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Assessment of paper metrics as predictors of quality for inkjet printing

Tadanobu Sato[1] *and Craig Revie*[2]

[1] Fujifilm, 2-26-30 Nishi Azabu Minato-ku, Tokyo 106-8620, Japan
[2] FFEI Limited, The Cube, Maylands Avenue, Hemel Hempstead, HP2 7DF UK

tadanobu.sato@fujifilm.com
craig.revie@ffei.co.uk

Abstract

Recent developments in inkjet technology have enabled the development of high-speed inkjet presses with similar quality and performance to conventional printing presses. These inkjet presses can print on a wide range of papers. Prints made on some papers are of high quality whereas on others are unacceptable. These print results vary from one digital press to another. The focus of this publication is the development of techniques to predict print quality from measurements of papers. Two studies were conducted. In the first, a set of around 250 papers were measured, prints were made on a single digital press and the print quality assessed. In the second, a set of 20 papers were measured, prints were made on three digital presses from different manufacturers and the print quality assessed for each. The studies were unable to identify or develop a single metric that can be used to predict print quality, however, a set of techniques is presented that have been found to be effective predictors of print quality where multiple metrics are used in combination and these methods and results are presented. Both studies adopted a 'black box' approach where only the paper measurements and the result of assessment were used to make predictions.

Keywords: inkjet press, print quality, paper property, logistic regression, quality prediction model

1. Introduction

For traditional printing where ink is pressed onto paper, we have observed as an industry that some physical behaviour of paper such as its ability to absorb ink quickly or the smoothness of its surface correlate well with print image quality. Paper properties have been identified that correlate with this physical behaviour, for example porosity (air permeability) and gloss. Paper manufacturers make measurements of these paper properties as part of the production process and use these to communicate with printers to help with paper selection.

For inkjet printing where ink is jetted onto paper, it has been observed that these conventional paper properties do not predict print image quality well. Understanding the physical interaction between ink and paper continues to be very important, and there are many scientific approaches in order to understand the physical interactions and their mechanism, for example Blohm and Åslund (2004), Kettle, Lamminmäki and Gane (2010), and Gigac, et al. (2014). The effect of calcium carbonate coating is explored in Možina and Franken (2018) and surface chemistry in general in Moutinho, Ferreira and Figueiredo (2010); the effects documented by these projects may be related to the surface measures in this paper. Krainer, Saes and Hirn (2020) explored the relationship between contact angle and ink spreading. These research projects have established some general principles that can be applied to the design of paper, however, the relationship between image quality and paper properties cannot yet be clearly described.

High-speed inkjet presses generally include two stages. In the first stage the paper is coated and in the second stage ink is jetted onto the coated surface. The first stage (precoating) modifies the characteristics of the paper surface to widen the window of paper properties that produce good print image quality. This is not intended to make the surface condition the same for all papers and the original paper properties still have a substantial influence following precoating. The time between precoating and inking is very small and usually the precoating does not completely dry before inking, therefore precoating and inking are continuous and dynamic processes and should not be considered separately. In addition, the method of precoating varies from one press to another as it is specific to the way in which ink is jetted onto the paper surface. For this reason, all measurements of the papers in this study were made before any precoating. From a practical perspective, it may be sufficient to find a direct correlation between measured properties (before any precoating step) and print acceptability based on print image quality.

The research described in this publication is one of the outcomes from a summit meeting held in April 2018 in conjunction with an ISO/TC 130 meeting where a range of industry experts discussed how the process of paper selection for high-speed inkjet presses might be improved. Attendees included representatives from paper manufacturers and from inkjet press manufacturers. In that meeting it was reported that considerable work had been done to try to find a simple metric that can be used to predict print image quality for inkjet presses without any success. At that meeting a group of industry experts including representatives from a number of inkjet press manufacturers (an ad-hoc group) agreed to work together to work on this problem. One inkjet press manufacturer, Fujifilm, conducted the research reported herein.

As this publication will show, while a single metric that predicts print image quality has not been identified, combinations of a relatively small number of metrics have been identified that enable prediction of print image quality with a high degree of confidence.

A study was conducted on a large set of papers printed on a single inkjet press (referred to as 'large study') to establish principles and methods of prediction. A second study was conducted on a small set of papers printed on three different inkjet presses (referred to as 'multi-press pilot study'). The results show that in all cases, a small set of predictor metrics produces high confidence in the prediction of print image quality. The best set of metrics for one press may not be the best set for another although there is significant overlap between these sets.

2. Methods

2.1 Paper selection

For the large study, a range of 250 commercially available papers were used, including cardboard, decorative and glossy papers. In a few cases, papers from different production lots were treated as different paper types.

For the multi-press pilot study, a set of 20 papers were selected by 7 inkjet press manufacturers. Each manufacturer selected at least one paper that produced good results and at least one that produced poor results using the best known press settings for that paper. The method of assessment in each case was the manufacturer's quality assurance process which was not disclosed and probably different for each manufacturer.

