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Higher-Order Probabilistic Models: Theory and Algorithms

Masterthesis

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Abstract

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Chapter 1

Introduction

In statistical theory and more applied disciplines as machine learning or artificial intelligence, it is fundamental to reduce the space of parameters. In this work we are going to consider multivariate categorical models, in other words, models that include variables with a discrete set of outcomes. More specifically, we are going to look at multivariate binary models or so called Ising Models, whose variables only have two possible outcomes. The parameter space of the entire model is growing exponentially with the number of variables. For instance, a binary model (a model with variables that have two possible outcomes) with n variables has $2^n - 1$ parameters, because each combination for all variables is encoded within one parameter. To fit a model to data, the general principle says that roughly ten times more observations than parameters are necessary in order to get a descriptive, meaningful model, but this requirement can often not be satisfied.

To meet this problem of a growing parameter space, we either have the option to use regularization methods as sparsity or low rank conditions, while fitting the model, with the purpose to set insignificant parameters to zero. On the other hand, we can use a different approach to model the data with fewer parameters from the beginning.

We will concentrate on a specific class of models that we are going to work with, where the focus is set on the interactions between the single variables. These type of modeling data combined with parameter space reduction methods is the objective we are willing to examine.

1.1 Idea of Variable Interactions

The idea of variable interactions is the based on the assumption that the outcome of one variable depends on the outcomes of the other remaining variables. That is encoded in a statistical model by an additional term which models the interaction. When we consider pairwise interactions, an interaction term of the variables x_i and x_j would have the shape

$$q_{ij}\ x_i\ x_j$$

with the interaction parameter q_{ij}. The interaction parameter indicates how much

the interaction between x_i and x_j influences the model. An interaction term of the the variables x_i, x_j, x_k would have the shape

$$q_{ijk}\ x_i\ x_j\ x_k$$

with interaction parameter q_{ijk}. Let $K = 3$ be the interaction order and $n = 3$ the dimension (number of variables). The entire model with the variables x_1, x_2 and x_3 would include the terms

$$q_1x_1 + q_2x_2 + q_3x_3 + q_{12}x_1x_2 + q_{13}x_ix_3 + q_{23}x_2x_3 + q_{123}x_1x_2x_3$$

with the parameter space $\Theta = (q_1,\ q_2,\ q_3,\ q_{12},\ q_{13},\ q_{23},\ q_{123})$. Here, we already get seven parameters for interaction order $K = 3$ and dimension $n = 3$.

Remark. The complexity of a model is equal to the size of the parameter space Θ (number of parameters) of the respective model.

Lemma 1.1. *Let K be the interaction order and n the number of variables, then the complexity of higher-order interaction models can be calculated with*

$$|\Theta| = \sum_{i=1}^{K} \binom{n}{i}, \quad \textit{where } \binom{n}{i} = 0 \textit{ for } i > n$$

Proof. TODO □

Conclusion 1.2. *We consider a binary model and the interaction order K is equal to the number of variables n, then the complexity of the higher-order interaction model is equal to the complexity of the entire categorical model and grows exponentially in n:*

$$|\Theta| = \sum_{i=1}^{n} \binom{n}{i} \ = \ 2^n - 1$$

Var. n \ Order K	2	3	4	5	6	$2^n - 1$
2	3	-	-	-	-	3
3	6	7	-	-	-	7
4	10	14	15	-	-	15
5	15	25	30	31	-	31
6	21	41	56	62	63	63

Table 1.1: Complexity for an interaction model of order K and dimension n. In comparison, the complexity for an entire binary model.

Hence, to model higher-order interactions between variables with an interaction order equal to the number of variables, the parameter space grows as fast as the complexity of the entire binary model as it is illustrated in table 1.1. Consequently, the order of interactions K should be held relatively small in comparison to the number of variables n to get a significant benefit. Therefore, we will mostly consider models with a rather low order of interaction in the following chapters. Later, we are going generalize these approach. Simultaneously, while fitting the model, we are going to use methods as regularization as a constraint in the objective function for model selection to reduce the complexity.

1.2 Pairwise Binary Interaction Models

1.2.1 Definitions and Conventions

In the following sections, we define and introduce a multivariate pairwise interaction model on binary variables and try to get a general understanding why it is reasonable to use that class of models.

Definition. Let $X = (X_1, ..., X_n)$ be a vector of random variables with the set of outcomes $\Omega = \{0, 1\}^n$. The distribution $p : \Omega \to [0, 1]$ of a *multivariate binary pairwise interaction model* has the form

$$p(x) \propto \exp(\sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij} x_i x_j)$$

with parameters $q_{ij} \in \mathbb{R}$, if the normalization condition

$$\sum_{x \in \Omega} p(x) = 1$$

is satisfied.

Remark. As we mentioned above, the parameter q_{ij} models the interaction between the variables x_i and x_j. Therefore, parameters with permuted index are equal. It is

$$q_{ij} = q_{ji}.$$

We presume a symmetric parameter space Θ.

Proposition 1.3. *For the interaction terms $q_i x_i$, $q_{ij} x_{ij}$ applies*

$$q_{ij} x_{ij} = \begin{cases} q_{ij} & , x_i = 1 \wedge x_j = 1 \\ 0 & , x_i = 0 \vee x_j = 0 \end{cases}$$

Before we proceed with model selection, in other words with fitting the parameters to data drawn from the respective model, we have a closer look at the normalization coefficient and the representation of the parameters.

The model distribution $p(x)$, as defined above, contains a normalization coefficient z to satisfy the normalization condition. The value of the normalization coefficient can be identified by rearranging the equation of the condition:

$$\begin{aligned} & \sum_{x\in\Omega} p(x) = 1 \\ \iff & \sum_{x\in\Omega} \frac{1}{z} \exp(\sum_{i=1}^{n} q_i x_i + \sum_{i=1}^{n}\sum_{j>i}^{n} q_{ij} x_{ij}) = 1 \\ \iff & z = \sum_{x\in\Omega} \exp(\sum_{i=1}^{n} q_i x_i + \sum_{i=1}^{n}\sum_{j>i}^{n} q_{ij} x_{ij}) \end{aligned}$$

Regarding the representation of the distribution of a multivariate binary pairwise interaction model, we would like to have a more intuitive, compact description of the parameter space Θ, therefore we write the parameters q_{ij}, in a matrix

$$Q = \{q_{ij}\}_{i,j=1,\dots,n}$$

and get

$$p(x) = \frac{1}{z} \exp(\sum_{i=1}^{n}\sum_{j=1}^{n} q_{ij} x_i x_j) = \frac{1}{z} \exp(\ x^{\mathsf{T}}\ Q\ x) =: p_Q(x)$$

Remark. We call Θ the parameter space and Q the matrix that contains the parameters. It is $\Theta = \{q_{11}, q_{12}, ..., q_{nn}\} = \{Q\}$. It is p_Q the distribution of the model with matrix Q that contains the parameters of the model.

After we introduced the general shape of a pairwise interaction binary model, we start to fit the parameters based on data which are distributed by a binary distribution p on Ω.

