



OptiPAQ - Software for Product Optimisation from Qi Statistics Ltd.

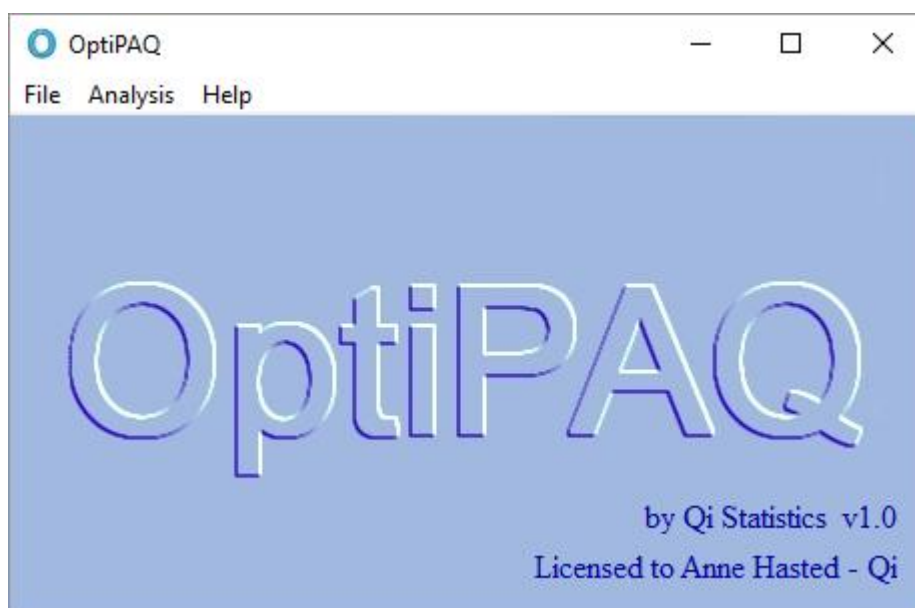
What it does

OptiPAQ fits response surface models to predict a consumer acceptability response from a set of quantitative descriptors using the first two components derived either using principal components or partial least squares. The recommended best fit to the data is plotted graphically and the user can then investigate the effect on product acceptability of modifying the descriptors

Data Requirements

An Excel data sheet containing at least 5 products with a single column measuring consumer acceptability (average liking score, purchase intent) and a set of quantitative descriptors (sensory panel mean scores, CATA percentages, analytic measures etc).

The sample data set is from a study on peanuts, 12 samples of peanuts profiled by a sensory panel plus additional results from a consumer test. Data sheet contains mean scores from the sensory panel plus average liking from a consumer test (120 consumers).



To input your data click on the **<File>** menu and then **<Open>**. Your data should then appear on the screen. The first step is to define the column containing product labels (turquoise), the consumer response (red) and descriptive data (purple). Note you can exclude data columns or rows (grey). To colour the columns select the top row (letters) and click on the appropriate category in the selection tab.

The Excel Worksheet Import Wizard dialog box is shown with the following data table:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Product	Overall Liking	Brown	Baked	Aromatic	Nutty	Raw	Dry	Stale	Tant	Sweet	Bitter	Rancid	Malt	Crispy	Crunchy	Hard
2	212	4.90	4.0	4.3	3.1	3.0	2.2	3.2	0.5	0.1	2.8	2.2	0.6	1.1	5.7	6.6	8.4
3	321	5.60	5.7	3.5	2.7	2.5	2.6	3.1	0.9	0.0	3.0	2.2	1.0	1.0	5.7	6.7	7.8
4	743	4.77	4.4	3.3	2.5	2.6	2.6	3.4	1.6	1.7	2.2	2.6	2.9	0.2	1.7	3.4	5.2
5	482	3.90	4.0	3.1	2.3	2.7	2.6	3.5	1.8	1.4	2.0	3.2	3.0	0.3	3.4	3.9	6.8
6	573	4.80	4.3	3.7	2.5	2.8	2.5	3.4	1.1	1.1	2.2	2.7	2.0	0.1	3.5	5.3	6.4
7	624	4.90	5.1	3.4	2.7	2.6	2.6	3.3	1.5	1.1	2.2	2.6	2.5	0.2	4.0	4.4	6.2
8	784	5.50	5.0	4.1	3.1	3.1	2.2	3.3	1.4	0.2	2.5	2.6	2.2	0.5	2.4	3.6	5.5
9	812	6.22	5.6	4.3	3.1	2.9	2.3	3.1	0.7	0.0	3.0	2.2	0.7	0.9	2.7	3.7	5.9
10	931	5.60	4.9	4.2	2.8	2.8	2.4	3.2	1.2	0.1	2.5	2.3	1.3	0.6	1.6	3.2	5.2
11	102	4.95	5.2	3.7	2.7	2.9	2.4	3.4	1.7	1.1	2.2	2.6	2.6	0.1	1.5	3.4	5.2
12	114	5.95	5.0	4.4	3.2	3.1	2.1	3.2	0.6	0.1	2.7	2.2	0.9	1.0	3.1	4.2	6.2
13	123	6.00	5.8	3.9	2.8	2.9	2.4	3.4	1.3	0.1	2.4	2.5	2.0	0.1	3.5	3.8	6.2