Papers were stored and measured in environments having temperature of 23 °C ± 1 °C and relative humidity of 50 % ± 2 %.

2.2 Measurement of paper properties

For the large study, all measurements were made by Fujifilm. For the multi-press pilot study, paper properties were measured in different laboratories that were made available to the project based on the capability of each laboratory. The set of paper properties measured for the large study and the set used by the multi-pres pilot study were slightly different from each other and the two sets of measurements made are described in Annex A.

2.3 Printing and visual assessment

For the large study, papers were printed on the Fujifilm Jet Press 720 which was optimised for each paper to produce the best reproduction possible in each case using Fujifilm's standard method. The overall print image quality was assessed using Fujifilm's standard quality assurance method. This was assessed from various perspectives such as image quality, quality of text, quality of solid areas and then each paper was classified as 'Accepted' or was assigned another category. The second category included a range from those that are never acceptable to those that may be acceptable for some uses. For the purpose of analysis, this second range of papers were combined into a single category.

For the multi-press pilot study, each paper in the set of papers was printed by three press manufacturers. In each case, the manufacturers applied their standard procedure for identifying the most suitable press setup for each. The way in which these presses were configured are not disclosed and this is likely to have been different for each manufacturer.

2.4 Prediction of print image quality

2.4.1 Background

The first step was to use a traditional approach and to look for a simple correlation between one of the paper metrics and print image quality assessment for each set of papers. When no such correlation could be identified, two possible options were considered.

The first option considered was to develop a new paper metric that provides a better correlation with print image quality. To date, it has not been possible to identify any existing metric or to develop any new metric of this kind that predicts print image quality. Steps to explore this option continue and may be fruitful in the longer term.

The second option was to look for correlation between print image quality and a combination of paper metrics. The initial investigation of this seemed to be promising but it was clear that at least three metrics are required to obtain a satisfactory prediction.

2.4.2 Model construction and prediction accuracy assessment

Logistic regression, a standard statistical method using linear regression for dimensionality reduction, was used as the method of prediction for this work. KNIME (see KNIME, 2020) was used as the platform to perform this analysis. Details of the use of logistic regression are described in Annex B.

For both studies, the method involves using a subset of papers to build a prediction model (the training set) and then testing the accuracy of this model using the remaining papers (the test set).

For the large study this was straightforward as it was possible to select 80 % of the papers at random as the training set used to build the model and then used the remaining 20 % of the papers as the test set to estimate the prediction accuracy of the model.

The technique used for the multi-press pilot study was different because of the small number of papers used. In this case, all of the papers except one were used as the training set to build the model and then the single paper was used as the test set to estimate prediction accuracy. This process was repeated for each paper in turn and so produced 20 predictions (one for each paper). This entire set of predictions was used when considering the overall accuracy of the model. This is a variant of k-fold cross-validation known as 'leave one out cross-validation' (LOOCV).

When considering logistic regression with more than three parameters, the method used to construct the model involved finding the minimum value of a multi-dimensional function and this can produce slightly different results each time and so it was also important to repeat each set of predictions to ensure consistent results.

2.4.3 Deciding which paper metrics to use

Since there are 16 paper metrics to choose from and if (for example) 4 metrics are selected for the model, there are almost 2 000 choices and it is not always practical to test every combination. It is therefore desirable to reduce the set of options and one way to do this is to identify the parameters that are independent from other parameters.

To do this the variance inflation factor (VIF) was calculated for the set of parameters and the parameter with the strongest correlation with other parameters was removed from the set. In this way the set of parameters was reduced to a more manageable set. The remaining metrics were then tested individually to determine their influence and the least important metric was removed.

3. Results

3.1 Traditional approach

When simple 2D plots were made, such as shown in Figure 1, in order to explore the relationship between the physical parameters of paper and parameters of image quality no clear correlation was apparent. Figure 1 shows an example of a 2D plot for a set of papers from the large study between a physical parameter of paper (the ink to paper contact angle recorded in 300 ms after the landing of ink) and a parameter of image quality (the maximum optical density of cyan). The dashed lines have been added to show slight trends in the data, for example there is a slight trend for a smaller contact angle to produce a higher maximum optical density, but these do not model the mechanism for ink–paper interaction.

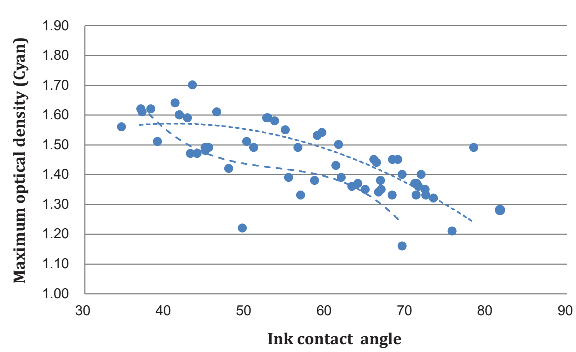

Figure 1: The 2D plot of cyan maximum optical density against ink contact angle

There may be a way to analyse such a relationship between the simple physical interaction between paper and ink, but as yet no satisfactory theory has been established.

