Ink Penetration, Isomorphic Colorant Mixing, and Negative Values of Yule-Nielsen *n*

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Abstract

As the number of inks used in printers increase beyond the traditional four, the "safe" profiling paradigm of factorial sampling of the ink levels combined with multi-dimensional interpolation grows exponentially in the number of samples required. The VHM-1, also known as the spectral Yule-Nielsen-modified Neugebauer model, and its derivatives are profiling alternatives that have demonstrated accuracy and enjoyed some popularity. Undoubtedly, part of the viability of these models stem from the use of the Yule-Nielsen parameter, n, as a fitting parameter, allowing the models to adapt to numerous situations.

This paper examines an aspect of this adaptability that is puzzling at best and defies reason at best, namely, negative values of n arising from fitting the model to measured spectra. Such values represent behavior even more extreme than n going to infinity, implying complete spreading of transparent ink.

Lewandowski, et al., have reported negative values of n when fitting the VHM-1 to spectra of halftones printed on ceramics, and the current author has provided the theoretical explanation of spreading of scattering ink. In this paper, the penetration of ink into the substrate is offered as an additional cause for this phenomenon. Both theoretical and empirical justification are offered to support this contention.

The theoretical justification is based on the remarkable similarity between the Yule-Nielsen formula with n = -1 and the ratio K/S used in colorant formulation work. Empirical data were generated by printing rather coarse halftone patterns on fiber inkjet paper, using ink jet with dye-based inks. The fitted value of n was approximately -3.8, versus fitted n values ranging from approximately +3.8 to +5.8 for prints produced on media that do not permit penetration.

The concept of isomorphic colorant mixing in briefly introduced to explain the similarity between VHM-1 with n = -1 and single-constant colorant formulation. This concept is an extension of the "linear function" introduced by Allen and mentioned by Kuehni and Tzeng. This concept is explained more completely in a separate publication.

KEYWORDS: Neugebauer, Yule-Nielsen, VHM-1, n value, ink penetration, isomorphic colorant mixing

Introduction

The VHM-1, or spectral [1, 2, 3] Yule-Nielsen corrected [4, 5]Neugebauer [6] model, for *k* colorants,

$$R_{\lambda} = \left[w_1 R_{1,\lambda}^{1/n} + w_2 \cdot R_{2,\lambda}^{1/n} + \dots + w_{2^k} \cdot R_{2^k,\lambda}^{1/n} \right]^n \tag{1}$$

and its variations are useful and well-regarded tools for predicting halftone color. Urban, Berns, and Rosen write that these



Figure 1. Relative isomorphisms for Yule-Nielsen/VHM-1 (u = -1) and K/S, with $R_p = 0.9$ and $R_s = 0.04$.

"have become the most popular models and are widely used today for printer characterization." [7] These authors cite the "simplicity and accuracy" [*ibid*] of these models as reasons for their success and popularity.

Such models become increasingly attractive as the number of inks used to produce a print increases. A standard $9 \times 9 \times ... \times 9$ factorial sampling plan for eight inks contains over 43 million patches. Even if 2000 patches were printed on each letter-sized page, the patches would fill over 21 500 such pages, enough to make a stack over two meters high. Printing this many pages would require a day and a half at 10 pages per minute. Even if 10 patches could be measured each second, measuring them would require 50 days, not counting downtime to position each page before measuring, remove it after measurement, periodically calibrate the instrument, etc.

The accuracy cited by Urban and colleagues seems to stem from two sources. First, the Yule-Nielsen correction relaxes the assumption implicit in uncorrected Neugebauer that the point spread function (PSF) of the paper has infinitesimal support, providing a more realistic model, even though Yule and Nielsen themselves refer to the the correction as semi-empirical. Secondly, the Yule-Nielsen correction involves a parameter, *n*, that is often used as a fitting parameter. In turn, this lends adaptability, resiliency, and flexibility to models based on the correction.

