Mathematics and Perfumery: An Examination of Arithmetical Methodology

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To many perfumers, the title of this article may suggest a shockingly heretical idea. Perfumery, after all, is very much an art form, in which the creativity and imagination of the perfumer is encouraged to the full in the design of perfumes of outstanding beauty. Mathematics is a science of extreme discipline, in which imagination is necessarily restricted, and creativity usually ends in disaster.

I would like, however, to submit that a facility with numbers, an easy familiarity with some simple arithmetical tools, can be a great aid to perfumers in their day to day work, not at all restricting artistry or imagination, but rather helping them to achieve final results that are the best obtainable, and proven to be so.

For many perfumers today, much of the fascination of the work is that it not only requires all the artistry that can be summoned up, but that at the same time, free-flowing creativity must be tempered, sometimes strictly, with a fiercely commercial attitude. Most perfumers are engaged in designing fragrances that they hope to sell in the world's markets, and these are now ruthlessly competitive places. For this reason, perfumers must ensure that each creation not only has the best odor and/or other technical attributes they are capable of giving it, but it must also be presented at the correct cost. This is where a little simple arithmetic can be extremely helpful.

To get the most out of math, I would advocate that perfumers should acquire a good calculator. Any type will be fine for the tasks at hand, but one feature is essential: the calculator should be able to add the results of multiplications in its memory. This will mean that costs can be simply calculated without having to write down long columns of numbers. An example will serve to illustrate the point. Here a perfumer wishes to find quickly the cost of the blend, the formula of which might be as in Table I.
A calculator with the required feature will be able to total the figures in the extension column, as the multiplications of quantity by cost are being performed. It is not necessary to write down the figures in the extension column, or to total them separately later, thus saving much time.

Many perfumers do not do their own costing. They write their trial formulae and hand them to a costing clerk for calculation. This certainly

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Table I

		Costs	Extension
Musk ketone	30	8.00	240
Coumarin	60	5.00	300
Benzyl acetate	200	1.50	300
Amyl cinnamic aldehyde	250	1.80	450
Terpineol	310	1.00	310
Hydroxycitronellal	150	9.00	1350
	1000		2950

saves time, and allows perfumers to get on with more creative tasks. Nevertheless, I feel that in certain circumstances, especially when a perfume has to be created to a specific price, neither more nor less, perfumers will find it advantageous to do at least some of the calculations themselves. They will have a closer feel for the value of their creation, a more intimate knowledge of where their money is being spent. They will be able to see more easily where changes can be made that will save money without affecting the performance of the creation. More importantly, it will give them an opportunity to perform tasks using mathematical tools that would be difficult or impossible otherwise.

As one can see from the previous example, the final price of this blend, assuming one is dealing in dollars and pounds, will be found by dividing the total of the extension column, 2950, by the total units in the formula, in this case 1000, thus giving a price of $2.95 per pound.

Now suppose this price is too expensive. A modification is required that will cost only $2.00 per pound. Assuming that no changes in the grades or qualities of the materials in the formula are possible or desirable, then there are two options open to the perfumer.

- the perfume can be diluted to the required price
- the quantities in the blend can be changed so that low-cost items are increased in quantity, and higher-cost materials are decreased

Use of dilution

The advantage of dilution is that the odor-character of the perfume remains the same, of course. The disadvantage is that it is weaker, and most diluents depress the fragrance more than seems mathematically logical. Also most perfumers do not wish to sell diluents, and most customers do not wish to buy them. Nonetheless, if a diluent is called for, here is a simple method of calculating exactly the correct quantity required to bring the dilution accurately to the desired price. By using the "X-Pattern" shown in figure 1, a logical step-by-step approach produces the answer swiftly, instead of by much trial and error.

The X-Pattern is used in the following way. Simple subtractions are all that are required. Subtract the "required cost" from the "cost of original perfume," and the result is the "quantity of diluent." Subtract the "cost of diluent" from the "required cost," and the result is the "quantity of original perfume!"

