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Using microwave metrology to count calories



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ABSTRACT

One non-destructive way to probe the caloric content of food is to examine the transmission spectra of low energy microwaves over a broad band (approximately 1–8 GHz). This paper proposes a simple, but generalizable, nearest neighbor scheme to estimate the calories of homogeneous mixtures of oil, sugar, and water. The approach's performance is empirically quantified and is also compared to the performance of an oracle estimator. We report that for this study the estimator achieves an average absolute error of approximately 10%. A heuristic extension of the nearest neighbor estimator is also discussed that can in some cases improve the average error performance. The work represents the first steps toward accurate and reliable calorie estimation techniques for complex, non-homogeneous foods of varying shapes and amounts.

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1. Introduction

In this paper, we explore the problem of estimating the total caloric content of simple water-based mixtures using microwave spectroscopy. The overall approach is based on a simple, yet profound observation that the calories within most common foods can be well approximated by only knowing the item's mass and the fractions of water and fat comprising it. The observation, reported by Webster and Neculaes [1] (see also Neculaes et al. [2]), comes from a simple linear regression of more than 6500 foods listed in the United States Drug Administration (USDA) National Nutrient Database [3]. Specifically, the total calories c in a food item can be approximated by

$$c \approx (8.89p_f + 3.79(1 - p_w - p_f))w, \quad (1)$$

where p_f and p_w denote the fraction of fat and water within the item, w denotes its weight/mass in grams, and the numerical constants have units of calories per gram (C/g).

This expression says that, with the exception of fat, all basic food constituents (complex carbohydrates, protein, and simple sugars) have essentially the same caloric density; fat, on the other hand, has over twice as many calories per gram.¹ Thus (1) reduces the problem of calorie estimation to the problem of estimating the water and fat content of a food item. (We assume the weight/mass of a food item can be readily measured.)

Here we propose and analyze a nearest neighbor estimator that estimates the constituent percentages of simple oil–water–sugar mixtures and thus, via (1), yields calorie estimates. The approach is based on creating a dictionary of representative microwave transmission spectra and defining an appropriate distance metric that maps a test spectrum to the dictionary element that best represents it (see Section 3 for details). For the class of mixtures studied, the estimator achieves average errors of 2.2%, 2.5%, 2.8% for oil, sugar, water respectively and 10.2% for calories. These results are on par with other estimators proposed in the literature for similar experiments [4–6] and are roughly

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¹ We assume that water as a basic food constituent has no calories.

within one percentage point of the performance of an oracle estimator for the constituent estimates and three percentage points for calories. This indicates that while some improvement may be gained by considering different distance metrics than the one proposed here, more sophisticated estimation methods will be necessary to improve average errors below approximately 1.4% for constituents and 7% for calories. However, for applications that can tolerate these levels of errors, the nearest neighbor estimator offers conceptual and computational simplicity.

1.1. Motivation

With the increasing prevalence of obesity worldwide and the growing associated costs (estimated to be \$147 billion USD in the US alone in 2008 [7]), a device that could reliably measure the calories in foods would presumably help individuals track caloric intake and help them maintain a healthy weight. Currently there are several commercial offerings able to monitor *burned* calories [8–10], but there are few, if any, precise and easy-to-use devices that measure caloric content of *non-homogeneous* foods (e.g. sandwiches and kebabs). Current optical devices (including near infrared) can yield accurate calorie counts of homogeneous foods [11], but because they only probe the food's surface, caloric estimation of non-homogeneous foods is problematic. Caloric intake can be tracked manually using publicly available nutritional information, but this approach is often tedious and error prone. The microwave spectroscopic approach presented here has the potential to overcome these problems and aims to fill this societal need.

1.2. Related work

In microwave spectroscopy, materials are delineated by differences in their complex permittivity. It is natural then to use the permittivity either directly or indirectly to infer information about a material's constituents. For example, Daschner et al. [6] estimate moisture content by performing a principal component regression over the measured dielectric spectra, i.e., over the real component of permittivity; Gibbs et al. [4] use time-domain features related to the received signal's delay, attenuation, and dispersion which are all characteristics related to complex permittivity; and Jean [12] leverages specific spectral characteristics to estimate the constituents of process materials. In contrast to these approaches which operate on a relatively small number of features (~ 10), the nearest neighbor estimator can be thought of as an estimator that uses a much larger set of features (~ 1000) because it operates on an entire measured spectrum. Alternatively, it can be thought of as an estimator only operating on a single object where the spectrum is thought of as being a signature of the food item and the goal is to search among a dictionary of signatures to find the best match.

