
◦◦◦◦◦◦◦ ◦◦◦◦◦◦◦◦◦◦◦◦◦◦◦ ◦◦◦◦◦◦◦◦●◦◦◦◦◦◦◦◦◦◦◦◦◦◦   ◦◦◦   ◦◦◦◦◦◦◦◦◦◦◦◦

Kolmogorov-Smirnov Statistic

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

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

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

Design Cat. Targets **Pred. Scores** Multinomial Cont. Targets Deployment Sum.

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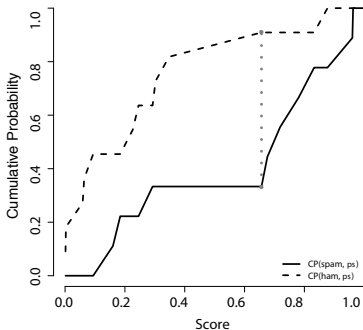
Figure: The K-S chart for the email classification predictions shown in Table 7 [30].

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○○ ○○○○○○○○●○○○○○○○○○○○○○○   ○○○   ○○○○○○○○○○○○

Kolmogorov-Smirnov Statistic

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

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

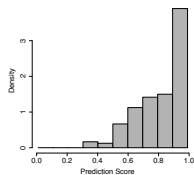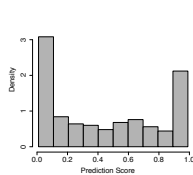| ID	Prediction Score	Positive ('spam') Cumulative Count	Negative ('ham') Cumulative Count	Positive ('spam') Cumulative Probability	Negative ('ham') Cumulative Probability	Distance
7	0.001	0	1	0.000	0.091	0.091
11	0.003	0	2	0.000	0.182	0.182
15	0.059	0	3	0.000	0.273	0.273
13	0.064	0	4	0.000	0.364	0.364
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
4	0.963	9	11	1.000	1.000	0.000
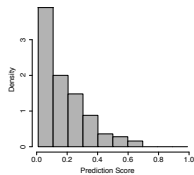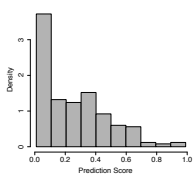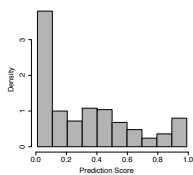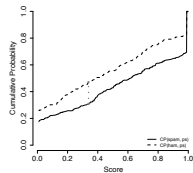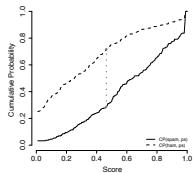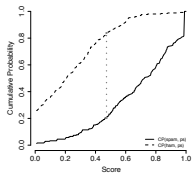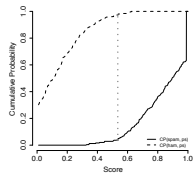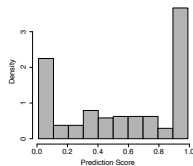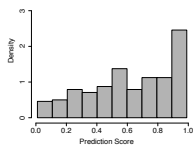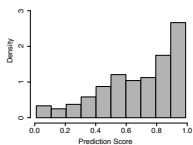
Figure: A series of charts for different model performance on the

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

Decile	ID	Target	Prediction	Score	Outcome
1st	9	spam	spam	0.960	TP
	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
	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
9th	15	ham	ham	0.059	TN
	13	ham	ham	0.064	TN
10th	7	ham	ham	0.001	TN
	11	ham	ham	0.003	TN

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.

Measuring Gain and Lift

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

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.