Statistical approaches were also tested, an example of which is shown in Figure 2 for the same measured parameter, namely ink contact angle. In this case, each dot represents assessment of print image quality for a single paper, being given a value of either 1 for accepted and 0 for not accepted. The green line shows the logistic regression curve in respect to ink contact angle after 300 ms after landing of ink, and it can be seen that many points would have been incorrectly classified based on this single parameter. Across all such parameters, no single parameter was found which could give a reliable prediction for the acceptability of print image quality.

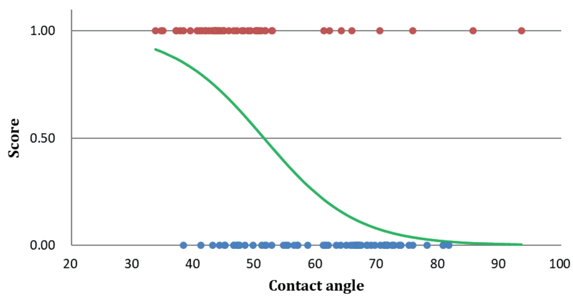

Figure 2: Example of logistic regression for the ink contact angle 300 ms after the landing of ink

3.2 Use of multidimensional linear methods

3.2.1 General approach

Since a simple relationship between parameters such as shown in Figure 1 could not be found an alternative approach was needed and multidimensional analysis was explored to determine whether this shows such a relationship.

Instead of looking for a relationship between physical parameters and image quality parameters a high-level approach was adopted. In this case it was assumed that the details of printing and assessment are unknown and that all that is known are the paper metrics and the result of assessment of print image quality. It was assumed that care has been taken to establish the best printing conditions for each paper and that a consistent process has been established for the assessment of print image quality. These assumptions mirror what happens in practice when manufacturers assess a new paper type for their press.

3.2.2 Prediction using all data sets and parameters

Logistic regression analysis was applied to the data. For the large study, predictions were calculated for 200 combinations randomly selected from the data set as the training set. An average accuracy of 0.80 and Cohen's kappa of 0.54 (Cohen, 1960) were obtained using the metrics shown in the first column of Table 1.

The first and second row of the table shows a good accuracy value, but a low value for Cohen's kappa. This difference indicates that the set of papers used to make predictions included more papers from one assessment category than the other. Since the selection process was random this was to be expected.

3.2.3 Removal of correlated parameters

In order to reduce the set of parameters used by the prediction model their independence was checked by calculating their VIF with all other parameters. The test results are shown in Table 2.

Table 1: Improvement in prediction accuracy and Cohen's kappa for each step

Condition	All metrics	VIF test	Test 1	Test 2	Test 3	Remove two papers (58 and 63)
Accuracy	0.803	0.808	0,827	0.833	0.840	0.869
Cohen's kappa	0.537	0.554	0.602	0.616	0.629	0.690
Contact angle (ink, 300 ms)	✓	✓	✓	✓	×	×
Contact angle (ink, 10 000 ms)	✓	✓	✓	✓	✓	✓
Contact angle (ink, 30 000 ms)	✓	×	×	×	×	×
Contact angle (H_2O, 300 ms)	✓	✓	✓	✓	✓	✓
Contact angle (H_2O, 10 000 ms)	✓	✓	✓	✓	✓	✓
Contact angle (H_2O, 30 000 ms)	✓	×	×	×	×	×
Surface pH	✓	✓	✓	×	×	×
Roughness	✓	✓	✓	✓	✓	✓
Thickness of coating layer	✓	✓	×	×	×	×
Si component	✓	✓	✓	✓	✓	✓
Al component	✓	×	×	×	×	×
Ca component	✓	✓	✓	✓	✓	✓
Ti component	✓	✓	✓	✓	✓	✓

Table 2: Variance inflation factors (the values above 2, 5 and 10 marked in green, yellow and red, respectively)