It will be seen that the difference between the price of the diluent and the desired price gives the quantity required of the original perfume. Conversely, the difference between the cost of the diluent and the desired price gives the quantity required of the original perfume. It is important to remember that one uses the price of the diluent to calculate the quantity of the concentrated perfume, and the price of the concentrate to produce the quantity of the diluent.

For example, in the previous illustration the perfumer wished to dilute a perfume costing $2.95 per pound to a blend costing $2.00 per pound. To achieve this, diethyl phthalate might be chosen as a diluent at a cost of, say, $1.00 per pound. The X-Pattern looks like figure 2.

Table II shows how one can prove the cost of the new dilution. Divide 3.90 by 1.95, and the answer is 2, that is, $2.00/lb.

The total diluted formula is 1.95, an awkward figure. By calculating a factor, one can create a formula totaling a round figure, say 1,000, and still have a formula with the same cost. Divide the required total, 1,000, by the current total, 1.95. This is easily done on a calculator; the result is 512.8 (see Table III). Multiply the quan-

Table II

		Costs	Extension
Concentrated perfume	1.00	2.95	2.95
Diethyl phthalate	.95	1.00	.95
	1.95		3.90

Table III

			Costs	Extension
Concentrated perfume	1.00 x 512.8	513	2.95	1513.35
Diethyl phthalate	.95 x 512.8	487	1.00	487.00
		1000		2000.35

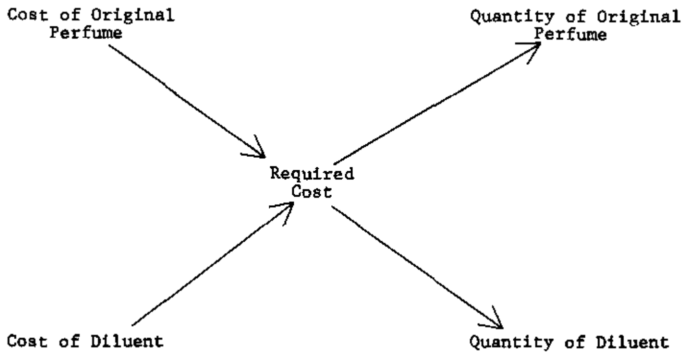

Figure 1

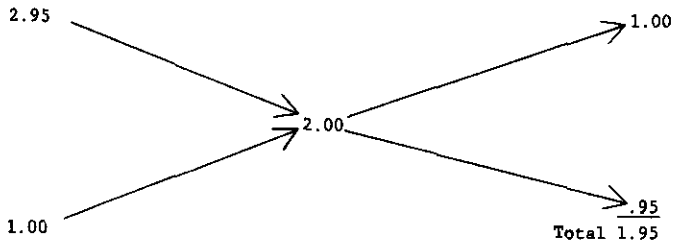

Figure 2

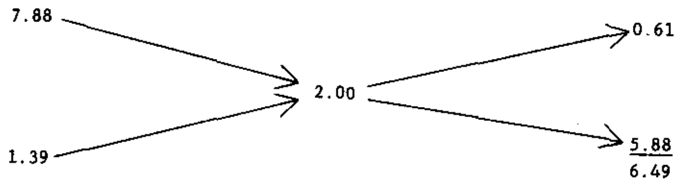

Figure 3

tities of concentrated perfume and diluent in the current formula by the factor, and a formula is created which totals a neat 1,000, and still costs $2.00 per pound, to within less than 1¢.

Dividing the extension total, 2000.35, by the formula total, 1,000, still gives a price of $2.00 per pound, despite the "rounding off" of the formula quantities.

By multiplying the quantities of materials in the original, concentrated perfume by the proportion in the diluted formula, a convenient, one stage formula can be created (see Table IV). Again, dividing the extension total by the diluted formula total gives a cost, rounded to the nearest cent, of $2.00 per pound.