Theoretical range of n and the Density Ratio

Yule and Nielsen derived their correction for the case n = 2, assuming transparent inks and complete diffusion of light within the substrate. Because their formula reduced to the single-ink version of Neugebauer's ¹ Ruckdeschel and Hauser [9] argued that the theoretical range of *n* should be the interval (1,2). Yule

¹This single-ink case had been independently derived by Davies (and reported by Murray). [8]



Figure 2. *n* and *u* as functions of tint density, for three area fractions, with $D_p = 0.1$ and $D_s = 1.4$. Top: Plot for Yule-Nielsen *n*. Bottom: Plot for u = 1/n.

and Nielsen [4] had mentioned that, for a single ink, as $n \to \infty$, the area fraction, *f*, approached the fraction:²

$$\frac{D_t - D_p}{D_s - D_p} \tag{2}$$

where D_t is the density of the tint, D_p is the density of the paper, and D_s is the density of the solid. This fraction shall be referred to here as the *Density Ratio*.

Pollack [10] recognized that having the colorant amount (here, the area fraction of the tint) equal to the density ratio is a consequence of the Bouguer-Lambert-Beer law, and corresponded to complete spreading of a transparent ink. The theoretical range of n could then be expanded to the interval $[1,\infty)$. For $D_t \neq D_p \neq D_s \neq D_t$, and n in this interval, the density ratio will be less than the area fraction, while the density ratio will exceed the area fraction for negative n.

The curious phenomenon of negative n

In a 1989 investigation, Pope [11] captured a set of halftone tints with a microscope-based image analysis system, and determined an area fraction for each tint using planimetric techniques. These area fractions were taken as ground truth. The tints were then measured with a densitometer, and Pope numerically solved for n for each measurement. In several instances, the value of n failed to converge, growing larger with



Figure 3. Halftone dots on fiber paper, 4X enlargement, showing distinct halftone pattern, indicating ink spread is incomplete.

each successive iteration and approaching floating-point overflow. Pope reported these instances as infinite n. Because the density ratio was greater than the area fraction for these cases, it is now recognized that they correspond to negative values of n.

This author had observed negative values of n when fitting the VHM-1 to spectra printed on newsprint for a corporate client. Lewandowski, et al., [12] have published an account of negative values of n when optimizing the model for wideband reflectances of halftone tints printed on ceramics. Permitting negative values of n is part of the adaptability and flexibility mentioned above, and may be justified particularly if physical reasons for this curious phenomenon. Viggiano [13] has shown that spreading of a scattering ink can cause negative n. Penetration of ink into the paper is offered in this investigation as an additional cause of negative n, and both empirical data and theoretical analysis are provided to support this statement.

Using u = 1/n as an alternative parameter

Throughout the remainder of this paper, the reciprocal of n, namely, u, will often be used instead of, or in addition to, n itself. This not only makes some of the formulae appear neater, but is also motivated by the discontinuous behavior in n and the relatively continuous (i.e., continuous save a removable singularity at u = 0) behavior in u. [12] This discontinuity when using n is apparent in Figure 2, as is the continuity when using u.

Ink Penetration as a Cause of Negative *n* Introduction to Isomorphic Colorant Mixing

The VHM-1 for a single ink may be inverted to obtain the area fraction of the halftone:

$$f = \frac{\frac{R_{p,\lambda}^{u} - R_{t,\lambda}^{u}}{R_{p,\lambda}^{u} - R_{s,\lambda}^{u}}}{\left(3\right)}$$

where *f* is the halftone tint's area fraction, u = 1/n, $R_{p,\lambda}$ is the spectral reflectance of the substrate (paper), $R_{s,\lambda}$ is the spectral reflectance of the solid print, and $R_{t,\lambda}$ is the spectral reflectance of the halftone tint.

Two salient features of this formula are:

²Actually, Yule and Nielsen assumed densities relative to the paper, as was the custom at the time. This would make $D_p = 0$, and the actual fraction they reported was D_t/D_s .

- 1. The area fraction *f*, may be written as the ratio $f = \phi_{YN}(R_{t,\lambda}) \div \phi_{YN}(R_{s,\lambda})$; and
- 2. The numerator and denominator may both be written as $\phi_{YN}(x) = \phi'_{YN}(x) \phi'_{YN}(R_{p,\lambda})$, where $\phi'_{YN}(R_{\lambda}) = R^{u}_{\lambda}$.