	Contact angle (ink, 300 ms)	Contact angle (ink, 10 000 ms)	Contact angle (ink, 30 000 ms)	Contact angle (H_2O, 300 ms)	Contact angle (H_2O, 10 000 ms)	Contact angle (H_2O, 30 000 ms)	Surface pH	Roughness	Thickness of coating layer	Si component	Al component	Ca component	Ti component
Contact angle (ink, 300 ms)	–												
Contact angle (ink, 10 000 ms)	4.034	–											
Contact angle (ink, 30 000 ms)	10.692	4.049	–										
Contact angle (H_2O, 300 ms)	1.367	1.269	1.300	–									
Contact angle (H_2O, 10 000 ms)	2.833	1.918	2.070	1.401	–								
Contact angle (H_2O, 30 000 ms)	2.861	1.996	2.257	1.407	23.454	–							
Surface pH	1.122	1.085	1.125	1.050	1.128	1.129	–						
Roughness	1.173	1.148	1.212	1.480	1.209	1.222	1.092	–					
Thickness of coating layer	1.031	1.015	1.038	1.013	1.004	1.004	1.037	1.003	–				
Si component	1.016	1.019	1.004	1.057	1.052	1.041	1.232	1.063	1.001	–			
Al component	1.012	1.016	1.003	1.044	1.039	1.030	1.373	1.052	1.011	5.953	–		
Ca component	1.006	1.001	1.012	1.000	1.005	1.007	1.872	1.039	1.007	2.063	2.170	–	–
Ti component	1.007	1.001	1.002	1.034	1.033	1.028	1.642	1.018	1.085	1.262	1.575	1.613	1.000

Strong correlations (VIF > 5) can be found between ink contact angles (300 ms and 30 000 ms), between water contact angles (10 000 ms and 30 000 ms) and between metal components (Si and Al). Based on this analysis, contact angle (ink, 30 000 ms), contact angle (H_2O, 30 000 ms) and Al component were removed from the model.

The results of predictions following the removal of these parameters are shown in the third column of Table 1. There is no dramatic change to the accuracy but the value of Cohen's kappa is improved. Following this step, the average of accuracy was 0.81 and the average Cohen's kappa was 0.55.

3.2.4 Removal of additional metrics using *k*-fold cross-validation

A method based on LOOCV was used to identify metrics with a low or negative effect on the model. For each LOOCV iteration, a single paper was used as the test set and all other papers used to build a logistic regression model. The prediction was recorded for each paper and this prediction compared with visual assessment. An LOOCV accuracy score was assigned for the set of metrics tested in this way as the ratio of correct predictions to the total number of papers.

This test was repeated multiple times, and each time one of the metrics was removed. The set of metrics with the highest LOOCV score was identified. This test was repeated three times (Test 1, Test 2 and Test 3 of Table 1) and each time the set of metrics with the best score was selected. Test 1 showed that removing the thickness of coating metric improved the accuracy and Cohen's kappa to 0.83 and 0.60, respectively. Test 2 showed that removing the surface pH metric improved the Cohen's kappa to 0.62. Test 3 showed that removing the contact angle (ink, 300 ms) metric the accuracy and Cohen's kappa improved to 0.84 and 0.63, respectively.

It was further observed that two papers seemed to be substantially different from the others in the set (papers 58 and 63). When these two papers were removed from the assessment, the accuracy and Cohen's kappa increased substantially to 0.87 and 0.69, respectively, as shown in the last column of Table 1. The reason for this is not completely clear and further investigation of this aspect is needed. It is possible that the visual assessment was incorrect or that there is some fundamental difference in these papers compared to the others.

4. Discussion

4.1 Prediction

These values for accuracy and Cohen's kappa seem to indicate that this provides a good basis for a prediction method for print image quality.

The studies considered only measurement values of physical paper properties when making predictions, but when data directly relating to image quality such as whiteness and gloss are also used in the prediction a different direction may be found.

Further investigation of this aspect is necessary including other measures such as those included in the ad-hoc data sets.

4.2 Verification of this prediction method

In order to confirm that this prediction method works well with data and assessments other than Fujifilm (the large study), predictions were also made using the data measured by the ad-hoc group. These predictions were done using 20 types of paper collected by the group. In this case, the number of data sets is very small and it is therefore necessary to reduce the set of parameters used for prediction.

Although VIF analysis is one direction to remove the parameters, only four parameters were eliminated from these data sets. Since *k*-fold cross-validation reduces the size of data sets, it is not an effective method for this prediction with small data sets. In the Equation [B.1] of logistic regression explained in Annex B, the coefficient β_i determines the extent to which the variable x_i contributes to the prediction. Therefore, if the coefficient β_i is close to zero, the variable x_i does not contribute to the prediction, and those parameters can be eliminated from the prediction. Table 3 shows the list of coefficients β_i for the printers by three different manufacturers.

Table 3: Coefficients obtained for each printer

No.	Parameters	Coefficient β_i Printer A	Printer B	Printer C
1.	Whiteness	−2.016	1.758	−0.454
2.	Gloss	−8.953	−8.100	−7.439
3.	Opacity	−2.722	5.899	−7.317
4.	Surface pH	1.688	−14.573	−2.134
5.	Liquid penetration	5.067	−3.184	0.662
6.	Setting homogeneity	−0.931	0.065	−2.976
7.	Surface roughness	7.060	1.348	3.220
8.	Mercury porosity	−3.187	0.507	−0.768
9.	Al component	2.659	6.619	0.944
10.	Si component	−0.425	9.345	0.988
11.	Ca component	7.976	1.905	−2.339
12.	Ti component	4.744	0.466	0.388
13.	Hygroexpansivity	−0.707	−7.721	4.507
14.	Contact angle 300 ms	5.967	0.862	1.943
15.	Contact angle 1100 ms	4.749	1.830	2.760
16.	Contact angle 3100 ms	6.315	0.853	3.399
17.	Constant	−3.845	7.415	2.193

Even with the same parameter, the coefficients are different depending on the printer. Here, the parameters with coefficients less than 1.0 were eliminated from the prediction. Tables 4 to 6 shows the results of the prediction using a small data set that has undergone the processes reducing the parameters used.