1.2.2 Pseudo-Log-Likelihood Function

We are given d data points $x^{(1)}, ..., x^{(d)}$ with each $x^{(i)} \in \{0,1\}, i = 1, ..., d$ and $\Omega = \{0,1\}^n$ that are independently drawn from a multivariate binary distribution p on Ω. To find the optimal choice of parameters, we minimize the negative likelihood function

$$\mathbf{p}_{ML} = \arg\min_{Q} -L(Q) = \arg\min_{Q} -\prod_{i=1}^{m} p_Q(x^{(i)}),$$

respectively minimizing the negative log-likelihood function

$$\mathbf{p}_{ML} = \arg\min_{Q} -\ell(Q) = \arg\min_{Q} -\sum_{i=1}^{m} \log p_Q(x^{(i)}).$$

Unfortunately, as far as we know, the minimization problem does not have an analytical solution, therefore we are going to use optimization algorithms to get a solution for the parameter estimation problem. Because the normalization factor is usually the sophisticated task for implementing a correctly working and high-performance optimization algorithm on categorical models, we are going to use the pseudo-likelihood function L_p instead. The pseudo-likelihood function is an approach to approximate the likelihood function, but with fewer complexity because the normalization constants are easier to track. We basically assume that

$$p_Q(x) = p_Q(x_1, ..., x_n) \approx p_Q(x_1|x_{-1}) \; ... \; p_Q(x_n|x_{-n}),$$

where

$$p_Q(x_r|x_{-r}) = p_Q(x_r|x_1, ..., x_{r-1}, x_{r+1}, ..., x_n) = \frac{\exp(2 \sum\limits_{j=1}^{n} q_{rj} x_r x_j - q_{rr} x_r x_r)}{1+\exp(q_{rr}+2 \sum\limits_{j=1, j\neq r}^{n} q_{rj} x_j)}.$$

Remark. We call the term $p_Q(x_r|x_{-r})$ the *node conditional* of the $r-th$ variable.

We get the maximum pseudo-likelihood parameter estimation with negative log-pseudo-likelihood function as follows:

$$\begin{aligned}
\mathbf{p}_{ML} &= \arg\min_Q -\ell(Q) \\
&\approx \arg\min_Q -\ell_p(Q) \\
&= \arg\min_Q -\sum_{i=1}^{d}\Big(\sum_{r=1}^{n} \log p_Q(x_r^{(i)}|x_{-r}^{(i)})\Big) \\
&= \arg\min_Q -\sum_{i=1}^{d}\Big(\sum_{r=1}^{n} \log\Big(\frac{\exp(2\sum\limits_{j=1}^{n} q_{rj} x_r^{(i)} x_j^{(i)} - q_{rr} x_r x_r)}{1+\exp(q_{rr}+2\sum\limits_{j=1, j\neq r}^{n} q_{rj} x_j^{(i)})}\Big)\Big) \\
&= \arg\min_Q -\sum_{i=1}^{d}\Big(\sum_{r=1}^{n}\Big(2\sum_{j=1}^{n} q_{rj} x_r^{(i)} x_j^{(i)} - q_{rr} x_r x_r\Big) \\
&\qquad\qquad - \log(1+\exp(q_{rr}+2\sum_{j=1, j\neq r}^{n} q_{rj} x_j^{(i)}))\Big)
\end{aligned}$$

Now, that we derived the optimization problem whose solution estimates the parameters Q, we will look at an example and try to fit a pairwise interaction model to binary data.

1.3 An Introductory Example

We are going to look at a concrete example where we apply a synthetic dataset to a multivariate binary pairwise interaction model by minimizing the negative log-pseudo-likelihood function. The generated dataset has three features $(X, Y, Z) \in \{0, 1\}^3$ and 10.000 entries. The frequency of the single occurrences can be seen in table 1.2:

(X, Y, Z)	(0,0,0)	(0,0,1)	(0,1,0)	(0,1,1)	(1,0,0)	(1,0,1)	(1,1,0)	(1,1,1)
#	983	2105	4172	1849	11	612	60	208

Table 1.2: Composition of the dataset with frequency of all occurrences.

If we used a categorical model with probability distribution p_c we would have one parameter for each occurrence and get its probability through maximum likelihood by

$$p_C(X, Y, Z) = \frac{\#(X, Y, Z)}{10.000}$$

We would have 8 different occurrences, so we would get 7 parameters.

Now, we fit the dataset to a multivariate binary pairwise interaction model. It has interaction order $K = 2$ and dimension $n = 3$. We minimize the negative log-pseudo-likelihood function

$$\arg\min_Q -\ell_p(Q)$$

and get for the the parameter space $\Theta = \{q_1, q_2, q_3, q_{12}, q_{13}, q_{23}\}$ the following result:

$$\Theta = \{-3.6605,\ 1.4626,\ 0.7821,\ -0.4238,\ 1.1982,\ -0.8032\}.$$

We computed the solution of the minimization problem with an optimization package that will be discussed in later chapters. The parameters space Θ can be written within a symmetric matrix

$$Q = \begin{pmatrix} -3.6605 & -0.4238 & 1.1982 \\ -0.4238 & 1.4626 & -0.8032 \\ 1.1982 & -0.8032 & 0.7821 \end{pmatrix}$$

which returns us the probability distribution p_Q of the multivariate binary pairwise interaction model as

$$p_Q(X, Y, Z) = \frac{1}{z}\ \exp(x^{\mathsf{T}} Q x)$$

with $x = (X, Y, Z)$ and normalization coefficient z. Now, we calculate the probability of each occurrence according to the model distribution p_Q to verify how close they are to the parameters of the p_c distribution:

(X, Y, Z)	(0,0,0)	(0,0,1)	(0,1,0)	(0,1,1)	(1,0,0)	(1,0,1)	(1,1,0)	(1,1,1)
p_C	0.0983	0.2105	0.4172	0.1849	0.0011	0.0612	0.0060	0.0208
p_Q	0.0969	0.2119	0.4185	0.1835	0.0025	0.0599	0.0046	0.0222

Table 1.3: Prediction according to the distribution p_C respectively p_Q for each possible occurrence in the dataset.

As we can see, we received acceptable results that are close to the real probabilities with one parameter less than in the categorical model. The idea is to save more and more parameters with increasing number of variables. Also, we will use further techniques like sparse and low-rank regularization in later chapters to find parameters which are expendable to describe the data. We can set them to zero and reduce the parameter space even more. Before, we will examine the model class for higher interaction orders.

Chapter 2

Binary Interaction Models of Order $K = 3$

In the following, we are going to extend the idea of pairwise interactions that we have seen in the previous chapter. Now, we are going to examine models of interaction order $K = 3$, where also interactions between three distinct variables can be specified.

2.1 Interaction Models of Order $K = 3$

Definition. Let $X = (X_1, ..., X_n)$ be a vector of random variables with the set of outcomes $\Omega = \{0, 1\}^n$. The distribution $p : \Omega \to [0, 1]$ of a *multivariate binary model of interaction order* $K = 3$ has the form

$$p(x) \propto \exp(\sum_{i,j,k}^{n} q_{ijk} x_i x_j x_k)$$

with parameters $Q = \{q_{ijk}\}_{i,j,k=1,...,n} \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n$, if the normalization condition

$$\sum_{x \in \Omega} p(x) = 1$$

is satisfied.