Measuring Gain and Lift

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

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

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○●○○○○○   ○○○   ○○○○○○○○○○○○

Measuring Gain and Lift

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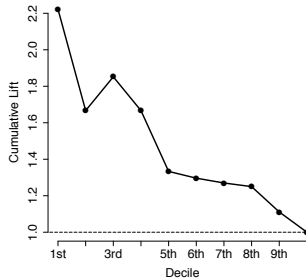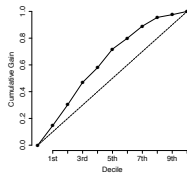
$$\tag{17}$$

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○●○○○○   ○○○   ○○○○○○○○○○○○

Measuring Gain and Lift
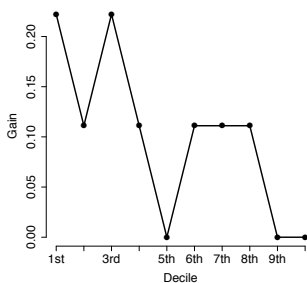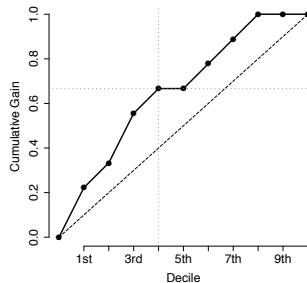
(a)   (b)

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

Design   Cat. Targets   **Pred. Scores**   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○ ○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○●○○○ ○○○ ○○○○○○○○○○○○

Measuring Gain and Lift

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

Design Cat. Targets **Pred. Scores** Multinomial Cont. Targets Deployment Sum.
○○○○○○○ ○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○○●○○ ○○○ ○○○○○○○○○○○○

Measuring Gain and Lift
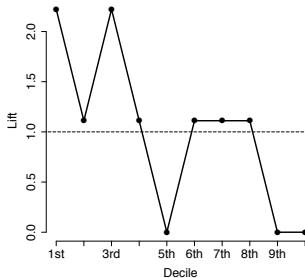
(a)   (b)

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

Design Cat. Targets **Pred. Scores** Multinomial Cont. Targets Deployment Sum.
〇〇〇〇〇〇〇 〇〇〇〇〇〇〇〇〇〇〇〇〇〇 〇〇〇〇〇〇〇〇〇〇〇〇〇〇●〇 〇〇〇 〇〇〇〇〇〇〇〇〇〇〇

Measuring Gain and Lift

$$\text{Cumulative lift}(dec) = \frac{\text{\% of positive instances in all deciles up to } dec}{\text{\% of positive test instances}}$$
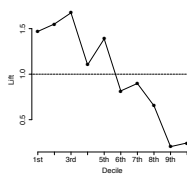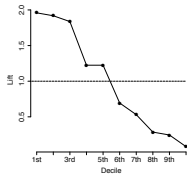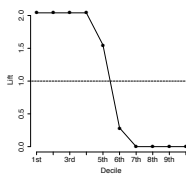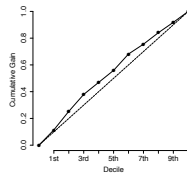(19)
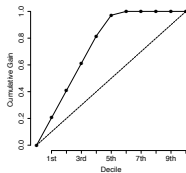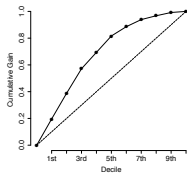
(a) Model 1 (b) Model 2 (c) Model 3 (d) Model 4
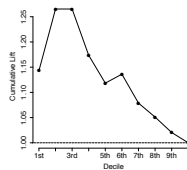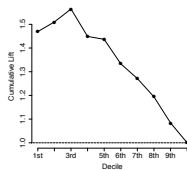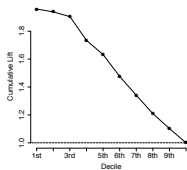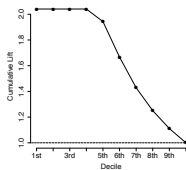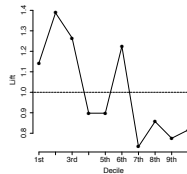
Performance Measures: Multinomial Targets

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

		\<br\>*level1*	Prediction\<br\>*level2*	\<br\>*level3*	$\cdots$	\<br\>*levell*	Recall
	level1	-	-	-		-	-
	level2	-	-	-		-	-
Target	*level3*	-	-	-		-	-
	$\vdots$				$\ddots$		$\vdots$
	levell	-	-	-		-	-
	Precision	-	-	-	$\cdots$	-	

$$\text{precision(l)} = \frac{TP(l)}{TP(l) + FP(l)} \qquad (20)$$

$$\text{recall(l)} = \frac{TP(l)}{TP(l) + FN(l)} \qquad (21)$$

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				**Recall**
		'durionis'	*'ficulneus'*	*'fructosus'*	*'pseudo.'*	
	'durionis'	5	0	2	0	0.714
Target	*'ficulneus'*	0	6	1	0	0.857
	'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

Design Cat. Targets Pred. Scores Multinomial **Cont. Targets** Deployment Sum.