Table 4: The results of predictions for small-size data for printerA

	Results of assessment	P (Acc)	P (NA)	Prediction
1	Acceptable	0.6492	0.3508	Acceptable
2	Not acceptable	1.0000	0.0000	Acceptable
3	Acceptable	0.9984	0.0016	Acceptable
4	Acceptable	1.0000	0.0000	Acceptable
5	Acceptable	1.0000	0.0000	Acceptable
6	Acceptable	1.0000	0.0000	Acceptable
7	Not acceptable	1.0000	0.0000	Acceptable
8	Not acceptable	0.0000	1.0000	Not acceptable
9	Acceptable	0.6347	0.3653	Acceptable
10	Acceptable	1.0000	0.0000	Acceptable
11	Not acceptable	0.0041	0.9959	Not acceptable
12	Acceptable	1.0000	0.0000	Acceptable
13	Acceptable	1.0000	0.0000	Acceptable
14	Not acceptable	0.0000	1.0000	Not acceptable
15	Not acceptable	0.9999	0.0001	Acceptable
16	Acceptable	0.0000	1.0000	Not acceptable
17	Not acceptable	0.0000	1.0000	Not acceptable
18	–	–	–	–
19	–	–	–	–
20	Acceptable	0.6181	0.3819	Acceptable

Table 5: The results of predictions for small size data for printer B

	Results of assessment	P (Acc)	P (NA)	Prediction
1	Acceptable	1.0000	0.0000	Acceptable
2	Acceptable	0.9998	0.0002	Acceptable
3	Acceptable	0.9999	0.0001	Acceptable
4	Acceptable	1.0000	0.0000	Acceptable
5	Not acceptable	0.4306	0.5694	Not acceptable
6	Not acceptable	0.0000	1.0000	Not acceptable
7	Not acceptable	0.0000	1.0000	Not acceptable
8	Not acceptable	0.0000	1.0000	Not acceptable
9	Not acceptable	0.0038	0.9962	Not acceptable
10	Not acceptable	0.0000	1.0000	Not acceptable
11	Not acceptable	1.0000	0.0000	Acceptable
12	Acceptable	1.0000	0.0000	Acceptable
13	Not acceptable	0.3097	0.6903	Not acceptable
14	Not acceptable	0.0000	1.0000	Not acceptable
15	Acceptable	0.0389	0.9611	Not acceptable
16	Not acceptable	0.0513	0.9487	Not acceptable
17	Acceptable	0.5966	0.4034	Acceptable
18	Acceptable	1.0000	0.0000	Acceptable
19	Not acceptable	1.0000	0.0000	Acceptable
20	Not acceptable	0.0717	0.9283	Not acceptable

Table 6: The results of predictions for small size data for printer C

	Results of assessment	P (Acc)	P (NA)	Prediction
1	Acceptable	1.0000	0.0000	Acceptable
2	Acceptable	1.0000	0.0000	Acceptable
3	Acceptable	0.9994	0.0006	Acceptable
4	Acceptable	0.9999	0.0001	Acceptable
5	Acceptable	1.0000	0.0000	Acceptable
6	Acceptable	1.0000	0.0000	Acceptable
7	Not acceptable	0.0000	1.0000	Not acceptable
8	Not acceptable	0.0000	1.0000	Not acceptable
9	Acceptable	1.0000	0.0000	Acceptable
10	Acceptable	0.9809	0.0191	Acceptable
11	Not acceptable	0.1736	0.8264	Not acceptable
12	Not acceptable	0.0007	0.9993	Not acceptable
13	Not acceptable	0.0289	0.9711	Not acceptable
14	Not acceptable	0.0712	0.9288	Not acceptable
15	Not acceptable	0.0001	0.9999	Not acceptable
16	Not acceptable	0.0000	1.0000	Not acceptable
17	Not acceptable	0.0000	1.0000	Not acceptable
18	Acceptable	0.9285	0.0715	Acceptable
19	Not acceptable	0.0000	1.0000	Not acceptable
20	Acceptable	0.9999	0.0001	Acceptable

All the predictions (P (Acc) for acceptable and P (NA) for not acceptable) have high accuracy, particularly, all predictions are correct for printer C.