2. Experimental data

Fig. 1 depicts the experimental setup. We used an Agilent vector network analyzer with two identical Cobham

spiral antennas to measure the transmission response of the mixtures (the top antenna being the transmitter and the bottom being the receiver). Each antenna has an effective bandwidth of 1.8–18 GHz and each has low dispersion characteristics. The analyzer was calibrated from 0.9 GHz to its maximum frequency of 8.5 GHz, and all measurements were referenced to the response of an empty beaker. For each experiment the analyzer swept through a uniform set of frequencies and recorded the received spectrum.

The mixtures were contained in a cylindrical beaker with a height and diameter equaling 75 cm and 150 cm, respectively. In order to minimize the effects of multipath and ensure that most of the transmitted energy passed through the sample, we chose a beaker that has a diameter three times larger than the largest dimension of the spiral antenna. The beaker contained homogeneous mixtures of distilled water, soybean oil (Fisher Scientific catalog number S25622), and a sucrose solution. The sugar/sucrose was purchased from a grocery store and solubilized as a 50% by weight solution of sugar and distilled water. The resulting syrup when added to the mixtures was considered to be 50% water and 50% sugar.

In total, the responses of 64 mixtures were recorded. The first 49 were considered dictionary elements and were created by combining different concentrations of oil and sugar by weight in 5% increments up to a maximum concentration of 30%. Fig. 2 graphically illustrates the different percentages. The remaining 15 samples were mixtures whose constituent percentages were randomly chosen within the same range as the dictionary samples (see Table 1). These mixtures were used to quantify the performance of the proposed estimator. Both the temperature and the volume of the mixtures were kept constant.

The peaks in the spectra and their general shape are controlled in large part by the frequency response of the system antennas and by the geometry of the measurement setup (see Fig. 3 for three prototypical spectral responses). The changing complex electrical permittivity of the samples modulates the spectral shape according to the frequency dependent attenuation for the mixtures and by an effective lens action on the wave front that is produced by delay and dispersion as the wave propagates through the material under test and its glass beaker container. The soybean oil is a fairly low loss, non-dispersive propagation medium over the frequency range used for the experiment. The complex permittivity of pure water exhibits a Debye frequency response that represents an increase in attenuation or loss factor with increasing frequency, up

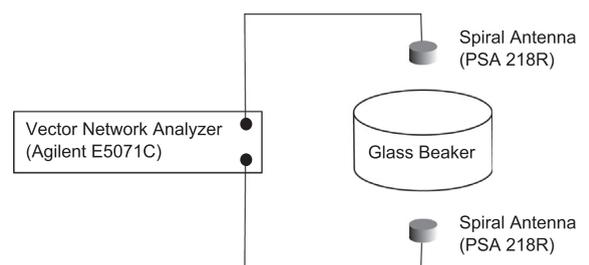


Fig. 1. Experimental setup.

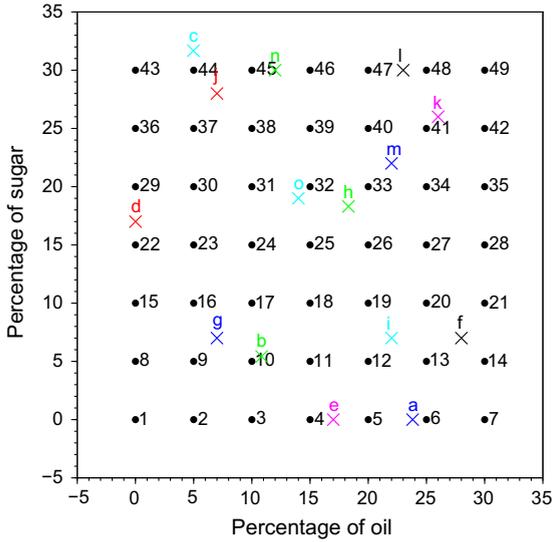


Fig. 2. The (x,y) coordinates of the dots equal the various oil and sugar percentages in the dictionary mixtures. The coordinates of the points marked with an 'x' are the oil and sugar percentages in the test mixtures.

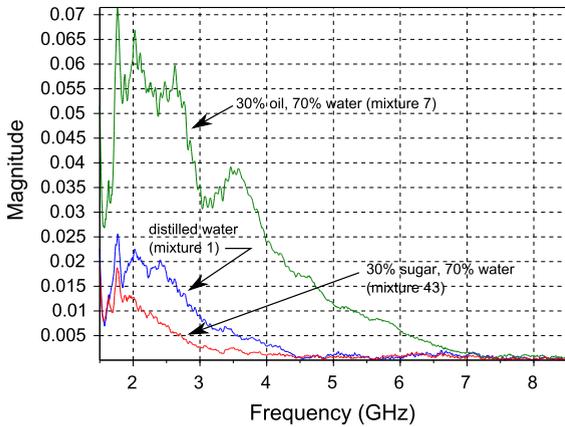


Fig. 3. Prototypical magnitude spectra for the experiments. Since oil is a low loss material, adding it to water lessens the attenuation across all frequencies (compare the response of mixture 1 to mixture 7). Adding sugar, increases attenuation as the conductivity of the mixture increases.