When you are happy with your selections press **<finished>**

The screen below appears:

The Analysis Options dialog box is shown with the following settings:

- Data Scaling:**
 - Centre
 - Normalise
- Retain R files:**
- Axes Method:**
 - PCA
 - PLS

Buttons: Cancel, Fit Model

Data Scaling

Select **Centre** if you want to analyse the descriptive data without rescaling.

Select **Normalise** if you want to centre and rescale the descriptive data to unit variance.

The modelling is carried out using R – if you want to save the R code and raw output - tick **<Retain R Files>**

Axes Method

Select **PCA** to derive the axes using Principal Components Analysis.

Select **PLS** to derive the axes using Partial Least Squares

And then click **<Fit Model>**

The software fits the four models below, the quadratic, elliptical and circular model are models with curvature and the vector model is linear, using the adjusted R squared value it suggests the most appropriate model (but you can make your own selection by changing the recommendation)

Vector Model

$$Y_i = b_0 + b_1F_{1i} + b_2F_{2i} + \varepsilon_i$$

Response changes linearly with either F1 or F2 or both F1 and F2

Circular model

$$Y_i = b_0 + b_1F_{1i} + b_2F_{2i} + b_3(F_{1i}^2 + F_{2i}^2) + \varepsilon_i$$

This model allows for curvature in the sensory space with circular contours (rate of change in response from the optimum is the same in both F1 and F2 directions)

Elliptical Model

$$Y_i = b_0 + b_1F_{1i} + b_2F_{2i} + b_3F_{1i}^2 + b_4F_{2i}^2 + \varepsilon_i$$

This model allows for curvature in the sensory space with elliptical contours (rate of change in response from the optimum is different in the F1 and F2 directions)

Quadratic Model

$$Y_i = b_0 + b_1F_{1i} + b_2F_{2i} + b_3F_{1i}^2 + b_4F_{2i}^2 + b_5F_{1i}F_{2i} + \varepsilon_i$$

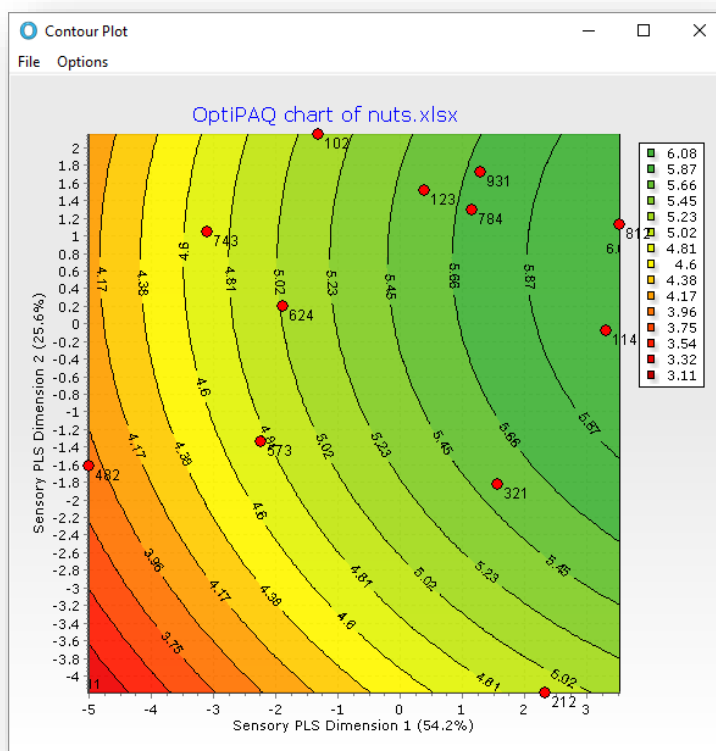
This model allows for curvature in the sensory space with elliptical contours (rate of change in response from the optimum is different in the F1 and F2 directions and there is a covariance between F1 and F2)

Here an elliptical model is recommended (the * indicates that the fit of the model is significant at the 5% level)

	R ²	Adjusted R ²		Recommended Model:
Vector Model	0.880 *	0.854	<input type="radio"/>	Elliptical
Circular Model	0.903 *	0.866	<input type="radio"/>	
Elliptical Model	0.924 *	0.881	<input checked="" type="radio"/>	
Full RSM Model	0.926 *	0.864	<input type="radio"/>	

OptiPAQ requires that you have at least 5 samples in order to fit a model. To avoid overfitting, only a vector model will be available in the screen above when there are either 5 or 6 samples. Similar restrictions apply for the models with curvature, at least 7 samples are required for a circular model, at least 8 for an elliptical model, and at least 9 samples for the Full RSM model.