According to these results, the method provides a good prediction of visual assessment. On the other hand, it is unlikely that a set of 20 papers is sufficient to provide an accurate prediction for all papers. For users of digital presses, however, even a lower level of prediction would be beneficial.

4.3 Extending the multi-press study

In an ideal world, a very large number of papers would be printed on a large number of digital presses and the result of printing carefully assessed by multiple experts. In practice this is difficult, as configuring the presses and assessing the result for a single paper can be quite time consuming. Different formats of printing presses, for example sheet sizes or roll versus sheet differences also need to be considered.

It has been helpful to hold the multi-printer pilot study with a small number of digital presses and papers in order to establish working methods that can be developed and where necessary modified for use in a larger study. Building on the experience gained from this study should inform future projects.

5. Conclusions

These studies have been able to demonstrate that a model can be developed where a relatively small number of paper metrics when combined produces a good prediction for print image quality. They have only demonstrated this for a limited number of digital presses and papers and further testing is necessary to ensure reliable application of this model.

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Whetzel, N, 2014. What is Hunter whiteness index? *HunterLab*, [online] Available at: <https://support.hunterlab.com/hc/en-us/articles/204255369-What-is-Hunter-Whiteness-Index-> [Accessed December 2020].

Annex A: Measurements and measurement methods

Table A.1 shows the set of paper measurements made by Fujifilm for use in the large study. This set of metrics was selected from a larger set of measurements made by Fujifilm and represents the set that has the most significant effect for the Fujifilm press used in present study.
Table A.2 shows measurements used for the multi-press pilot study made by members of the ad-hoc group. In some cases, the measurement methods differ slightly even where the same name is used.

Table A.1: Description of measurements used for the large study

Measurement name	Description
Contact angle (ink, 300 ms) Contact angle (10 000 ms) Contact angle (ink, 30 000 ms) Contact angle (H_2O, 300 ms) Contact angle (H_2O, 10 000 ms) Contact angle (H_2O, 30 000 ms)	Measured by an automated contact angle tester for ink and water, at intervals of 300 ms, 10 000 ms and 30 000 ms after the ink or water landed on the surface. See IEC 62899-201:2016 Amendment 1 (summary) and TAPPI/ANSI T 558 om-15 (full description).
Surface pH	Measured by pH meter with flat-head electrode. See IEC 62899-201:2016+AMD1:2018, Amendment 1.
Roughness	Surface roughness was measured by Parker-Print-surf (PPS) method. See ISO 8791-4:2007.
Thickness of coating layer	Evaluated by observation from a scanning electron microscope (SEM). The details including the preparation of cross-sections are specified in IEC 62899-201:2016+AMD1:2018, Amendment 1.
Si component Al component Ca component Ti component	The composition was analysed by X-ray fluorescence spectrometry (XRF) and the amounts of Al, Si, Ca and Ti were measured. Units are kilo count per second (kcps) according to the Kα ray of each metal. See IEC 62899-201:2016+AMD1:2018, Amendment 1.

Citations Table A.1

International Electrotechnical Commission, 2018.
Technical Association for the Pulp and Paper Industry, 2015.
International Organization for Standardization, 2007.

Table A.2: Description of measurements used for the multi-press pilot study

Measurement name	Description
Whiteness	Based on adopted Hunter Whiteness Index calculated from CIELAB: $$Whiteness = 100 - \sqrt{(100 - L^*)^2 + {a^*}^2 + {b^*}^2} \qquad [A.1]$$ where L^*, a^* and b^* are the components of CIELAB (see Whetzel, 2014).
Gloss	The 60° gloss measurement using Byk micro-TRI gloss meter. See ISO 2813:2014
Opacity	Measured by the diffuse reflectance method using L&W Elrepho 070. The illuminant/observer was C/2°. See ISO 2471:2008.
Surface pH	Measured by the pH meter with flat-head electrode. See IEC 62899-201:2016+AMD1:2018.
Liquid penetration	Automatic scanning liquid absorptometer based on Bristow's method (see Bristow, 1967) was used.
Setting homogeneity	The surface of tested papers was coated entirely with purple ink in a thick layer. The two minutes later all excess ink was wiped off and its uniformity assessed by a group of experts from Fogra and ISO/TC 130. Ink used: 'wipe test ink' from Flint Group Germany.
Surface roughness	Surface roughness was measured by Parker-Print-surf (PPS) method. See ISO 8791-4:2007.
Mercury porosity	Measured by Mercury porosimetry; the mercury pressure was up to 345 MPa (50 000 psi). See ISO 15901-1:2016.
Al component Si component Ca component Ti component	The composition was analysed by X-ray fluorescence spectrometry (XRF) and the amounts of Al, Si, Ca and Ti were measured. Units are kilo count per second (kcps) according to the Kα ray of each metal. See IEC 62899-201:2016+AMD1:2018.
Hygroexpansivity	Dimensional stability for moisture is measured as hygroexpansivity. See ISO 8226-1:1994.
Contact angle 300 ms Contact angle 1100 ms Contact angle 3100 ms	Measured by an automated contact angle tester for water at intervals of 300 ms, 1100 ms and 3100 ms after the water landed on the surface. See IEC 62899-201:2016+AMD1:2018, Amendment 1 (summary) and TAPPI/ANSI T 558 om-15 (full description).