Remark. It stands $\sum_{i_1,...,i_K}^{n}$ for $\sum_{i_1=1}^{n} ... \sum_{i_K=1}^{n}$.

Remark. We call Q of the previous definition a *tensor* of order $K = 3$ of the multivariate binary model of interaction order $K = 3$. The dimension of the model and of the tensor is n and indicates the number of variables x_i.

As it was pointed out in the previous chapter, a parameter q_{ijk} describes the interaction between the variables x_i, x_i and x_k. Therefore, we consider parameters $q_{\sigma(i)\sigma(j)\sigma(k)}$ with permuted indexes as equal, because they describe the same interaction. It is

$$q_{ijk} = q_{ikj} = q_{jik} = q_{jki} = q_{kij} = q_{kji}.$$

It also follows, that the indexes of a parameter indicate the affected variables. Therefore, we are going to shorten the parameters q_{ijk} in a way that no index occurs more than once, because we only need to know if a variable x_i is affected by a parameter or not. We write

$$q_{iii} := q_i, \quad q_{iij} := q_{ij}.$$

For instance, when we regard a model of interaction order $K = 3$, the parameter q_{ij} stands for the parameters q_{iij} and q_{ijj} but we write it as one, because both describe the same interaction between variable x_i and x_j. Altogether it leads to a strong symmetry concept for the tensor Q, where also

$$q_{iij} = q_{iji} = q_{jii} = q_{ijj} = q_{jij} = q_{jji}.$$

If we only required normal symmetry (equality of permuted indexes), it would be

$$q_{iij} \neq q_{ijj}$$

because on the left there are two i which is not in the permutation group of a index with one i (on the right). But for shortened notation, where only one index of each is displayed, they are each other's permutation. Therefore, it is a stronger property. We call the tensor Q *strongly symmetric* which is presumed in the following sections.

Example. We consider a multivariate binary model of interaction order $K = 3$ and dimension $n = 3$. The associated tensor Q has $3^3 = 27$ parameters that are summarized in 7 distinct parameters, namely

$$q_1,\ q_2,\ q_3,\ q_{12},\ q_{13},\ q_{23},\ q_{123},$$

that describe the model.

2.2 Representation of the Node Conditional

As we proceeded in the first chapter, we are also going to look at the pseudo-likelihood function in order to estimate the parameters of the respective model. Therefore, we have to pick up on first the node conditional of the $r-th$ variable in the binary model of interaction order $K = 3$. The node conditional $p(x_r|x_{-r})$ describes slices that we cut out of the tensor Q for the $r-th$ variable. In other words, we are interested in all parameters that contain index r. When we regard strong symmetry of the associated tensor Q, it turns out that also in the node conditional some parameters have more than one occurrence. These occurrences can be counted, categorized into groups and summarized as one expression.

Example. We consider the tensor Q for $K = 3$ and $n = 3$. We derive the node conditional for $r = 1$. We list all parameters that contain index $r = 1$ and categorize them by using the shortened parameter notation and strong symmetry:

$$\begin{aligned}
6\ q_{123} &= q_{123} + q_{132} + q_{213} + q_{231} + q_{312} + q_{321} \\
6\ q_{12} &= q_{112} + q_{121} + q_{211} + q_{122} + q_{212} + q_{221} \\
6\ q_{13} &= q_{113} + q_{131} + q_{311} + q_{133} + q_{313} + q_{331} \\
q_1 &= q_{111}
\end{aligned}$$

For the node conditional (without normalization) we get

$$p(x_1|x_{-1}) \propto \exp(\ 6\ q_{123}x_1x_2x_3 + 6\ (q_{12}x_1x_2 + q_{13}x_1x_3) + q_1x_1).$$

Let us generalize the previous approach with the following lemma.

Lemma 2.1. *For the node conditional of the $r-th$ variable in a multivariate binary model of interaction order $K = 3$, we get*

$$p_Q(x_r|x_{-r}) \propto \exp(\ 6 \sum_{i<j, i\neq r, j\neq r}^{n} q_{rij}x_rx_ix_j + 6\sum_{i\neq r}^{n} q_{ri}x_rx_i + q_rx_r)$$

Proof. We are going to count the occurrences for each m partition of $K = 3$. To count the combinations for the first term $\sum q_{rij}x_rx_ix_j$, we are going to look at the $m = 3$ partition of $K = 3$. We only have one partition:

$$3 = 1 + 1 + 1$$

This means all parameters are different. We count the combinations that are represented by q_{rij}:

$$q_{rij} = q_{rji} = q_{irj} = q_{ijr} = q_{jri} = q_{jir}$$

We get $6 = 3!$ different combinations for the $m = 3$ partition of $K = 3$.

The next step is to count combinations for the second term $\sum q_{ri}x_rx_i$ of the $m = 2$ partition of $K = 3$. We get two partitions:

$$3 = 2 + 1 = 1 + 2$$

We count the combinations that are represented by the parameter q_{ri}:

$$q_{rri} = q_{rir} = q_{irr} = q_{rii} = q_{iri} = q_{iir}$$

We get $6 = 2 \cdot \binom{3}{2}$ different combinations.

For the last of the possible partitions, the $m = 1$ partition of $K = 3$, trivially we get only one combination q_{rrr} that is represented by q_r. □

Unfortunately, the formula we derived is difficult to use in terms of implementation. Because of its restrictions in the sums it would lay kind of skewed in the memory and therefore high-performance techniques as vectorization would become complicated to apply. But, we can also think of the node conditional $p(x_r|x_{-r})$ as slices that we cut out of n-dimensional tensor of order K at the $r - th$ position for the $r - th$ variable. That approach leads to an easier formula for the node conditional which we will introduce in the following proposition and lemma.

Remark. In all following sums, the index r is fixed, except it is explicitly told.

Proposition 2.2. *It is*

$$\sum_{i,j}^{n} q_{rij}x_r x_i x_j = 2\sum_{i<j,i\neq r,j\neq r}^{n} q_{rij}x_r x_i x_j + 3\sum_{i\neq r}^{n} q_{ri}x_r x_i + q_r x_r$$
$$\sum_{i}^{n} q_{ri}x_r x_i = \sum_{i\neq r}^{n} q_{ri}x_r x_i + q_r x_r$$

Remark. The findings of proposition 2.2 are simply a result of counting the occurrences of the single terms.