Use of restructuring

The second option in accomplishing the task of reducing the perfume's price is changing the quantities of the terms in the formula, that is, restructuring the fragrance. The advantage to this method is that no diluent is used, so the perfume is not weakened or depressed, but the disadvantage is that the balance is altered. Without

Table IV

	Original Formula	Factor	Diluted Formula	Costs	Extension
Musk ketone	30	0.513	15	8.00	120
Coumarin	60	0.513	31	5.00	155
Benzyl acetate	200	0.513	103	1.50	154.5
Amyl cinnamic aldehyde	250	0.513	128	1.80	230.4
Terpineol	310	0.513	159	1.00	159
Hydroxycitronellal	150	0.513	77	9.00	693
	1000				
Diethyl phthalate			487	1.00	487
			1000		1998.9

Table VA. Low Cost Base

		Costs	Extension
Benzyl acetate	200	1.50	300
Amyl cinnamic aldehyde	250	1.80	450
Terpineol	310	1.00	310
	760		1060

Cost of this base = $\frac{1060}{760}$ = \$1.39/lb.

Table VB. High Cost Base

		Costs	Extension
Musk ketone	30	8.00	240
Coumarin	60	5.00	300
Hydroxycitronellal	150	9.00	1350
	240		1890

Cost of this base = $\frac{1890}{240}$ = \$7.88/lb.

care and skill, which can only be acquired by experience, a lower-priced blend will smell cheap, rough, and out of balance. Mathematical methods can help a perfumer's work, but they can never supersede skill, knowledge of materials, and expertise in blending them.

On returning to the original formula, it will be seen that three items have costs above the required cost of \$2.00 per pound, and three have costs below it. The perfumer should now design two separate formulae, which can be called "Low Cost Base" and "High Cost Base" (see Table VA and VB). These 2 bases are only needed for calculation purposes. They are not actually compounded, so the fact that, for instance, the high-cost base contains too much crystalline material, and is therefore uncompoundable, is of no importance.

Now, using the X-Pattern, one can calculate how much of each base is needed to form a final blend costing \$2.00/lb (see fig. 3).

Table VI

		Costs	Extension
Low Cost Base 0.61 x 154.08 =	906	1.39	1259.34
High Cost Base 5.88 x 154.08 =	94	7.88	740.72
	1000		2000.06

Cost of this blend = $\frac{2000.06}{1000}$ = \$2.00/lb

To make the final formula total 1,000, one should multiply the required quantities by $\frac{1000}{6.49}$ = 154.08. This gives the formula in Table VI.

To prepare the compoundable total formula, one multiples the low-cost materials by one factor, and the high-cost materials by another. In the original formula there were 760 parts of low-cost items, but in the new formula, 906 parts are required so one multiplies the quantities of low-cost items by $\frac{906}{760}$ = 1.192 (see Table VII).

Table VII

	Old Formula	Factor	New Formula	Costs	Extension
Musk ketone	30	0.3916	12	8.00	96.0
Coumarin	60	0.3916	23	5.00	115.0
Benzyl acetate	200	1.1920	238	1.50	357.0
Amyl cinnamic aldehyde	250	1.1920	298	1.80	536.4
Terpineol	310	1.1920	370	1.00	370.0
Hydroxycitronellal	150	0.3916	59	9.00	531.0
			1000		2005.4

Similarly, the original formula called for 240 parts of high-cost items, but the new formula requires 94 parts. Therefore, one should multiply the quantities of high-cost items by $\frac{94}{240}$ = 0.3916. (see Table VII)

Again, dividing 2005.4 by 1,000 gives a cost of \$2.00 per pound for the new blend. The process of 'rounding out' is advocated because it produces simple, compoundable formulae. Without it, one becomes caught in a welter of figures; with it, the final results are usually extremely close to those desired; quite close enough for any commercial purposes.