This author has developed [14] a framework termed "Isomorphic Colorant Mixing," wherein the metric colorant amount (here, the area fraction f) may be expressed as such a ratio. The function $\phi'(*)$ is termed a "Type 1 Isomorphism;" it is a generalization of the "linear function" introduced by Allen, [15] and mentioned by Kuehni [16] and Tzeng. [17] Further, $\phi(*)$ (without the prime) is referred to as a "Type 2 Isomorphism." Type 2 isomorphisms are simply Type 1 isomorphisms minus the Type 1 Isomorphism applied to the case with zero colorant, and assume a value of zero when no colorant is present. Finally, a metric colorant amount may be obtained by dividing the Type 2 isomorphism of a spectrum produced using a single colorant by the corresponding Type 2 isomorphism of that same colorant at unit colorant amount.

A Type 1 isomorphism for single-constant colorant mixing is: [16]

$$\phi'_{K/S}(R) = \frac{(1-R)^2}{2R} \tag{4}$$

while the corresponding Type 2 isomorphism is:

$$\phi_{K/S}(R) = \frac{(1-R)^2}{2R} - \frac{(1-R_p)^2}{2R_p}$$
$$= \frac{(R_p - R)(1-R_p R)}{2R_p R}$$
(5)

The ratio of the Type 2 isomorphism of a tint relative to that of the solid print is then:

$$f_{K/S} = \frac{R_s}{R} \cdot \frac{(R_p - R)(1 - R_p R)}{(R_p - R_s)(1 - R_p R_s)}$$
(6)

This ratio, as well as the corresponding ratio for the VHM-1 with n = u = -1, is plotted in Fig 1 for $R_p = 0.9$ and $R_s = 0.04$, both typical values. The similarity of the two functions is striking.

The similarity of the two isomorphisms suggests that some form of colorant mixing process may cause an optimized value for *n* to be negative. One of the things the colorant can mix with is the substrate, through penetration.

Experimental Approach

Fiber-based media permit penetration of aqueous inks; cellulose is a polar molecule, and not only the fibers themselves but also the voids between them provide many capillaries to draw in water. On the other hand, photo-grade substrates for ink jet printing often have transparent top coatings that reduce or eliminate altogether the penetration of ink into the optically scattering material below. However, such papers generally have point spread functions that are quite compact, resulting in photon diffusion properties very different from that produced by fiber-based papers. One may combine absolute ink hold-out



Figure 4. Verso (unprinted side) of test print on fiber paper over dark background, showing significant penetration.

with photon diffusion similar to that produced by a fiber-based paper by printing halftone patterns on a transparent substrate, backing the resulting print with fiber-based paper, printed side in contact with the paper, and viewing or measuring in reflection mode.

To test the hypothesis that the penetration of ink into a scattering portion of the substrate can induce negative u, halftone tints may be produced on these substrates, one of which permits such penetration and others of which preclude it. The VHM-1 may be fitted to the spectra of these tints, using area fraction and u as optimization parameters, and a spectral error metric as the objective function of the optimization. It should be sufficient to utilize patches printed from individual inks, rather than multi-ink patches.

Hypothesis

It is hypothesized that halftone patterns printed with identical inks at identical screen frequencies will tend to produce fitted values of u closest to -1 using a fiber-based substrate, fitted values of u closest to -1/2 when printed on a photo-grade ink jet paper, and between the other two values when printed on a transparent base and measured in reflection mode backed by unprinted the same fiber-based paper used to produce the first print.

Experimental Methodology

To test this hypothesis, printing was performed using a Canon BJC-3000 ink jet printer using dye-based from a retail refill kit. Default halftoning was employed. Printing of the Postscript test page was performed at 360 spots per inch from Open SuSE 10.3 Gnu/Linux using the Foomatic s400a1 print driver. All three substrates were printed using the same driver-level options; only the thickness setting on the printer itself was changed for the thicker (glossy photo) medium.

