Quadratic Multidimensional Regression

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Considering a structured dataset consisting of N sets $\{\mathbf{X}_k, f_k, \sigma_{y_k}\}$, where $\mathbf{X}_k$ is the feature vector of dimension 2 and f_k the target behaviour. Lets assume ae multinomial model model:

$$f_k = a + b^i x_{(i,k)} + c^{ij} x_{(i,k)} x_{(j,k)} \tag{1}$$

wjere $x_{(k)}$ with $k = 1, 2, \cdots, \mathbb{D}$, reprsents the k-th feature of the vector $\mathbf{X}_k$. Here, we are using the Einstein sum notation. The constants a, b^i and c^{ij} are the parameters wich values we want to find.

A general totally symmetric matrix M of rank R and dimension $\mathcal{D}$ has a number of independent componentes given by

$$\text{number of components } = \binom{\mathbb{D} + R - 1}{R}.$$

where $\binom{\cdot}{\cdot}$ is the binomial coefficient. From (1), we can see clearly that c^{ij} is the components of a symmetric matrix. Because of this, we can write:

$$\text{number of components of } c^{ij} = \binom{\mathbb{D} + 2 - 1}{2}$$

The total number of independent coefficients of (1) is:

$$\text{number of parameters} = \binom{\mathbb{D} - 1}{0} + \binom{\mathbb{D}}{1} + \binom{\mathbb{D} + 1}{2}. \tag{2}$$

For a general regression problem, where the maximum order of the multinomial is $\mathbb{O}$, the number of parameter is:

$$n_P = \sum_{k=0}^{\mathbb{O}} \binom{\mathbb{D} + k - 1}{k}.$$

The expression of the square of (1) is:

$$\begin{aligned} f_k^2 =& a^2 + 2ab^i x_{(i,k)} + \left(2ac^{ij} + b^i b^j\right) x_{(i,k)} x_{(j,k)} + \\ &+ \left(2ad^{ijl} + 2b^i c^{jl}\right) x_{(i,k)} x_{(j,k)} x_{(l,k)} + \\ &+ \left(2b^i d^{jlr} + c^{ij} c^{lr}\right) x_{(i,k)} x_{(j,k)} x_{(l,k)} x_{(r,k)} \\ &+ \left(2c^{ij} d^{lrs}\right) x_{(i,k)} x_{(j,k)} x_{(l,k)} x_{(r,k)} x_{(s,k)} + \\ &+ \left(d^{ijl} d^{rst}\right) x_{(r,k)} x_{(s,k)} x_{(t,k)} x_{(i,k)} x_{(j,k)} x_{(l,k)} \end{aligned}$$

Assuming that the data are uncorrelated, the Chi Squared function can be writen as:

$$\chi^2 = \sum_k \frac{1}{\sigma_k^2} \left[f_k - f\left(x_{(k)}\right)\right]^2$$

or

$$\chi^2 = \sum_k \left(\frac{1}{\sigma_k^2} f_k^2 - \frac{2}{\sigma_k^2} f_k f + \frac{1}{\sigma_k^2} f^2 \right) . \tag{3}$$

Defining the functions

$$A := \sum_k \frac{1}{\sigma_k^2} \quad B_i := \sum_k \frac{1}{\sigma_k^2} x_{(i,k)} \quad C_{ij} := \sum_k \frac{1}{\sigma_k^2} x_{(i,k)} x_{(j,k)} \quad ; \tag{4}$$

$$D_{ijl} := \sum_k \frac{1}{\sigma_k^2} x_{(i,k)} x_{(j,k)} x_{(l,k)} \quad E_{ijlr} = \sum_k \frac{1}{\sigma_k^2} x_{(i,k)} x_{(j,k)} x_{(l,k)} x_{(r,k)} \tag{5}$$

and

$$H := \sum_k \frac{f_k}{\sigma_k^2} \quad I_i := \sum_k \frac{f_k}{\sigma_k^2} x_{(i,k)} \quad J_{ij} := \sum_k \frac{f_k}{\sigma_k^2} x_{(i,k)} x_{(j,k)} \quad Z := \sum_k \frac{f_k^2}{\sigma_k^2}, \tag{6}$$

the χ^2 can be written as:

$$\begin{aligned} \chi^2 =& Z - 2aH - 2b^i I_i - 2c^{ij} J_{ij} + \\ &+ a^2 A + 2ab^i B_i + \left(2ac^{ij} + b^i b^j\right) C_{ij} + \\ &+ \left(2b^i c^{jk}\right) D_{ijk} + \left(c^{ij} c^{kr}\right) E_{ijkr} \end{aligned}$$

Minimizing with respect to a, b's and c's, we have the following system of equations:

$$aA + b^i B_i + c^{ij} C_{ij} + d^{ijk} D_{ijk} = H \tag{7}$$

$$aB_v + \left(b^j\right) C_{vj} + c^{jk} D_{vjk} + d^{ijk} E_{vijk} = I_v \tag{8}$$

$$aC_{vw} + b^i D_{ivw} + c^{ij} E_{ijvw} + d^{ijk} F_{vwijk} = J_{vw} \tag{9}$$

In matrix notation, this system can be rewritten as

$$
\begin{bmatrix}
A & B_1 & \cdots & B_{\mathbb{D}} & C_{11} & \cdots & C_{\mathbb{D}\mathbb{D}} \\
B_1 & C_{11} & \cdots & C_{1\mathbb{D}} & D_{111} & \cdots & D_{1\mathbb{D}\mathbb{D}} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
B_D & C_{\mathbb{D}1} & \cdots & C_{\mathbb{D}\mathbb{D}} & D_{\mathbb{D}11} & \cdots & D_{\mathbb{D}\mathbb{D}\mathbb{D}} \\
C_{11} & D_{111} & \cdots & D_{\mathbb{D}111} & E_{1111} & \cdots & E_{11\mathbb{D}\mathbb{D}} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
C_{\mathbb{D}\mathbb{D}} & D_{a\mathbb{D}\mathbb{D}} & \cdots & D_{\mathbb{D}\mathbb{D}\mathbb{D}} & E_{11\mathbb{D}\mathbb{D}} & \cdots & E_{\mathbb{D}\mathbb{D}\mathbb{D}\mathbb{D}}
\end{bmatrix}
\begin{bmatrix}
a \\ b^1 \\ \vdots \\ b^{\mathbb{D}} \\ c^1 \\ \vdots \\ c^{\mathbb{D}}
\end{bmatrix}
=
\begin{bmatrix}
A \\ G^1 \\ \vdots \\ G^{\mathbb{D}} \\ H^{11} \\ \vdots \\ H^{\mathbb{D}\mathbb{D}}
\end{bmatrix}
\tag{10}
$$