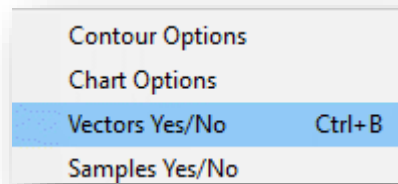
The response surface is plotted as a contour plot, the contour levels indicate predicted liking. The samples tested are positioned on the plot.



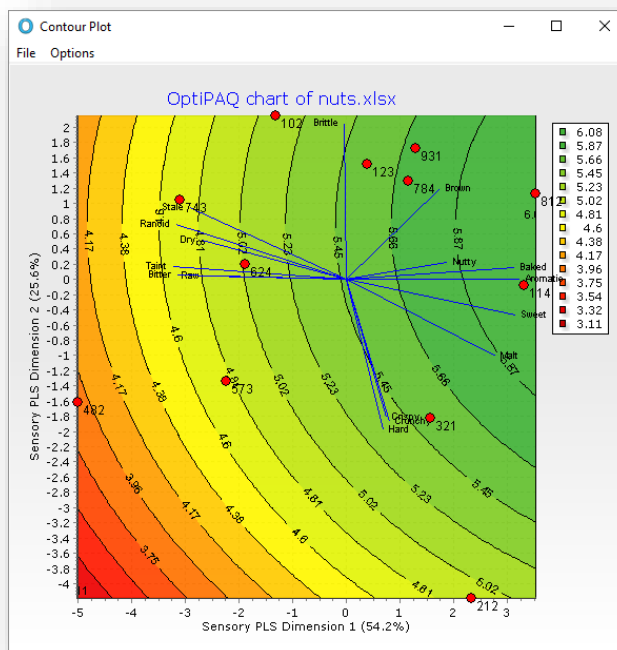
If you click on options, you have options to:

- Change the number of contours (Contour options)
- Change the colours (Chart Options)
- Add Sensory Vectors (Vectors Yes/No)

- Remove samples from plot (Samples Yes/No)

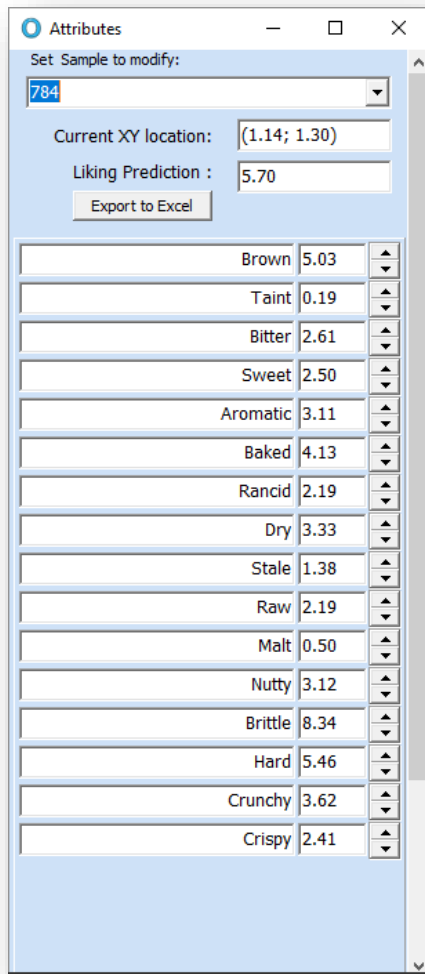


Below is a plot with sensory vectors superimposed:



The plots can be saved as graphic files (<File Menu>)

Additionally the user can select a sample of interest, change the sensory properties (within the sensory range investigated) either using the up and down arrows or by typing numbers directly. The sample is repositioned on the graph and the predicted liking calculated.



The screenshot shows a software window titled 'Attributes'. At the top, there is a dropdown menu for 'Set Sample to modify:' with '784' selected. Below this are two input fields: 'Current XY location:' with the value '(1.14; 1.30)' and 'Liking Prediction:' with the value '5.70'. A button labeled 'Export to Excel' is positioned below these fields. The main area of the window contains a table with 16 rows, each representing an attribute and its corresponding value. Each row has a small up/down arrow icon to its right.

Brown	5.03
Taint	0.19
Bitter	2.61
Sweet	2.50
Aromatic	3.11
Baked	4.13
Rancid	2.19
Dry	3.33
Stale	1.38
Raw	2.19
Malt	0.50
Nutty	3.12
Brittle	8.34
Hard	5.46
Crunchy	3.62
Crispy	2.41

Selecting the option **<Export to EXCEL>** produces an EXCEL file – saved in the same folder as the original data file.

This file contains details of the model fit (R^2 Q^2 and VIP statistics) and predicted liking of the selected product.