Lemma 2.3. *The node conditional of the $r-th$ variable in a multivariate binary model of interaction order $K=3$ can also be represented as*

$$p_Q(x_r|x_{-r}) \propto \exp(\ 3\sum_{i,j}^{n} q_{rij}x_r x_i x_j - 3\sum_{i}^{n} q_{ri}x_r x_i + q_r x_r).$$

Proof. We will show this by using the terms from proposition 2.2. We rearrange the equations

$$\sum_{i<j,i\neq r,j\neq r}^{n} q_{rij}x_r x_i x_j = \frac{1}{2}\sum_{i,j}^{n} q_{rij}x_r x_i x_j - \frac{3}{2}\sum_{i\neq r}^{n} q_{ri}x_r x_i - \frac{1}{2}q_r x_r$$
$$\sum_{i\neq r}^{n} q_{ri}x_r x_i = \sum_{i}^{n} q_{ri}x_r x_i - q_r x_r$$

and use them for the node conditional:

$$\begin{aligned} p_Q(x_r|x_{-r}) &\propto \exp(\ 6\sum_{i<j,i\neq r,j\neq r}^{n} q_{rij}x_r x_i x_j + 6\sum_{i\neq r}^{n} q_{ri}x_r x_i + q_r x_r) \\ &= \exp(\ 3\sum_{i,j}^{n} q_{rij}x_r x_i x_j - 3\sum_{i\neq r}^{n} q_{ri}x_r x_i - 2q_r x_r) \\ &= \exp(\ 3\sum_{i,j}^{n} q_{rij}x_r x_i x_j - 3\sum_{i}^{n} q_{ri}x_r x_i + q_r rr) \end{aligned}$$

□

To illustrate the previous proof, we are going to look at a example for $n=4$.

Example. Let $n=4$ and $K=3$. We would like to cut out the node conditional for the $r-th$ variable for $r=2$. We have the tensor Q and want to extract all parameters $q_{rij}, i,j=1,...,4$, that contain the index $r=2$. It is illustrated in Figure 2.1 and Figure 2.2.

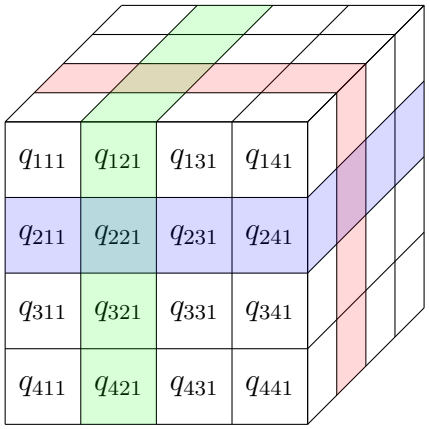


Figure 2.1: A 4-dimensional tensor of order $K = 3$ with marked node conditionals for $r = 2$.

After we cut out the slices that all include index $r = 2$ (first sum in the formula), we notice that we get too many of some parameters. As we can see in Figure 2.2, the rows $q_{22i} = q_{2i}$, $q_{2i2} = q_{2i}$ and $q_{i22} = q_{2i}, i = 1, 2, 3, 4$ appear twice, that makes

$$2q_{22i} + 2q_{2i2} + 2q_{i22} = 6q_{2i},\ i = 1, 2, 3, 4$$

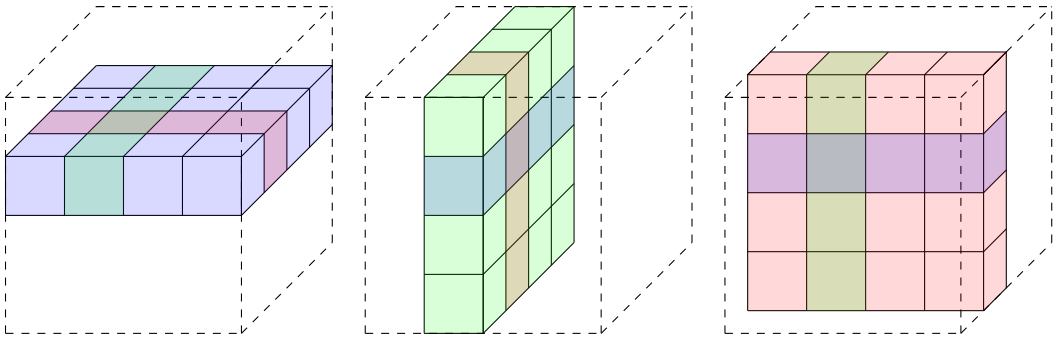
even though we need each of them only once. Therefore, we have to subtract them three times (second summand in the formula). That makes

$$2q_{22i} + 2q_{2i2} + 2q_{i22} - q_{22i} - q_{2i2} - q_{i22} = 6q_{2i} - 3q_{2i},\ i = 1, 2, 3, 4$$

and we get

$$q_{22i} + q_{2i2} + q_{i22} = 3q_{2i},\ i = 1, 2, 3, 4$$

which is the correct number of occurrences of q_{2i}. But then, we subtracted the remaining summand q_{222} one time too much, therefore we add it another time (third summand in the formula). That procedure reminds us on the inclusion exclusion principle in combinatorics which generalizes the familiar method of obtaining the number of elements in the union of finite sets. It is clarified by Figure 2.3.



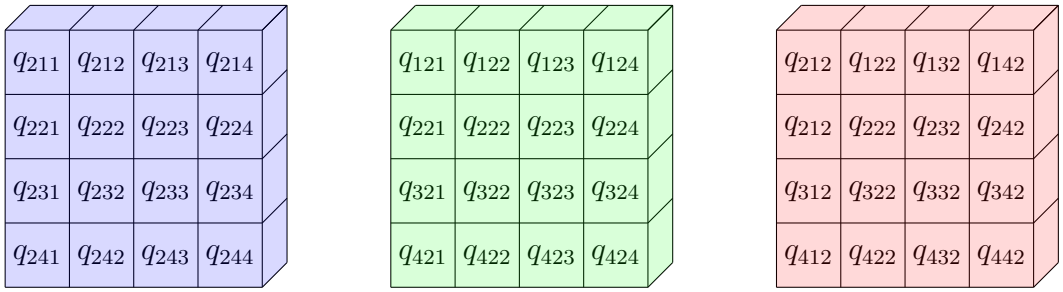


Figure 2.2: Slices that we cut out of the tensor Q that contain index $r = 2$.

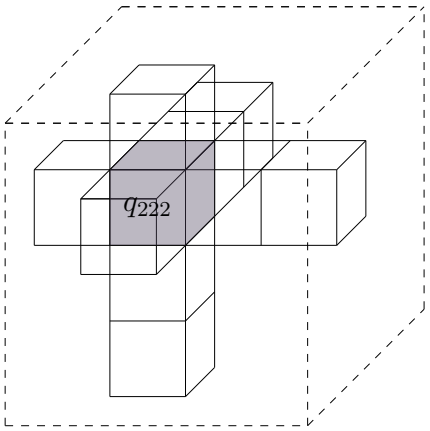


Figure 2.3: Illustration of the parameters that appear more than once when we cut out the slices for the node conditional for $r = 2$.

Remark. In the change of representation of the node conditional $p_Q(x_r|x_{-r})$ we went from picking out the single parameters from the tensor Q to using an alternating sum of tensors whose order is getting lower.

2.3 Unregularized Optimization Problem

After we formulated the node conditional for multivariate binary models of interaction order $K = 3$, we can do the next step and derive the pseudo-likelihood function to fit the parameter space $\Theta = \{Q\}$ to data. Before, we define various notations that will be used in the following.