Basic Measures of Error

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

$$\text{mean squared error} = \frac{\displaystyle\sum_{i=1}^{n} (t_i - \mathbb{M}(\mathbf{d}_i))^2}{n} \qquad (23)$$

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

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

ID	Target	Linear Regression		k-NN	
		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**

Design Cat. Targets Pred. Scores Multinomial **Cont. Targets** Deployment Sum.
ooooooo ooooooooooooooo ooooooooooooooooooooooo ooo ● oooooooooooo

Domain Independent Measures of Error

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

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

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:

1. The performance of the model measured using appropriate performance measures
2. The distributions of the outputs of a model
3. The distributions of the descriptive features in query instances presented to the model

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.

Monitoring Changes in Performance Measures

- 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.

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.
0000000 000000000000000 0000000000000000000000   000   000000000000   00●00000000000

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.

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.

Monitoring Model Output Distributions

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

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

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.

Monitoring Model Output Distributions

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].

Target	Original		New Sample 1			New Sample 2		
	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**

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.
○○○○○○○   ○○○○○○○○○○○○○○○   ○○○○○○○○○○○○○○○○○○○○○○○○○   ○○○   ○○○○○○●○○○○○○
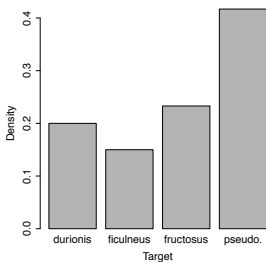
Monitoring Model Output Distributions

$$
\begin{aligned}
\text{stability index} \;=\; & \left(\frac{7}{30} - \frac{12}{45}\right) \times log_e\left(\frac{7}{30}\Big/\frac{12}{45}\right) \\
& + \left(\frac{7}{30} - \frac{8}{45}\right) \times log_e\left(\frac{7}{30}\Big/\frac{8}{45}\right) \\
& + \left(\frac{11}{30} - \frac{16}{45}\right) \times log_e\left(\frac{11}{30}\Big/\frac{16}{45}\right) \\
& + \left(\frac{5}{30} - \frac{9}{45}\right) \times log_e\left(\frac{5}{30}\Big/\frac{9}{45}\right) \\
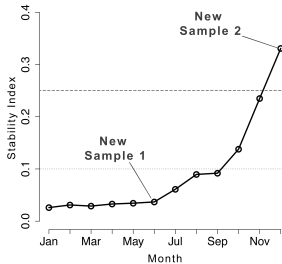=\; & 0.026
\end{aligned}
$$
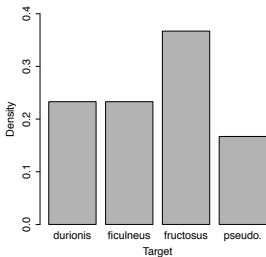
(a) Original
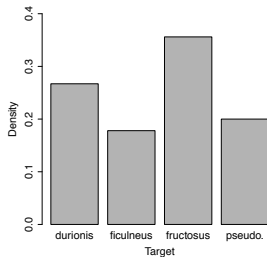
(b) New Sample 1

(c) New Sample 2

(d) Monitoring Over Time

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   Deployment   Sum.
○○○○○○○   ○○○○○○○○○○○○○○○○ ○○○○○○○○○○○○○○○○○○○○○○○○   ○○○   ○○○○○○○●○○○○○

Monitoring Descriptive Feature Distribution Changes

- 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.

Design Cat. Targets Pred. Scores Multinomial Cont. Targets **Deployment** Sum.

Monitoring Descriptive Feature Distribution Changes

- 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.

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.

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).

Week	Control Group (Random Selection)	Treatment Group (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

Design   Cat. Targets   Pred. Scores   Multinomial   Cont. Targets   **Deployment**   Sum.

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