Blends of diluted bases and restructured bases

At this stage one has two formulae, both modifications of the original, both costing the required amount; in this example, \$2.00/lb. Both of these formulae should now be compounded in sufficient quantities to enable one to make several blends with them, and have these blends tested in the final base required, be it soap, lotion, antiperspirant, detergent, or some other product. From these two bases a series of blends can now be prepared (See Table VIII).

As both the diluted base and the "altered" base have the same cost, in this example \$2.00 per pound, all the blends in the series must necessarily also cost the same $2.00 per pound.

These seven blends should now be tried out, and also stability-tested in the required medium. Finally, a careful organoleptic assessment should be carried out by perfumer, evaluator, salesperson, customer, panelist, or any desired combination. This careful assessment will produce a definitive answer that is proven mathematically to be the best obtainable. If it is felt that the ideal answer lies between two samples, further blends of diluted base and restructured base can be tried.

Now comes the final stage of producing a tidy, convenient formula for production. Suppose that testing has shown that the ideal blend consist of 300 parts of diluted base and 700 parts of restructured base. This ratio is the best compromise between the weakness of the diluted base and the altered odor of the restructured base. The final formula is produced by writing a total formula containing the required parts of each material from both the diluted formula and the restructured formula. Table IX shows how to do this. Table X shows the costing of the final formula.

As one may see, the cost price, $\frac{1999.6}{1000}$ = 1.996 or $2.00 per pound to the nearest cent, is accurately retained despite the rounding off of figures for the convenience of compounding.

Table VIII

Diluted base	0	100	300	500	700	900	1000
Restructured base	1000	900	700	500	300	100	0
	1000	1000	1000	1000	1000	1000	1000

Table IX

	Diluted Formula	Diluted Formula x 0.300	Restructured Formula	Restructured Formula x 0.700	Final Formula
Musk ketone	15	4.5	12	8.4	13
Coumarin	31	9.3	23	16.1	25
Benzyl acetate	103	30.9	238	166.6	198
Amyl cinnamic aldehyde	128	38.4	298	208.6	247
Terpineol	159	47.7	370	259.0	307
Hydroxycitronellal	77	23.1	59	41.3	64
Diethyl phthalate	487	146.1		—	146
		300.0		700.0	1000

Table X

	Final Formula	Costs	Extension
Musk ketone	13	8.00	104
Coumarin	25	5.00	125
Benzyl acetate	198	1.50	297
Amyl cinnamic aldehyde	247	1.80	444.6
Terpineol	307	1.00	307
Hydroxycitronellal	64	9.00	576
Diethyl phthalate	146	1.00	146
	1000		1999.6

This final formula can be confidently offered to customers as the best possible compromise between dilution and altering the balance of the formula.

In the example, it was assumed that no changes in materials were possible or desirable. However, it cannot be stated too strongly that before any mathematically derived formulae are calculated, the original formula should be reworked to produce the best possible compromise, using lower-cost materials. More reasonably-priced versions of many essential oils should be substituted, or even synthetic replacements may be tried, if the perfumer feels that their use is justified.

Line Extension

Often, cost reductions are required when line extension work is requested, starting with a successful cologne or extrait perfume. If the orginal perfume is modified, substituting more reasonably-priced materials for the high-cost items in the cologne oil, some progress is made in reducing the price to the figure requested. At this stage the previously described arithmetical tools can be employed to further reduce costs to produce an optimum blend, accurately costed to the required figure.

Usually line extensions are needed for other media than extrait, such as soap, dusting powder, antiperspirant, even shampoos or hair conditioners. Here stability of materials is obviously of great importance, so selection of substitute materials must not only take price into consideration, but also odor and color stability, and the odor-suppressing or enhancing effect that many cosmetic and toiletry bases have on certain perfumery materials.