Definition. Let $Q = \{q_{i_1 \dots i_K}\}_{i_1,\dots,i_K=1,\dots,n} \in \underbrace{\mathbb{R}^n \times \dots \times \mathbb{R}^n}_{K-times}$ be a tensor of order K. Then, we define the *K-times tensor-vector multiplication* of Q and an arbitrary vector $x \in \mathbb{R}^n$ as

$$Q[x]^K = Q[\underbrace{x, x, \dots, x}_{K-times}] := \sum_{i_1,\dots,i_K}^{n} q_{i_1,\dots,i_K} x_{i_1} \dots x_{i_K}.$$

Definition. Let $Q = \{q_{i_1 \dots i_K}\}_{i_1,\dots,i_K=1,\dots,n} \in \underbrace{\mathbb{R}^n \times \dots \times \mathbb{R}^n}_{K-times}$ be a tensor of order K. Then, we call

$$Q_{m,r}, \quad m \in \{1, \dots, K\}, r \in \{1, \dots, n\}$$

the *m-th subtensor* of Q with order $K - m$ and fixed index r. It is

$$Q_{K,r} = q_{\underbrace{r \dots r}_{K-times}} = q_r.$$

Example. Let $Q \in \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n$ be a tensor of order $K = 3$ and $x \in \mathbb{R}^n$. Then, it is

$$Q[x]^3 = Q[x, x, x] = \sum_{i,j,k}^{n} q_{ijk}\ x_i x_j x_k.$$

and

$$Q_{1,r}[x]^2 = Q_{1,r}[x, x] = \sum_{i,j}^{n} q_{rij}\ x_r x_i x_j = x^\mathsf{T} Q_{1,r}\ x$$

the first subtensor of Q of index r.

Remark. In figure 2.2, the first subtensor for $r = 2$, $Q_{1,2}$, of the respective tensor Q is displayed and is equal to the slices we cutted out of the tensor. Because of the strong symmetry of Q, all possible subtensors $Q_{m,r}$ for fixed m and r (three in figure 2.2) are equal.

Now, we can write the derived node conditional of lemma 2.3 for a multivariate binary model of interaction order $K = 3$ as

$$\begin{aligned} p_Q(x_r|x_{-r}) &= \frac{\exp(\ 3\sum_{i,j}^{n} q_{rij}x_r x_i x_j - 3\sum_{i}^{n} q_{ri}x_r x_i + q_r x_r)}{1 + \exp(\ 3\sum_{i,j}^{n} q_{rij}x_i x_j - 3\sum_{i}^{n} q_{ri}x_i + q_r)} \\ &= \frac{\exp(\ 3\ Q_{1,r}[x]^2 - 3\ Q_{2,r}[x] + Q_{3,r}x_r)}{1 + \exp(\ 3\ Q_{1,r}[x|_{x_r=1}]^2 - 3\ Q_{2,r}[x|_{x_r=1}] + q_r)}. \end{aligned}$$

Again, are given d data points $x^{(1)}, \dots, x^{(d)}$ with each $x^{(i)} \in \{0, 1\}, i = 1, \dots, d$ and $\Omega = \{0, 1\}^n$ that are independently drawn from a multivariate binary distribution p on Ω. We start with the maximum likelihood approach and end up in minimizing the negative log-pseudo-likelihood function ℓ_p. We formulate the optimization problem:

$$\begin{aligned} \mathbf{p}_{ML} &= \arg\max_{Q}\ L(Q) \\ &\approx \arg\min_{Q} -\ell_p(Q) \\ &= \arg\min_{Q} -\sum_{i=1}^{d}\sum_{r=1}^{n} \log p_Q(x_r^{(i)}|x_{-r}^{(i)}) \\ &= \arg\min_{Q} -\sum_{i=1}^{d}\sum_{r=1}^{n} \frac{3\ Q_{1,r}[x^{(i)}]^2 - 3\ Q_{2,r}[x^{(i)}] + Q_{3,r}x_r^{(i)}}{\log(1 + \exp(\ 3\ Q_{1,r}[x^{(i)}|_{x_r=1}]^2 - 3\ Q_{2,r}[x^{(i)}|_{x_r=1}] + q_r))} \end{aligned}$$

The entire, formulated optimization problem can be implemented and fits a multivariate binary model of interaction order $K = 3$. As we can see, it is getting complex and also the space of parameters is growing, but stays below the complexity of an entire binary model. In the next chapter, we want to generalize the approach for arbitrary interaction orders.

Chapter 3

Binary Interaction Models of Higher Orders

Now, we move on to generalize the approaches we discussed in the previous chapters. We assume an arbitrary interaction order $1 < K \leq n$, define the corresponding multivariate binary interaction model and derive the node conditional that mainly depends on K. To estimate the parameter within the tensor Q of order K, we also will formulate the optimization problem in the end.

3.1 Interaction Models of Order K

Definition. Let $X = (X_1, ..., X_n)$ be a vector of random variables with the set of outcomes $\Omega = \{0, 1\}^n$. The distribution $p : \Omega \to [0, 1]$ of a *multivariate binary model of interaction order* K has the form

$$p(x) \propto \exp(\sum_{i_1,...,i_K}^{n} q_{i_1...i_K}\, x_{i_1} ... \, x_{i_K}\,) = \exp(\, Q[x]^K\,)$$

with parameters $Q = \{q_{i_1...i_K}\}_{i_1,...,i_K=1,...,n} \in \underbrace{\mathbb{R}^n \times ... \times \mathbb{R}^n}_{K-times}$, if the normalization condition

$$\sum_{x \in \Omega} p(x) = 1$$

is satisfied.

Definition. We formally define the shortened parameter representation of a parameter of a multivariate binary model of interaction order K as

$$q_{i_1,i_2,...,i_m} := q_{\underbrace{i_1, ..., i_1, i_2, ..., i_2, ..., i_m, ..., i_m}_{\#\,K}}$$

where each index appears only once and actually stands for all a m-partitions of K. That means, the absolute number of indexes is K.

Example. Let Q be a tensor of order $K = 5$. Then, the shortened parameter q_{1234} stands for

$$q_{11234} = q_{12234} = q_{12334} = q_{12344}$$

which are necessarily equal.

Definition. Let Q be a tensor of order K. Then, we call Q *symmetric* when

$$q_{i_1,...,i_K} = q_{\sigma(i_1),...,\sigma(i_K)}$$

for all permutations σ of the set $\{i_1, ..., i_K\}$. That means all entries in Q with permuted indexes are equal. Furthermore, we call Q *strongly symmetric* when

$$q_{i_1,...,i_m} = q_{\sigma(i_1),...,\sigma(i_m)}$$

for all $m \in \{1, ..., K\}$ for all permutations σ of the set $\{i_1, ..., i_m\}$. That means all entries in Q with permuted indexes are equal for all shortened parameters.

Hence, in some way normal symmetry and the shortened parameter representation induce strong symmetry of a tensor. As in the previous chapter, we use the shorten parameter notation and we presume strong symmetry of the tensor Q.

3.2 Node Conditional

Before we get to the general node conditional, we define two different ways to represent them. It follows the findings from the previous chapter where we already defined them for interaction order $K = 3$. Now, we are going to generalize this approach.