Table 1
Test samples.

Test sample	Oil (%)	Sugar (%)	Water (%)	Weight (g)	Calories (C)
a	23.81	0.00	76.19	835.50	1758.53
b	10.84	5.42	83.74	832.40	972.02
c	4.98	31.67	63.35	925.90	1542.36
d	0.00	17.00	83.00	897.90	590.73
e	17.00	0.00	83.00	814.80	1224.48
f	28.00	7.00	65.00	817.50	2244.94
g	7.00	7.00	86.00	855.00	760.69
h	18.30	18.30	63.40	857.50	1994.48
i	22.00	7.00	71.00	809.70	1794.05
j	7.00	28.00	65.00	915.40	1558.38
k	26.00	26.00	48.00	891.80	2947.04
l	23.00	30.00	47.00	899.50	2873.18
m	22.00	22.00	56.00	866.30	2422.35
n	12.00	30.00	58.00	907.10	2015.39
o	14.00	19.00	67.00	878.90	1733.98

to the molecular relaxation frequency that occurs in the range of 18 GHz, depending on temperature. Any conductivity caused by ionic impurities in the water cause attenuation to increase with decreasing frequency. The sugar, which was dissolved in the water, lowers the real part of the complex permittivity of the mixture and increases its conductivity on a volumetric basis. There are no interfacial effects for the three-component mixtures. Oil–water emulsions can exhibit such effects, but no agents were added to cause the water and oil to emulsify. The oil, sugar, and water were mechanically mixed to create a roughly homogeneous distribution such that the effective permittivity of the mixtures varied according to the percent volume of the constituents.

As the results in Section 3 show, the different complex permittivities of the mixtures and the effects they have on the spectral responses are sufficient to mathematically distinguish one response from another. This fact is the basis for the nearest neighbor estimator.

3. Calorie estimation

In this section, we first introduce the notion of an oracle estimator whose performance serves as a benchmark for the nearest neighbor estimator. We then define and empirically quantify the performance of the proposed nearest neighbor estimator. We also present an extension to the estimator that leverages the known weight (mass) of a test sample.

3.1. Oracle estimates

An oracle estimate is a type of nearest neighbor estimate where one assumes that the constituent percentages of the test samples are *known*. This is clearly an unrealistic scenario, but oracle estimators are useful because their performance bounds the performance of realistic estimators. Let $p_o, p_s,$ and p_w denote the fraction of oil, sugar, and water, respectively, in a given test sample and let $p_o^{(j)}, p_s^{(j)},$ and $p_w^{(j)}$ denote the same fractions in dictionary sample j . We define an oracle estimate as the dictionary

Table 2
Oracle estimates.

Test samples	Oracle index	Oracle oil (%)	Oracle sugar (%)	Oracle water (%)	Oracle calories (C)	Oil error (%)	Sugar error (%)	Water error (%)	Calories error (%)
a	6	25.00	0.00	75.00	1856.90	-1.19	0.00	1.19	-5.59
b	10	10.00	5.00	85.00	897.74	0.84	0.42	-1.26	7.64
c	44	5.00	30.00	65.00	1464.31	-0.02	1.67	-1.65	5.06
d	22	0.00	15.00	85.00	510.46	0.00	2.00	-2.00	13.59
e	4	15.00	0.00	85.00	1086.54	2.00	0.00	-2.00	11.27
f	14	30.00	5.00	65.00	2335.19	-2.00	2.00	0.00	-4.02
g	16	5.00	10.00	85.00	704.09	2.00	-3.00	1.00	7.44
h	26	20.00	15.00	65.00	2012.12	-1.70	3.30	-1.60	-0.88
i	13	25.00	5.00	70.00	1953.00	-3.00	2.00	1.00	-8.86
j	44	5.00	30.00	65.00	1447.71	2.00	-2.00	0.00	7.10
k	41	25.00	25.00	50.00	2827.01	1.00	1.00	-2.00	4.07
l	48	25.00	30.00	45.00	3021.87	-2.00	0.00	2.00	-5.18
m	34	25.00	20.00	55.00	2582.01	-3.00	2.00	1.00	-6.59
n	45	10.00	30.00	60.00	1837.78	2.00	0.00	-2.00	8.81
o	32	15.00	20.00	65.00	1838.22	-1.00	-1.00	2.00	-6.01