Citations Table A.2

International Electrotechnical Commission, 2018.

International Organization for Standardization, 1994; 2007; 2008; 2014; 2016.

Technical Association of the Pulp and Paper Industry, 2015.

Annex B: Summary of the use of logistic regression

B.1 General

The general equation for a logistic regression model is shown in Equation [B.1].

$$p = \frac{1}{1 + b^{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 ... + \beta_i x_i)}} \quad \text{[B.1]}$$

where in this case,
p is the probability of prints made on the paper having good print image quality,
β_i are the parameters of the model,
x_i are the predictors of the model, in this case the selected paper property measurements,
b is a base which in this case is the base of the natural logarithm (e).

This equation can be thought of as having two steps: a dimensionality reduction step which maps the multiple dimensions x_i to a single dimension (y), and a mapping step which maps y which has range ($\pm\infty$) to the range [0 1].

These two steps can be written as shown in Equations [B.2] and [B.3].

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 ... + \beta_i x_i \quad \text{[B.2]}$$

$$p = \frac{1}{1 + e^{-y}} \quad \text{[B.3]}$$

Consider the case of two paper properties, x_1 = Contact angle and x_2 = Ca content. Each paper can be plotted as shown in Figure B.1 according to the measurement of each of these two properties. In this case, green circles indicate papers that produce good print image quality and red crosses those that do not.

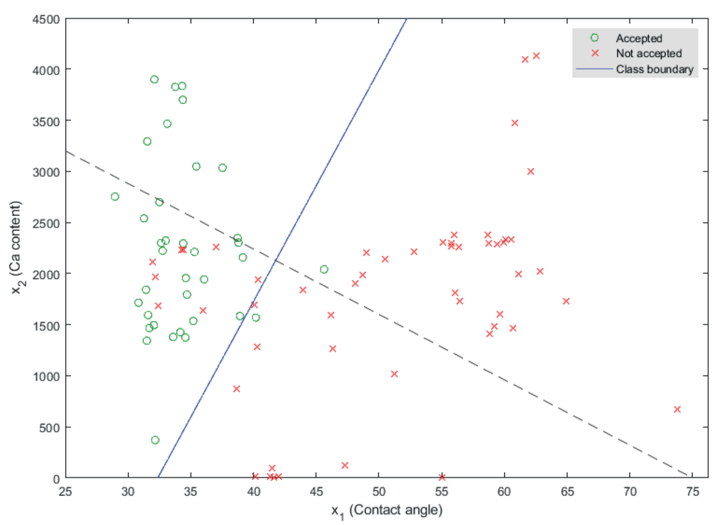

Figure B.1: Assessment relative to two paper metrics

The set of values corresponding to y = 0 for the first step of the equation is illustrated by the blue line. The region to the left of the line is predicted by the model as **Acceptable** and the region to the right is predicted as **Not acceptable**.

Each circle or cross has a y value corresponding to its distance from this line. The result of this mapping is shown in Figure B.2 which shows the values of y on a number line and Figure B.3 which shows the corresponding probability p.