It will be seen that the production of modifications is work demanding a high degree of skill and knowledge of raw materials. Perfumers need an armory of carefully chosen or cleverly designed substitutes for materials used in perfumes. Their list of substitutes must not only include lower-priced replacements for all the expensive items that they love to use in their "cost no object" creations; it must also include materials that they can use to replace those items that would discolor many cosmetic bases; or would be olfactorily unstable in oxidizing media, or those bases with either high or low pHs.

An important point that must be remembered when using mathematical methods for assiting in the creation of perfume modifications is that, for many combinations of raw materials or accords, there is a balance point where the quantities of the chosen materials complement each other perfectly. By changing the proportions, as in the previously described "X-Pattern" of price alteration, this balance-point may be lost, and a rough fragrance may result in which various notes predominate, producing an undesirable, unfinished, or "grey" note in the perfume. This effect must obviously be avoided, and here again, any mathematical methods used must be tempered with the perfumers' intimate knowledge of their materials, and their experience in creating well-rounded blends with all the parts correctly balanced.

In practice, the above problem of lack of balance seems only to occur when one is using the X-Pattern to alter the pricing of fairly simple blends, containing less than fifteen or twenty items. The more sophisticated perfumes, containing thirty, forty, or more items will rarely develop a "grey" or unbalanced character when their costings are altered mathematically.

The above assertion may surprise many perfumers, and is certainly open to much argument and questioning. It seems to go against accepted rules of creating balance and accord in perfumes. This writer's only defense would be that, having used mathematical methods in cost-modification work for many years, the final results have been most pleasing, and salable: The practical results belie the theoretical objections. Used with common sense, a good basic knowledge of the materials in the blends, and an eye for spotting obvious discrepancies, unbalanced or "rough" perfumes seem to occur very seldom.

So far, I have written only about reducing costs of perfumes using the X-Pattern. Is this mathematical tool also applicable in those happy cases where a richer, more sophisticated version of a perfume is required, at a higher price? Yes, indeed! Firstly, the formula is worked through, replacing lower-cost items with chemicals or naturals of higher price and better quality. Then, using this more expensive version of the formula, one can balance up to the required price using the mathematical methods previously described. They work in exactly the same way, whether costs are being reduced or increased.

A possibly unsuspected advantage of the X-Pattern is that this writer has found it most helpful in creating some well-known fragrance types at costs that were previously thought to be unattainably low. By using the restructuring method, in which constituent quantities are altered without the use of diluents, it has been found possible to create household and toiletry fragrances at extremely competitive prices, displaying the characteristic notes of some very sophisticated perfumes, and at the same time using no diluents, thus maintaining the highly desirable power and lift that are so necessary in today's markets.

Working to Round Figures

As the reader will have noticed, in the previous examples, I have tried at all times to make the formulae total 1,000. This habit of working to a round figure, be it 100 or 1,000, is one that I would strongly encourage a perfumer to develop. It has many advanages.

- A formula totalling 1,000 is much easier to compound than one with an odd total. Multiplying by a simple factor produces a batch formula to any required size, and the quantities of each item that the compounder has to add will be simple figures, involving no decimal points. If you love your Compounding Department, total your formulae to a round figure!

- Formulae totalling 100 or 1,000 will help perfumers learn the correct dosages of their raw materials. It is an excellent mental habit to get into, to constantly think in terms of formulae totalling 100 or 1,000. (Personally, this writer advocates 1,000, as in most cases it removes the necessity of working with decimal points.) If one wished to add aldehyde C.10 to the blend and one knows that it usually achieves the correct effect at 1 part in 1,000, how convenient it is to add it again to a perfume totalling 1,000, and how inconvenient to have to judge the quantity for a formula totalling say, 763 or 1,359.