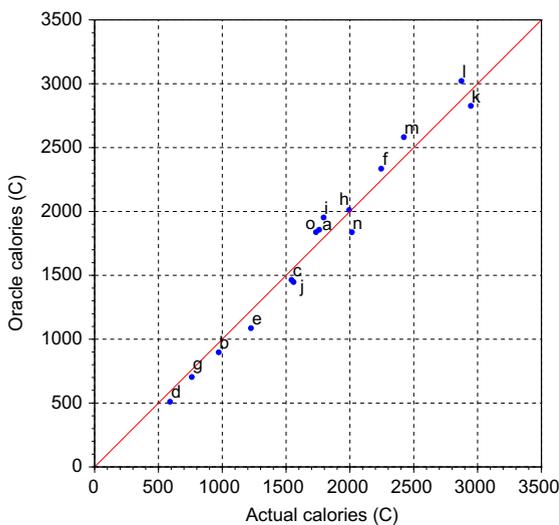
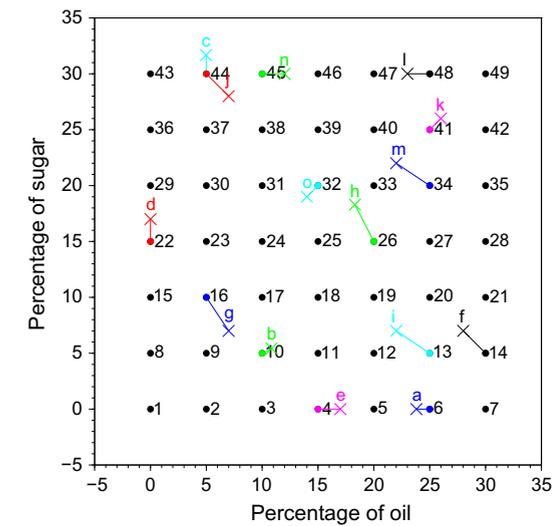


Fig. 4. Oracle performance. Left panel: Like Fig. 2 the dots represent the dictionary samples and the 'x's represent the test samples. The lines connect the test samples to their oracle estimate. Right panel: Plot of the oracle estimated calories versus the actual calories for the test samples.

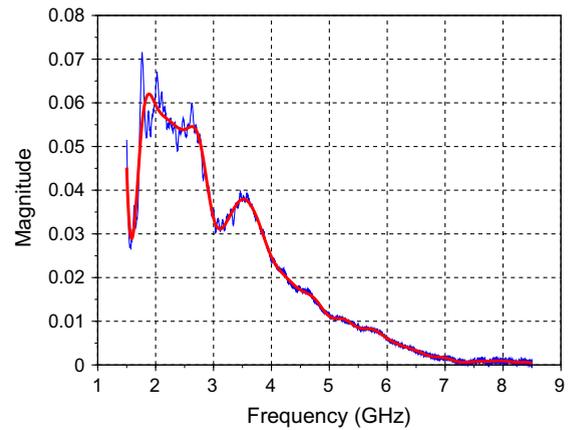


Fig. 5. Cubic spline approximation (thick smooth curve) overlaid on a dictionary spectrum.

sample that best matches the test sample in terms of its constituent percentages,

$$j^\circ := \arg \min_{j \in \{1, \dots, 49\}} \|p_j - p\| \quad (2)$$

where $p = [p_o, p_s, p_w]^T$, $p_j = [p_o^{(j)}, p_s^{(j)}, p_w^{(j)}]^T$, $\|\cdot\|$ denotes the ℓ_2 norm of a vector, and j° is the index denoting an oracle estimate (T denotes transpose). The corresponding oracle calorie estimate is

$$c^\circ := (8.89p_o^\circ + 3.79p_s^\circ)w, \quad (3)$$

where w denotes the weight or mass of the test sample and p_o° is shorthand notation for $p_o^{(j^\circ)}$ (likewise for p_s°). Table 2 and Fig. 4 capture the performance results of the oracle estimator. Note in interpreting Table 2 we conclude that the constituent percentage errors of any nearest neighbor estimator is bounded below by approximately 3%.