Test form

Tonescales in cyan, magenta, and yellow were created. Each had 16 steps, including the plain paper and the solid patches. The plain paper was designated Step 0, and the solid patches as Step 15. The steps were evenly spaced in design area fraction, with

	Substrate		
	Fiber	Glossy	TX over Fiber
и	-0.2631	0.2634	0.1720
n	-3.801	3.797	5.815
ΔE_{94}^* Statistics			
Minimum	0.05	0.05	0.06
Q1	0.22	0.19	0.22
Median	0.41	0.37	0.32
Q3	0.55	0.63	0.46
D9	0.72	0.850	0.78
Maximum	1.12	1.05	1.36
Mean	0.421	0.429	0.390
Std. Dev.	0.228	0.270	0.248

Table 1. Fitted values of u, five-number summaries, upper deciles, means, and standard deviations of $\Delta E_{q_4}^*$, by substrate

a spacing of 1/15, equal to 17 digital counts in standard 8-bit encoding. Two tonescales were printed in each color using a different pseudo-random ordering for both.

Measurement

The test page was measured using a Gretag-Macbeth Spectrolino spectrophotometer on a Spectroscan X-Y table, driven by the program Measure from the Profile Maker suite. An ultraviolet blocking filter was used to reduce the effects of fluorescence. A white backing was made from enough sheets of the unprinted paper to be visually opaque over a black background. (In the case of the transparent samples, the fiber-based paper was used as the backing.)

For each page, six measurements of the unprinted substrate were made (one in each tonescale), and were averaged. The two solids for each ink were also averaged together.

The wavelength range measured was 380 to 730 nanometers. Low signal at 380 and 390 nanometers for the photo paper was noted, and was attributed to a combination of the tungsten source used in the spectrophotometer, the use of the ultraviolet-blocking filter, and possibly the use of titanium dioxide as a white pigment in this medium. Accordingly, the wavelength range was reduced to 400 to 730 nanometers for all measurements.

Numerical fitting

A numerical optimization was performed on the collected measurements, using a proprietary tool. For each substrate, all six measurements of A single value of u, together with an optimized area fraction for each tint, was computed. The optimization criterion was to minimize the sum of squared weighted reflectance errors; the weighting functions used are described in Viggiano. [18, 19]



Figure 5. Box-and-whisker plots of ΔE_{94}^* for the optimized fits on the three substrates.

Results

Complete spread of the ink could be ruled out because the dot pattern was still quite visible, as shown in Fig 3. Penetration of the ink into the paper was evident from the considerable showthrough; refer to Fig 4.

A summary of the optimizations appear in Table 1 and Figure 5. The statistics included in the table are for ΔE_{94}^* between the measured and fitted spectra for each tint, and comprise the minimum, first quartile (25th percentile), median, third quartile (75th percentile), ninth decile (90th percentile), maximum, mean, and standard deviation. The statistics indicate reasonably good fit quality, though the distribution of color differences seemed slightly anomalous for the transparency backed by fiber paper. The slightly larger range for this sample may have been caused by incomplete contact between printed dot and backing, perhaps as a result of local topology of the backing. Nevertheless, the fit quality is good.

Optimized values of u were -0.2631 for the fiber-based paper, 0.2634 for the glossy photo paper, and 0.1720 for the transparency backed by the fiber paper, corresponding to n-values of -3.801, 3.797, and 5.815, respectively. This supports the hypothesis that penetration of the ink contributed to negative u (and n).

The CIE 1994 ΔE_{94}^* color differences between measured and fitted spectra for the print on fiber paper were sorted, and the patches with the third quartile error and ninth decile error were selected for plotting. Fig 6 shows a comparison of the measured and observed spectra for the patch with the upper quartile error. This was patch 8 in a yellow tonescale, with a design area fraction of 8/15 and a ΔE_{94}^* of 0.55. In Fig 7, the comparison is shown for the patch with the upper decile error, patch 3 from a cyan tonescale, having a design area fraction of 0.2 and a ΔE_{94}^* of 0.72.

Discussion

The inks used were dye-based, hence minimally scattering and posessing nearly complete transparency. Inks that exhibit considerably greater scattering were able to produce negative n (or u) only some of the time. [13] Non-transparency of the inks could not have played a large role in causing the negative values observed here, and is ruled out as the dominant cause.