Splitting Out a Base

Sometimes it is desirable to "split out" a base when modifying a perfume. Unnecessary complication in perfumery is always to be avoided, so it is often a good practice, when modifying a perfume, to work through any bases, such as jasmins, roses, and so forth, and include only those parts that are of olfactory value. Items which, in the base, may be of value in creating the required odor, will often be found to be so dilute when that base is used in the final formula that they no longer have any practical value, and may be discarded from one's final modification. If both the original formula and the bases in it total 1,000, this process of splitting out may be accomplished comparatively easily. If they do not, a mathematical nightmare develops: awkward and time consuming.

So far I have written about modifying perfumes to an accurate desired price. This is often required by the customers of the perfumery house, and for this reason I have described the X-Pattern to help perfumers achieve this result.

Pro Rata Calculations

Sometimes the customer will give perfumers the freedom to choose their own price and dose-rate, only stipulating the maximum amount of money to be spent per unit of finished product. This gives the perfumer the opportunity to calculate the price and dose-rate on a pro rata basis. Familiarity and ease with pro rata calculations is very helpful in perfumery work. An example will illustrate how pro rata calculations may be easily performed.

Having found out how much the customer wishes to pay to fragrance one hundredweight of the product, for instance, a shampoo, it is necessary to calculate the raw-material cost of perfuming one hundredweight of the product. This is done by dividing the customer's price per hundredweight by the required mark-up. Let us assume that this calculation gives a quantity of $2.50 worth of perfume per hundredweight at raw material cost price. Now a hundredweight is 100 pounds, so one can spend $2.50 to perfume 100 lbs of shampoo base, or 2½ cents to perfume 1 pound. In this case it is assumed that three perfumes with different raw material costs have been designed, and one wishes to calculate the percentages at which they should be added to the base to achieve the maximum pro-rata effect.

The point to remember here is that, for a range of prices, the price times the dose-rate must always be the same. In the example, if one had a perfume with a cost of $4.00/lb, then $4.00 x dose-rate = 2½ cents. This may be written as

$$\text{dose-rate} = \frac{\$0.025}{4} = 0.00625$$

so the dose-rate in this case is 0.00625 per unit. Moving the decimal point two places to the right gives a dose-rate of 0.625%. In other words, for this example, if the cost price is $4.00/lb, then one should add the perfume at 0.625% to the shampoo base to achieve a raw material cost of $2.50 per hundredweight for perfume.

From the above, one may see that a useful general formula for calculating pro rata dose-rate has been evolved.

$$\%\text{Dose Rate} = \frac{\text{Raw Material Cost Per Hundredweight}}{\text{Cost of Perfume Per Pound}}$$

Suppose the two other perfumes cost $7.60/lb and $8.20/lb, respectively. Then the correct dose-rates are obtained as follows.

$$\begin{array}{l} \text{\% Dose Rate for} \\ \text{\$7.60/lb perfume} \end{array} = \frac{2.5}{7.6} = 0.329\%$$

$$\begin{array}{l} \text{\% Dose Rate for} \\ \text{\$8.20/lb perfume} \end{array} = \frac{2.5}{8.2} = 0.305\%$$

Of course, these inconvenient figures should be rounded off to produce figures that the customer can easily work with.

It is well, before starting to design or select perfumes for a base for which the customer has given a pro rata option, to calculate the maximum and minimum dose rates that might be acceptable. In other words, one should choose a lower dose-rate below which most perfumes are unlikely to be strong enough to do the job, and a higher dose-rate above which perfumes are likely to cause problems by changing the viscosity or color of the base, or by being deleterious in other ways. Having chosen upper and lower limits, one should calculate the cost prices for these units. When choosing or designing perfumes for this job, one should not go outside these upper and lower price units. The exact dose-rate for each fragrance may be calculated as before.

Conclusion

In the day-to-day work of the Perfumery Department, many problems will arise, besides those that I have mentioned here, where a little simple arithmetic can be of great assistance. In the same way that perfumers would be well advised never to totally abandon balance work, so they will gain by exercising their mathematical skills. All perfumers wish to design that magnificent winner that will astound the industry. Perhaps a little math will help to achieve this goal.