3.2. Nearest neighbor estimates

Nearest neighbor estimates are found by searching among the dictionary elements for the best matches to

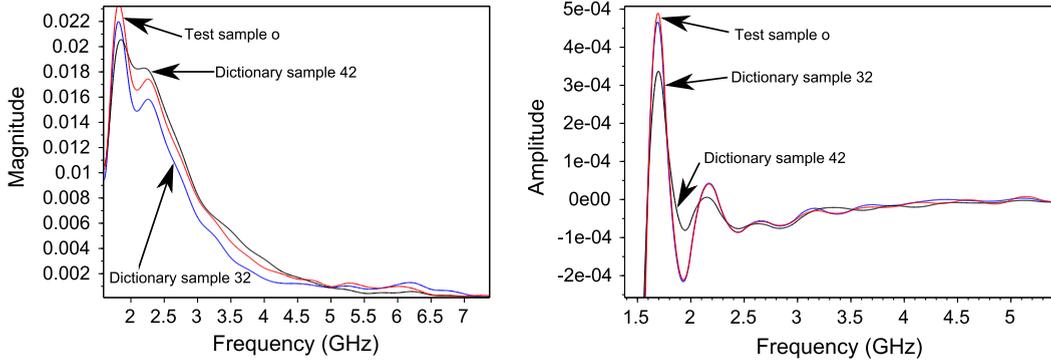


Fig. 6. The left panel shows the spline approximation of two dictionary spectra and one test spectrum. Dictionary element 32 is indeed the oracle estimate of test sample ‘o’, but 32 is further away (in the ℓ_2 sense) than dictionary element 42. Thus for the nearest neighbor estimate to decode properly the norm of the error of the spectra’s derivatives need to be taken into account. The right panel illustrates the point and shows that the distance between the derivatives of dictionary element 32 and test sample ‘o’ is smaller than that of dictionary element 42.

Table 3
Nearest neighbor estimates.

Test samples	NN index	NN oil (%)	NN sugar (%)	NN water (%)	NN calories (C)	Oil error (%)	Sugar error (%)	Water error (%)	Calories error (%)
a	12	20.00	5.00	75.00	1643.85	3.81	-5.00	1.19	6.52
b	10	10.00	5.00	85.00	897.74	0.84	0.42	-1.26	7.64
c	44	5.00	30.00	65.00	1464.31	-0.02	1.67	-1.65	5.06
d	29	0.00	20.00	80.00	680.61	0.00	-3.00	3.00	-15.22
e	4	15.00	0.00	85.00	1086.54	2.00	0.00	-2.00	11.27
f	27	25.00	15.00	60.00	2281.64	3.00	-8.00	5.00	-1.64
g	9	5.00	5.00	90.00	542.07	2.00	2.00	-4.00	28.74
h	32	15.00	20.00	65.00	1793.46	3.30	-1.70	-1.60	10.08
i	26	20.00	15.00	65.00	1899.96	2.00	-8.00	6.00	-5.90
j	37	5.00	25.00	70.00	1274.24	2.00	3.00	-5.00	18.23
k	42	30.00	25.00	45.00	3223.41	-4.00	1.00	3.00	-9.38
l	47	20.00	30.00	50.00	2622.04	3.00	0.00	-3.00	8.74
m	34	25.00	20.00	55.00	2582.01	-3.00	2.00	1.00	-6.59
n	46	15.00	30.00	55.00	2240.99	-3.00	0.00	3.00	-11.19
o	32	15.00	20.00	65.00	1838.22	-1.00	-1.00	2.00	-6.01

the test samples. But instead of directly comparing magnitude spectra, we first approximate them. In particular, each magnitude spectrum is approximated by a cubic spline (piecewise polynomial) where the polynomial coefficients in each segment are chosen to minimize the squared error between the approximation and the original spectrum [13,14]. The frequency points defining the endpoints of the different piecewise segments (i.e. the knot sequence) are taken to be elements of a uniform sub-sequence of the frequencies at which the data were originally collected. The purpose of taking spline approximations is to obtain smooth representations of the spectra that preserve the curves’ overall shape. Fig. 5 shows an example of one such approximation.

Let $r_j \in \mathfrak{R}^n$, $n = 1400$, denote the cubic spline approximation of the j th dictionary spectra ($j = 1, \dots, 49$) and let $s \in \mathfrak{R}^n$ denote the spline approximation of one of the test spectra. A natural way to quantify the distances between $\{r_j\}$ and s is to compute the ℓ_2 norm of the error between s and all of the dictionary elements,

$$\|r_j - s\| = \left(\sum_{k=1}^n |r_j(k) - s(k)|^2 \right)^{1/2}, \quad j = 1, \dots, 49, \quad (4)$$

where smaller error indicates higher similarity. However, empirical experiments suggest that this measure does not yield very accurate nearest neighbor estimates. Thus we augment (4) by considering the spectra’s difference signals. Let Δr_j and Δs denote the difference signals of r_j and s ,

$$\Delta r_j(k) = r_j(k + 1) - r_j(k), \quad k = 1, \dots, n - 1 \quad (5)$$

$$\Delta s(k) = s(k + 1) - s(k), \quad k = 1, \dots, n - 1. \quad (6)$$

These difference signals are the first order finite difference approximation to the derivative of the spectra as a function of frequency [15–17]. Hence the norm of the error $\|\Delta r_j - \Delta s\|$ is a measure of similarity between a test spectrum’s derivative and the derivatives of the dictionary spectra. Comparing derivatives allows one to compare the general shape of the spectra even if two spectra significantly differ in magnitude. To understand this statement, consider the example in Fig. 6. The plot in this figure shows a test spectrum and two dictionary spectra. The dictionary element that is most similar in shape to the test spectrum (dictionary sample 32) is the oracle estimate and thus is