Figure 6. Measured and fitted spectra, upper quartile (75th percentile) CIE 1994 color difference between measured and fitted on fiber paper. This is a yellow patch with nominal area fraction of 8/15; $\Delta E_{94}^* = 0.55$.



Figure 7. Measured and fitted spectra, upper decile error (90th percentile) CIE 1994 color difference between measured and fitted on fiber paper. This is a cyan patch with nominal area fraction of 3/15; $\Delta E_{q_A}^* = 0.72$.

Similarly, ink spread was incomplete; the halftone patterns were visible using only modest magnification. This factor can also be ruled out as the dominant cause.

Although it was not identified as a possible cause, fluorescence is unlikely to have played a major role here, because the ultraviolet component had been filtered from the source.

Of the factors identified, only penetration of ink into a scattering medium remains. Either this was the dominant cause of the negative Yule-Nielsen parameter, or some as yet unidentified agent was responsible. However, prints in which penetration of ink had been reduced or eliminated, and these did not produce negative u. It is therefore concluded that it is likely that penetration of the inks into the substrate played a dominant role in the negative values of u observed here.

It is noted, for the case where penetration was significant, that the fitted value of u was closer to zero than the -1 suggested by the similarities of the isomorphisms. However, spatially partite mixing was still present. What was produced, measured, and observed was a portmanteau, a mash-up, of single-constant Duncan colorant mixing and halftoning. Prints with less distinct halftoning may produce u closer to -1, as long as penetration is essentially complete.

Accordingly, it is predicted that complete penetration of non-scattering inks into a scattering paper, combined with complete spread, would result in fitted values of *u* closer to -1.

For Future Work

One may ask how, if penetration occurred in solids as well as in tints, would penetration of ink into a scattering substrate cause negative *n*? The spectrum of the solid will be affected by penetration, and the effect on the spectra of tints printed from that solid should have been accounted for by the effect on the solid. Apparently, the tints are affected to a degree disproportionately larger than their area fraction. Why?

The hypothesis tentatively adopted is that the proportion of ink penetrating is greater for the tints because it can diffuse laterally and down about the perimeter of each dot, while, for a solid patch, except at its margins, penetration can only occur in the downward direction. Capillary attraction at the perimeter of dots should cause a greater fraction of the deposited ink to be drawn into the substrate.

Summary

Penetration of ink into the substrate has been offered as an explanation for negative values of the Yule-Nielsen parameter *n*. This was motivated by the similarity of the isomorphism for *K*/*S*, from single-constant colorant mixing, to the isomorphism for the Yule-Nielsen model with n = -1. Examination of plots of the isomorphisms for u = 1/n = -1 and *K*/*S* revealed a striking resemblance, and it was hypothesized that negative *n* could arise even with transparent inks that have undergone nominal spread, if the inks were to mix with the substrate, through penetration.

Empirical data have been presented that support for this theoretical prediction. While prior literature cites complete spread of optically scattering inks as a cause of negative *n*, the halftones analyzed were produced using non-scattering dye-based inks, and the spread of the inks was clearly minimal because the halftone pattern was very distinct, even to the naked eye. The previous cause may therefore be ruled out in this instance, and it was concluded that ink penetration was the most likely cause.

Lewandowski, et al., have suggested using this author's parameter, u, the reciprocal of n, in place of n to maintain continuity during optimization. Plots shown here bear out the continuity when u is used, rather than n.

Acknowledgments

The author thanks Dr Franziska Frey, Dr Vincent Amuso, and Dr Mark Fairchild, all of RIT, as well as Dr Jean-Pierre Van de Capelle of Xerox, and Dr Philipp Urban of the Technical University of Darmstadt, Germany, for serving as his dissertation committee. Dr Jon Arney had originally served as the author's research advisor. Dr Stefi Baum, Director of the Center for Imaging Science at RIT, arranged for assistantships for the author. Dr David Wyble of the Munsell Color Science Laboratory at RIT arranged for use of equipment. A portion of this work was funded under a Center for Imaging Science/Kodak Innovation grant. The anonymous reviewers made several valuable suggestions that have improved the quality of this paper.

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