Definition. Let p_Q be the distribution of a multivariate binary model of interaction order K with strongly symmetric tensor Q. We call

$$p_Q(x_r|x_{-r}) \propto \exp(\sum_{m=1}^{K} \tau_{K,m} \sum_{i_1<...<i_m,\, \forall i_l : i_l \neq r}^{n} q_{r i_1 ... i_m}\, x_r x_{i_1} ... \, x_{i_m})$$

the *standard representation* for the $r - th$ node conditional with integer coefficients $\tau_{K,m}, m = 1, ..., K$.

Definition. Let p_Q be the distribution of a multivariate binary model of interaction order K with strongly symmetric tensor Q. We call

$$p_Q(x_r|x_{-r}) \propto \exp(\sum_{m=1}^{K} \pi_{K,m} \sum_{i_1,...,i_m}^{n} q_{r i_1 ... i_m}\, x_r x_{i_1} ... \, x_{i_m})$$

the *slice representation* for the $r - th$ node conditional with integer coefficients $\pi_{K,m}, m = 1, ..., K$.

Remark. The difference between these two types of representation and their coefficients $\tau_{K,m}$ and $\pi_{K,m}$ lays in the second sum. In contrast to the slice representation we do not have the same index in a single summand twice in the standard representation.

The coefficients $\tau_{K,m}, \pi_{K,m}$ in the previous definitions are the result of counting occurrences of differently categorized parameters, which needs to be done for each K. In the following, we are going to analyze systematically the behavior of these coefficients and try to find a generalized expression to calculate them for each K and m. We will follow a similar strategy as we did it in the chapter before for interaction order $K = 3$.

3.2.1 Standard Representation

At first, we are going to analyze the coefficients $\tau_{K,m}$ of the standard representation. When we consider our observations from the previous chapter and take a closer look at the proof of lemma 2.1, we recognize that the coefficients $\tau_{K,m}$ correspond with the m partitions of K.

Definition. Let

$$P_{K,m} := \{(k_1, ..., k_m) \mid K = k_1 + ... + k_m,\ k_1 \geq k_2 \geq ... \geq k_m \geq 1,\ k_i \in \mathbb{N}\}$$

be the set of all m partitions of K.

Definition. Let $(k_1, ..., k_m) \in P_{K,m}$ be a m partition of K. Then we define the *counting vector* for a partition $(k_1, ..., k_m)$ as

$$a_{(k_1,...,k_m)} := (a_1, ..., a_K),\ a_i \text{ is the number of occurrences of } i \in (k_1, ..., k_m),$$

that represents the occurrences of each integer in $(k_1, ..., k_m)$.

Proposition 3.1. *It is*

$$\sum_{i=1}^{K} a_i = m$$

for a counting vector $a_{(k_1,...,k_m)}$ of a m partition of K.

Example. Let us consider the 3 partitions of 6. They are summarized in the set

$$P_{6,3} = \{(4, 1, 1),\ (3, 2, 1),\ (2, 2, 2)\}$$

and its elements have the counting vectors

$$a_{(4,1,1)} = (2, 0, 0, 1, 0, 0),\ a_{(3,2,1)} = (1, 1, 1, 0, 0, 0),\ a_{(2,2,2)} = (0, 3, 0, 0, 0, 0).$$

Before we get to the lemma where we will count the number of permutations of indexes for each m partition of K, we will look at an example to understand how we are going to count and categorize them. The proof afterwards follows the same principle.

Example. Let $K = 5$ and $m = 3$. We count all permutations of indexes for the partitions in $P_{5,3} = \{(3,1,1),\ (2,2,1)\}$. Let us first look at $5 = 3 + 1 + 1$. We get 20 elements that are:

$$rrrij,\ rrijr,\ rijrr,\ ijrrr,\ rrirj,\ rirjr,\ irjrr,\ rirrj,\ irrjr,\ irrrj$$

$$rrrji,\ rrjir,\ rjirr,\ jirrr,\ rrjri,\ rjrir,\ jrirr,\ rjrri,\ jrrir,\ jrrri$$

This is the case because we first choose three r's from five, then we choose one i from two and then one j from one:

$$\tbinom{5}{3} \cdot \tbinom{2}{1} \cdot \tbinom{1}{1} = 10 \cdot 2 \cdot 1 = 20$$

This correspondents with the *multinomial coefficient*:

$$\tbinom{5}{3,1,1} = \tfrac{5!}{3!1!1!} = \tbinom{5}{3} \cdot \tbinom{2}{1} \cdot \tbinom{1}{1}$$

However, we also need to consider that each index is different. That means we also count the cases where i occurs three times and j three times. That multiplicities can be expressed with the multinomial coefficient of the counting vector

$$a_{(3,1,1)} = (2,0,1,0,0),$$

that can be considered as a 2 partition of 3 with $3 = 2+1$. Its multinomial coefficient would be:

$$\tbinom{3}{2,1} = \tfrac{3!}{2!1!} = 3$$

Finally, we get the number of permutations of indexes for the partition $(3,1,1)$ as a product of the multinomial coefficient of the partition and the multinomial coefficient of its the counting vector:

$$\tbinom{5}{3,1,1} \cdot \tbinom{3}{2,1} = 20 \cdot 3 = 60$$

The same can be done with the other partition $(2,2,1) \in P_{5,3}$. Together with its counting vector $a_{2,2,1} = (1,2,0,0,0)$, we get

$$\tbinom{5}{2,2,1} \cdot \tbinom{3}{2,1} = \tfrac{5!}{2!2!1!} \cdot \tfrac{3!}{2!1!} = 30 \cdot 3 = 90$$

permutations of the indexes. Overall, for the set $P_{5,3}$, we get

$$\tbinom{5}{3,1,1} \cdot \tbinom{3}{2,1} + \tbinom{5}{2,2,1} \cdot \tbinom{3}{2,1} = 60 + 90 = 150$$

permutations of indexes.

Lemma 3.2. *Let $K \in \mathbb{N}$ be arbitrary and $m \in \{1,...,K\}$. Let $P_{K,m}$ be the set of all m partitions of K and $\tau_{K,m}$ the coefficients of the standard representation of the $r-th$ node conditional. Then*

$$\tau_{K,m} = \sum_{(k_1,...,k_m) \in P_{K,m}} \tbinom{K}{k_1,...,k_m} \tbinom{m}{a_1,...,a_K}$$

where $a_{(k_1,...,k_m)} = (a_1,...,a_K)$ is the corresponding counting vector of $(k_1,...,k_m)$.

Proof. Let $(k_1, ..., k_m)$ be a m partition of K and $a_{(k_1,...,k_m)} = (a_1, ..., a_K)$ its corresponding counting vector. To count the permutations of

$$K = k_1 + ... + k_m$$

without regarding the order, we need to calculate:

$$\binom{K}{k_1} \cdot \binom{K-k_1}{k_1} \cdot ... \cdot \binom{K-k_1-...-k_{m-1}}{k_m} = \frac{K!}{k_1! \, ... \, k_m!} = \binom{K}{k_1,...,k_m}.$$

However we have different indexes, therefore we have to regard the order of the partition as well. For instance for $k_1 \neq k_2$, the permutations of indexes of $(k_1, k_2..., k_m)$ and $(k_2, k_1, ..., k_m)$ must be counted individually. For counting the permutations, we use the counting vector that displays the multiplicities of the single k_i. Because it is $\sum_{i=1}^{K} a_i = m$, the non zero elements of the counting vector can be seen as a partition of m. Therefore we get the multinomial coefficient to count the permutations in the initial permutation $(k_1, ..., k_m)$:

$$\binom{m}{a_1,...,a_K}$$

Together we get the number of the permutations of the indexes of a m partition of K as a product of

$$\binom{K}{k_1,...,k_m} \cdot \binom{m}{a_1,...,a_K}.$$

This needs to be done for all m permutations of K. □

The proofs shows us how the single permutation of indexes must be counted and gives us the remaining formula. When we compute the coefficients $\tau_{K,m}$, it generates a triangle that can be seen in figure 3.1.