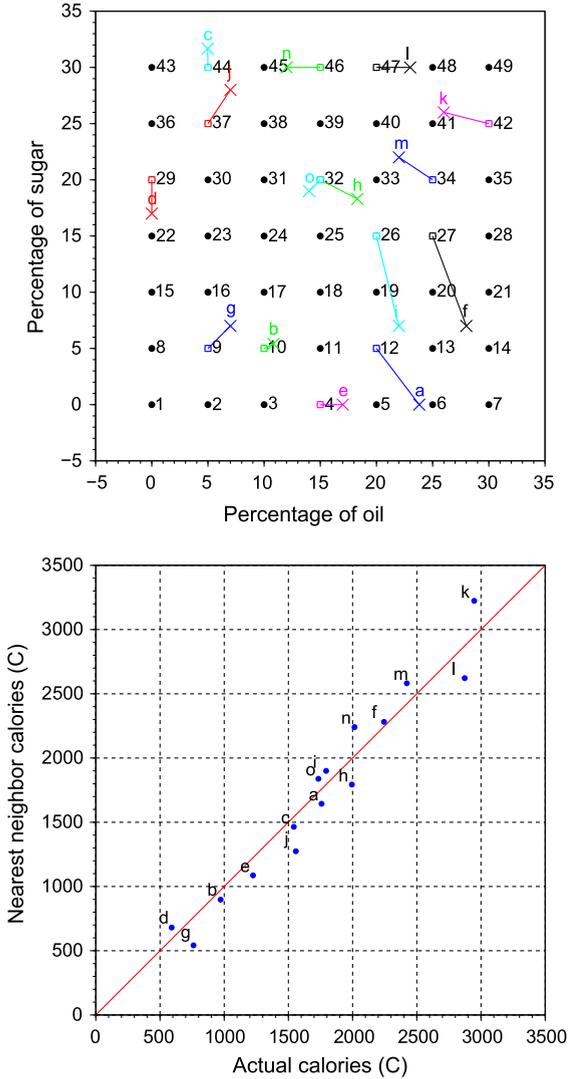


Fig. 7. Nearest neighbor performance. Left panel: Dots represent the dictionary samples and the 'x's represent the test samples. The lines connect the test samples to their nearest neighbor estimate (marked as squares). Right panel: Plot of the estimated calories versus the actual calories for the test samples.

the spectrum we want to choose as the test sample's nearest neighbor; however, the other dictionary spectrum (dictionary element 42) has a smaller ℓ_2 error, i.e.,

$$\|r_{42} - s\| < \|r_{32} - s\|. \quad (7)$$

The right hand panel in Fig. 6 shows the difference signals of the same three spectra. Note that in this plot the difference signal of the oracle estimate more closely matches the test signal as compared to the other dictionary signal. This example demonstrates a limitation of using the norm of the spectral error alone to compute a nearest neighbor estimate and motivates the use of a nearest neighbor estimate of the form

$$\arg \min_j \|r_j - s\| + \|\Delta r_j - \Delta s\|, \quad (8)$$

where the minimizer would be the index of the dictionary spectrum deemed to be the nearest neighbor of s . To apply this rule, however, the two terms in (8) need to be normalized such that their contributions are equally weighted.

Letting

$$\tilde{F} = \min_j \|r_j - s\| \quad \hat{F} = \max_j \|r_j - s\|$$

$$\tilde{G} = \min_j \|\Delta r_j - \Delta s\| \quad \hat{G} = \max_j \|\Delta r_j - \Delta s\|,$$

we normalize the norms to the unit interval

$$\mu_j = \frac{\|r_j - s\| - \tilde{F}}{\hat{F} - \tilde{F}} \quad (9)$$

$$v_j = \frac{\|\Delta r_j - \Delta s\| - \tilde{G}}{\hat{G} - \tilde{G}}. \quad (10)$$

The proposed nearest neighbor rule is then

$$j^* := \arg \min_{j \in \{1, \dots, 49\}} \mu_j + v_j. \quad (11)$$

The constituent fractions of the optimal spectrum r_{j^*} are the nearest neighbor estimates, denoted by $p_o^{(j^*)} = p_o^*$, $p_s^{(j^*)} = p_s^*$, and $p_w^{(j^*)} = p_w^*$ for oil, sugar, and water respectively. The nearest neighbor calorie estimate is computed as

$$c^* := (8.89p_o^* + 3.79p_s^*)w. \quad (12)$$

Table 3 contains the results of applying this estimator to the 15 test samples. Fig. 7 graphically shows the pairing between the test samples and their nearest neighbor. The average absolute error for the calorie estimates is 10.15% with the minimum and maximum absolute errors being 1.64% and 28.74%. The sample mean and variance are 0.027 and 0.015.