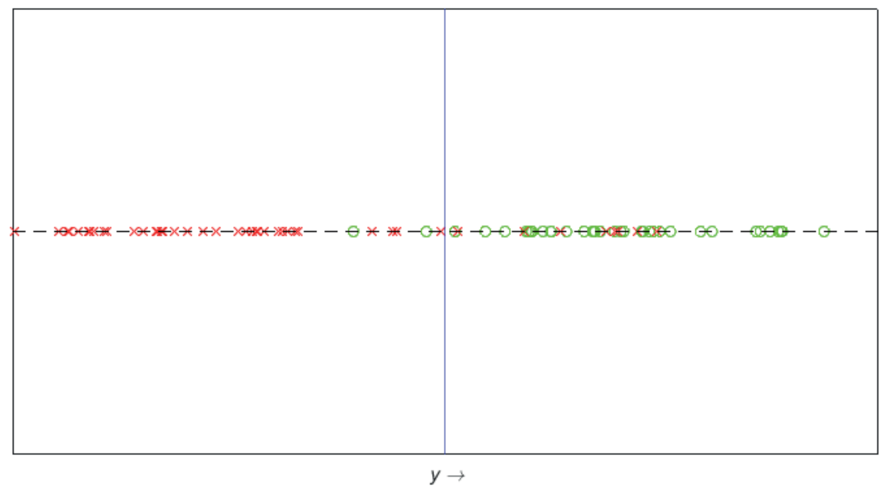

Figure B.2: Distance (y) from class boundary for each paper

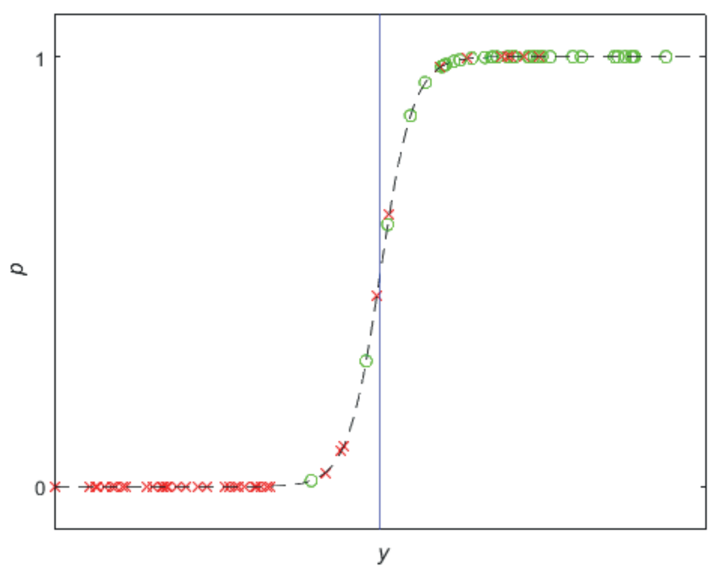

Figure B.3: Relationship between logistic regression probability and distance

As can be seen, the results for these two paper properties are quite good but can be improved. For example, visual inspection shows that eight papers that were classified as **Not acceptable** have been predicted by the model as being **Acceptable** (the red crosses to the left of the model class boundary in Figure B.1) and similarly two papers that were classified as being **Acceptable** have been predicted by the model as being **Not acceptable** (green circles to the right of the model class boundary in Figure B.1).

B.2 Measuring the performance of the model

A confusion matrix, also known as an error matrix, is a specific table layout that allows visualization of the performance of statistical algorithms. In this case the confusion matrix for Figure B.1 is shown below in a more usual form.

Table B.1: Confusion matrix for example of Figure B.1

		Predicted print quality	
Confusion matrix		**Acceptable**	**Not acceptable**
Assessed print quality	Acceptable	34	2
	Not acceptable	8	44

One way to measure the performance of the model is by the percentage of correct predictions (p_0) which is calculated as shown in Equation [B.4].

$$p_0 = \frac{(34+44)}{(34+8+2+44)} = 88.6\ \% \qquad [B.4]$$

This is an important measure but, in this case, there are 36 papers which are **Acceptable** and 52 which are **Not Acceptable** and so the results are likely to be biased. In order to avoid this problem, Cohen's kappa (κ) was used which takes into account the probability of chance agreement. This is done by measuring the probability that either the print is assessed or predicted as **Acceptable** (p_A) and the probability that the print is assessed or predicted as **Not acceptable** (p_N) and taking their sum (p_e) as shown in Equations [B.5], [B.6] and [B.7].

$$p_A = \frac{34+8}{34+8+2+44} \times \frac{34+2}{34+8+2+44} = 0.477 \times 0.409 = 0.195 \qquad [B.5]$$

$$p_N = \frac{2+44}{34+8+2+44} \times \frac{8+44}{34+8+2+44} = 0.523 \times 0.591 = 0.309 \qquad [B.6]$$

$$p_e = 0.195 + 0.309 = 0.504 \qquad [B.7]$$

Cohen's kappa is then defined as shown in Equation B.8.

$$\kappa = \frac{p_0 - p_e}{1 - p_e} = \frac{0.886 - 0.504}{1 - 0.504} = 0.770 \qquad \text{or } 77\ \% \qquad [B.8]$$

B.3 Extending to higher dimensions

The studies have found that the model can be significantly improved when four paper properties were used in combination. It is not possible to show a plot in this case but these same metrics can be used to measure the performance of the model for any number of paper properties.

B.4 Testing the model for large and small data sets

The discussion so far has assumed that the model is built and tested using the same data set but this is not generally useful when the objective is to predict the result for other papers. To do that, it is usual to split the data set into two and use one part to build the model and the other part to test it.

For the large data set this can be done relatively successfully and (for example) 80 % of the samples (in this case 70 samples) can be used to build the model and the remaining 20 % (in this case 18 samples) to test the model's performance.

For the smaller data set, which has just 20 samples, this is not possible and the approach must be modified somehow and, in this case, *k*-fold cross-validation was used. The data set was partitioned into (say) 19 samples and 1 sample and this is done in all possible ways – there are 20 ways to do this. A model is built for each of these cases using 19 samples and then tested using 1 sample and the result recorded. The average value of the results for all 20 tests is then taken as the overall result.