K							
1				1			
2			1		2		
3		1		6		6	
4	1		14		36		24
5		1		30		150		240		120
6		1		62		540		1560		1800		720
7	1		126		1806		8400		16800		15120		5040

Figure 3.1: Coefficients $\tau_{K,m}$ for $K = 1, ..., 7$, in the K-th row and m-th position

Proposition 3.3. *For a fixed K ($K-th$ row of the triangle in figure 3.1), the coefficients $\tau_{K,m}$ can also be used to calculate potencies with any basis n as a sum of binomial coefficients:*

$$n^K = \sum_{i=1}^{K} \tau_{K,i} \cdot \binom{n}{i}$$

Proposition 3.4. *The coefficients $\tau_{K,m}$ can also be calculated recursively with*

$$\tau_{K,m} = (\tau_{K-1,m-1} + \tau_{K-1,m}) \cdot m$$

whereby it is $\tau_{K,K} = K!$ and $\tau_{K,1} = 1$.

Remark. The results of propositions 3.3 and 3.4 are solutions of general combinatorial problems that are described in QUELLE (wikipedia: pascalsches dreieck)

Remark. The term in proposition 3.3 also expresses the number of parameters in a n-dimensional tensor of order K and its distribution of the single multiplicities.

Example. Let $K = 4$ and $n = 6$. The parameters of a 6-dimensional tensor of order 4 are distributed as follows:

$$\begin{aligned} 6^4 &= 1 \cdot \binom{6}{1} + 14 \cdot \binom{6}{2} + 36 \cdot \binom{6}{3} + 24 \cdot \binom{6}{4} \\ &= 1 \cdot 6 + 14 \cdot 15 + 36 \cdot 20 + 24 \cdot 15 \\ &= 6 + 210 + 720 + 360 \\ &= 1296 \end{aligned}$$

Thereby we can recognize that there are 6 parameters with one index, 210 parameters with two different indexes, 720 parameters with three different indexes, 360 parameters with four different indexes and all together 1296 indexes.

3.2.2 Slice Representation

After we introduced the standard representation and calculated their coefficients $\tau_{K,m}$, we get to the second type of representation and derive the coefficients $\pi_{K,m}$ for the slice representation. As it was pointed out before, the slice representation is mainly used for a highly efficient implementation, because the occurring entire sums are simply tensor-vector products. To attain the transition between the two representations, we have to express tensor-vector product of the $m - th$ subtensor of Q of order K and the vector x

$$Q_{m,r}[x]^{K-m} = \sum_{i_1,\dots,i_{K-m}}^{n} q_{ri_1\dots i_{K-m}} x_r x_{i_1} \dots x_{i_{K-m}}, \; m \in \{1, \dots, K\}$$

as a term of sums from the standard representation. As we indicated the terms for $K = 2$ and $K = 3$ in proposition 2.2, we will do it for higher $K's$ as well. Again, it is simply a matter of counting the different types of parameters and assign them to the correct group. Before we formulate the transition from both representations for arbitrary K's, we look at an example.

Example. Let $K = 3$, $n = 4$, $r = 1$ and Q be the tensor of order K of the respective model. Then, the tensor-vector product of the first subtensor of Q can be expressed

as

$$\begin{aligned}
Q_{1,1}[x]^2 &= \sum_{i,j}^{4} q_{1ij} x_1 x_i x_j \\
&= q_{111}x_1x_1x_1 + q_{112}x_1x_1x_2 + q_{113}x_1x_1x_3 + q_{114}x_1x_1x_4 + q_{121}x_1x_2x_1 \\
&\quad + q_{122}x_1x_2x_2 + q_{123}x_1x_2x_3 + q_{124}x_1x_2x_4 + q_{131}x_1x_3x_1 + q_{132}x_1x_3x_2 \\
&\quad + q_{133}x_1x_3x_3 + q_{134}x_1x_3x_4 + q_{141}x_1x_4x_1 + q_{142}x_1x_4x_2 + q_{143}x_1x_4x_3 \\
&\quad + q_{144}x_1x_4x_4 \\
&= q_1x_1 + 3q_{12}x_1x_2 + 3q_{13}x_1x_3 + 3q_{14}x_1x_4 + 2q_{123}x_1x_2x_3 \\
&\quad + 2q_{124}x_1x_2x_4 + 2q_{134}x_1x_3x_4 \\
&= q_1x_1 + 3\sum_{i\neq 1}^{4} q_{1i}x_1x_i + 2\sum_{i<j,\, i,j\neq 1}^{4} q_{1ij}x_1x_ix_j.
\end{aligned}$$

For the tensor-vector product of the second subtensor of Q, we get

$$\begin{aligned}
Q_{2,1}[x] &= \sum_{i}^{4} q_{11i}x_1x_1x_i \\
&= q_{111}x_1x_1x_1 + q_{112}x_1x_1x_2 + q_{113}x_1x_1x_3 + q_{114}x_1x_1x_4 \\
&= q_1x_1 + \sum_{i\neq 1}^{4} q_{1i}x_1x_i.
\end{aligned}$$

For the tensor-vector product of the third subtensor of Q, we get

$$Q_{3,1}x = q_1x_1.$$

Now, we generalize the approach in the following proposition.

Proposition 3.5. *Let $K \in \mathbb{N}$, $m \in \{1, ..., K\}$ and Q a tensor of order K. Then, the tensor-vector product of the $m-th$ subtensor of Q can be expressed as*

$$Q_{m,r}[x]^{K-m} = \psi_{K-m+1,\,1}\; q_1x_1 + \sum_{j=1}^{K-m} \psi_{K-m+1,\,j+1} \sum_{i_1<\ldots<i_j,\,\forall i_l : i_l\neq r}^{n} q_{ri_1\ldots i_j}x_r x_{i_1}\ldots x_{i_j}$$

with coefficients $\psi_{K,m} \in \mathbb{N}$ and it is $\psi_{K,1} = 1$ for all $K \in \mathbb{N}$.

We always assume a determined tensor Q with fixed order K. From there, we get the coefficients $\psi_{K,m}$ for $m \in \{1, ..., K\}$ for the tensor-vector product of the first subtensor of Q, the coefficients $\psi_{K-1,m}$ for $m \in \{1, ..., K-1\}$ for the tensor-vector product of the second subtensor of Q until the coefficient $\psi_{1,1}$ for the tensor-vector product of the $K-th$ subtensor of Q.