Note that the oracle constituent errors listed in Table 2 do indeed lower bound the nearest neighbor constituent errors. However, the same is not true for the oracle calorie estimates. Because (1) is a many-to-one mapping there are times when the error of a nearest neighbor calorie estimate is smaller than the error of an oracle estimate. For example, this happens with test sample 'f'.

3.3. Leveraging measured weight

There is no reason to expect that the weight of the dictionary samples, or rather the weight of any potential nearest neighbor estimate, should be the same as the measured weight of a test sample. But because all the mixtures in these particular experiments had constant volume, a weight difference between a test sample and its nearest neighbor estimate directly implies a difference among the true constituent percentages and the nearest neighbor constituent percentages.² Thus this weight difference provides additional information that can be used to calculate a new calorie estimate from the nearest neighbor estimate. In this section, we propose a heuristic extrapolation scheme based on this potential weight difference.

² This is true provided the test sample does not lie on a line of equal weight.

Table 4
Estimates leveraging measured weights.

Test samples	Extrapolated oil (%)	Extrapolated sugar (%)	Extrapolated water (%)	Extrapolated calories (C)	Oil error (%)	Sugar error (%)	Water error (%)	Calories error (%)
a	19.18	4.59	76.23	1569.89	4.63	-4.59	-0.04	10.73
b	9.22	4.68	86.10	829.84	1.62	0.74	-2.36	14.63
c	6.18	30.00	63.82	1561.48	-1.20	1.68	-0.47	-1.24
d	0.00	19.92	80.08	677.88	0.00	-2.92	2.92	-14.75
e	16.44	0.00	83.56	1190.82	0.56	0.00	-0.56	2.75
f	23.24	14.42	62.34	2135.71	4.76	-7.42	2.66	4.87
g	6.43	5.55	88.02	668.62	0.57	1.45	-2.02	12.10
h	14.59	19.93	65.49	1759.71	3.71	-1.63	-2.09	11.77
i	16.27	13.89	69.83	1597.81	5.73	-6.89	1.17	10.94
j	6.83	25.14	68.03	1427.76	0.17	2.86	-3.03	8.38
k	28.63	24.83	46.53	3109.38	-2.63	1.17	1.47	-5.51
l	19.74	30.00	50.26	2601.57	3.26	-0.00	-3.26	9.45
m	25.81	20.18	54.01	2650.42	-3.81	1.82	1.99	-9.42
n	14.61	30.00	55.39	2209.17	-2.61	-0.00	2.61	-9.61
o	15.94	20.17	63.89	1917.33	-1.94	-1.17	3.11	-10.57

Let $\delta = w - w^*$ denote the difference of the weight of the test sample and the weight of the nearest neighbor estimate. The proposed scheme apportions a particular fixed fraction of δ to the constituent weights of the nearest neighbor estimate such that the extrapolated weight equals the test sample's measured weight. Mathematically, this adjustment is expressed as

$$w_o^b := w^* p_o^* + (8.89/12.68)\delta \tag{13}$$

$$w_s^b := w^* p_s^* + (3.79/12.68)\delta \tag{14}$$

for $w_o^b > 0$ and $w_s^b > 0$ where w_o^b, w_s^b represent the extrapolated oil and sugar weight in the test sample, p_o^* and p_s^* denote, respectively, the fraction of oil and sugar for the nearest neighbor estimate, and w^* denotes the nearest neighbor estimate's weight. The fractions 8.89/12.68 and 3.79/12.68 are the ratios of the caloric densities. The extrapolated calorie estimate c^b is then computed as,

$$c^b := 8.89w_o^b + 3.79w_s^b. \tag{15}$$

Note that if $\delta = 0$, c^b equals the nearest neighbor estimate. Also note that when this scheme is implemented care must be taken to ensure the boundary conditions are satisfied, i.e., ensure that the method does not produce negative (non-physical) weights.

Because the weight difference does not provide any information as to how the constituent proportions should be changed, there is no guarantee that this scheme reduces the calorie error. The extrapolation works best when the weight difference is caused by differences in the percentages of oil and gas and not in the percentage of water.

Like the nearest neighbor results, Table 4 and Fig. 8 contain the results of this extrapolation procedure for the test samples. The average absolute error for the calorie estimates is 9.11% with the minimum and maximum absolute errors being 1.24% and 14.75%, respectively. The sample variance of the calorie errors is 0.010 which is a 33% decrease than the nearest neighbor estimates. However, because of the heuristic nature of the scheme, there are instances where performance worsens. For example, for

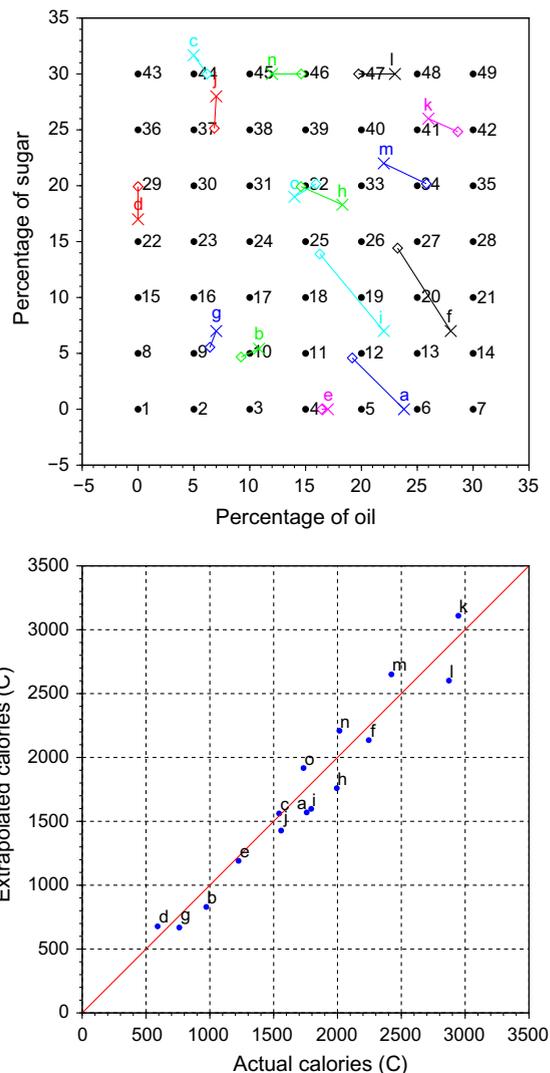


Fig. 8. Extrapolation performance. Left panel: Dots represent the dictionary samples and the 'x's represent the test samples. The lines connect the test samples to their nearest neighbor extrapolated estimate (marked as diamonds). Right panel: Plot of the estimated calories versus the actual calories for the test samples.

test sample 'a' the calorie error increased from 6.52% to 10.73%. On the other hand, the maximum nearest neighbor error of 28.74% for test sample 'g' reduced to 12.10%. In this case, both the sugar and oil concentrations moved closer to the true constituent percentages consequently reducing the error.

4. Conclusion

While the results reported here are only for simple mixtures of oil, sugar, and water, the approach of estimating calories by finding nearest neighbor estimates from within a set of dictionary elements generalizes to more complicated food items. In particular, the definition of the nearest neighbor estimator in (11) remains applicable as the constituent list grows larger, and it can be easily tailored to take advantage of different spectral aspects (e.g., different regularization terms can be added). The efficacy of the approach for more complicated foods is still however an open question.

In some sense, it is remarkable that a nearest neighbor approach worked as well as it did because the spectra are high dimensional objects ($n = 1400$), and for such spaces, it is typically difficult to create dictionaries large enough that guarantee sufficient performance.³ The fact that the proposed estimator worked reasonably well suggests that the spectra lie in a very small subspace in \mathbb{R}^n that can be well-represented by a small dictionary. An important question moving forward is how large does this subspace become when more complicated foods are considered. If it becomes too large, nearest neighbor estimators will no longer be practical; if on the other hand the subspace remains small, nearest neighbor estimators offer a simple solution.

The nearest neighbor methodology also informs more sophisticated machine learning [18,19] and neural network approaches [20] in their application to calorie estimation. For both approaches, features are first extracted from the data of interest (in this case the transmission spectra) and they are in turn used to train a classifier or an estimator. Performance thus depends on the chosen set of features. When considering more complicated food items, and even for simple mixtures, it is unclear a priori which set of features should be used and what number of features is sufficient to achieve a target performance. The results reported here directly suggest two features (the norm of the spectra error and the norm of the difference signals) and indirectly suggest features related to the shape of a spectrum (e.g., slopes and curvatures) as candidate features for more complicated food items. The results also suggest that with only these two features machine learning and neural network techniques should be able to achieve a 10% (or better) average error for simple mixtures.

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³ To maintain a fixed distance among dictionary elements, the required number of elements grows exponentially in n .