Remark. In the example above, we already got $\psi_{3,1} = 1$, $\psi_{3,2} = 3$, $\psi_{3,3} = 2$ in the first equation, $\psi_{2,1} = 1$, $\psi_{2,2} = 1$ in the second equation and $\psi_{1,1} = 1$ in the last equation.

Lemma 3.6. *Let $K \in \mathbb{N}$ and $m \in \{1, ..., K\}$. Let $P_{K,m}$ be the set of all m partitions of K and $\psi_{K,m}$ the coefficients for the representation of the $m-th$ subtensor of Q. Then*

$$\psi_{K,m} = \frac{1}{m} \sum_{(k_1,...,k_m) \in P_{K,m}} \binom{K}{k_1,...,k_m} \binom{m}{a_1,...,a_K} = \frac{\tau_{K,m}}{m}$$

where the $\tau_{K,m}$'s stand for the coefficients of the standard representation of the $r-th$ node conditional and $a_{(k_1,...,k_m)} = (a_1, ..., a_K)$ is the corresponding counting vector of $(k_1, ..., k_m) \in P_{K,m}$.

Proof. TODO □

Proposition 3.7. *The coefficients $\psi_{K,m}$ can also be calculated recursively with*

$$\psi_{K,m} = (\ (m-1)\ \psi_{K-1,m-1} + m\ \psi_{K-1,m}\ )$$

whereby it is $\psi_{K,K} = K!$ and $\psi_{K,1} = 1$.

K							
1					1		
2				1		1	
3			1		3		2
4		1		7		12	6
5	1		15		50	60	24
6		1	32	180	390	360	120
7	1	63	602	2100	3360	2520	720

Figure 3.2: Coefficients $\psi_{K,m}$ for $K = 1, ..., 7$, in the K-th row and m-th position

Proposition 3.8. *For a fixed K ($K-th$ row of the triangle in figure 3.2), the coefficients $\psi_{K,m}$ can also be used to calculate potencies with any basis n as a sum of binomial coefficients:*

$$n^{K-1} = \sum_{i=1}^{K} \psi_{K,i} \cdot \binom{n}{i-1}$$

Remark. The results from propositions 3.7 and 3.8 follow directly from the corresponding propositions about the coefficients $\tau_{K,m}$ in the previous section.

After calculating the coefficients $\psi_{K,m}$, we are going to examine the coefficients $\pi_{K,m}$. As we did it in section 2.2, we are going from the standard representation of the node conditional to the slice representation. The triangle in figure 3.2 will support us. First, we will look at an example.

Example. Let $K = 4$ and $n > K$ be arbitrary. We get the term of the standard representation for the $r - th$ node conditional from the triangle in figure 3.1 as follows:

$$24 \sum_{i<j<k,\, i,j,k\neq r}^{n} q_{rijk} x_r x_i x_j x_k + 36 \sum_{i<j,\, i,j\neq r}^{n} q_{rij} x_r x_i x_j + 14 \sum_{i\neq r}^{n} q_{ri} x_r x_i + q_r x_r$$

Now, we can derive the coefficients $\pi_{K,m}$ from the coefficients $\tau_{K,m}$ with the help of the coefficients $\psi_{K,m}$ in the triangle in figure 3.2:

$$\begin{aligned}
&= 4 \sum_{i,j,k}^{n} q_{rijk} x_r x_i x_j x_k - 12 \sum_{i<j,\, i,j\neq r}^{n} q_{rij} x_r x_i x_j - 14 \sum_{i\neq r}^{n} q_{ri} x_r x_i - 3\, q_r x_r \\
&= 4 \sum_{i,j,k}^{n} q_{rijk} x_r x_i x_j x_k - 6 \sum_{i,j}^{n} q_{rij} x_r x_i x_j + 4 \sum_{i\neq r}^{n} q_{ri} x_r x_i + 3\, q_r x_r \\
&= 4 \sum_{i,j,k}^{n} q_{rijk} x_r x_i x_j x_k - 6 \sum_{i,j}^{n} q_{rij} x_r x_i x_j + 4 \sum_{i}^{n} q_{ri} x_r x_i - q_r x_r
\end{aligned}$$

We get the slice representation of the $r - th$ node conditional for $K = 4$:

$$p_Q(x_r|x_{-r}) \propto \exp(\, 4 \sum_{i,j,k}^{n} q_{rijk} x_r x_i x_j x_k - 6 \sum_{i,j}^{n} q_{rij} x_r x_i x_j + 4 \sum_{i}^{n} q_{ri} x_r x_i - q_r x_r)$$

$$= \exp(4\, Q_{1,r}[x,x,x] - 6\, Q_{2,r}[x,x] + 4\, Q_{3,r}[x] - Q_{4,3} x_r)$$

Lemma 3.9. *Let $K \in \mathbb{N}$ be arbitrary and $m \in \{1, ..., m\}$. Let $\pi_{K,m}$ be the coefficients of the slice representation of the $r - th$ node conditional of a multivariate binary model of interaction order K, then*

$$\pi_{K,m} = (-1)^{K-m} \binom{K}{m-1}$$

Proof. TODO □

Remark. The coefficients $\pi_{K,m}$ correspond with the values of the pascal's triangle.

K							
1				1			
2			-1		2		
3		1		-3		3	
4	-1		4		-6		4
5		1		-5		10		-10		5
6		-1		6		-15		20		-15		6
7	1		-7		21		-35		35		-21		7

Figure 3.3: Coefficients $\pi_{K,m}$ for $K = 1, ..., 7$, in the K-th row and m-th position

3.3 Unregularized Optimization Problem

After we derived the coefficients $\pi_{K,m}$ for the slice representation, we can formulate the node conditional with normalization for a generalized multivariate binary model of interaction order K:

$$p_Q(x_r|x_{-r}) = \frac{\exp(\sum_{m=1}^{K} \pi_{K,m}\, Q_{m,r}[x]^{K-m})}{1 + \exp(\sum_{m=1}^{K} \pi_{K,m}\, Q_{m,r}[x|_{x_r=1}]^{K-m})}$$

We are given d data points $x^{(1)}, ..., x^{(d)}$ with each $x^{(i)} \in \{0,1\}, i = 1, ..., d$ and $\Omega = \{0,1\}^n$ that are independently drawn from a multivariate binary distribution p on Ω. We start with the maximum likelihood approach and end up in minimizing the negative log-pseudo-likelihood function ℓ_p. We formulate the optimization problem:

$$\begin{aligned}
\mathbf{p}_{ML} &= \arg\max_Q \; L(Q) \\
&\approx \arg\min_Q -\ell_p(Q) \\
&= \arg\min_Q -\sum_{i=1}^{d}\sum_{r=1}^{n} \log p_Q(x_r^{(i)}|x_{-r}^{(i)}) \\
&= \arg\min_Q -\sum_{i=1}^{d}\sum_{r=1}^{n} \frac{\sum_{m=1}^{K} \pi_{K,m}\, Q_{m,r}[x^{(i)}]^{K-m}}{\log(1 + \exp(\sum_{m=1}^{K} \pi_{K,m}\, Q_{m,r}[x^{(i)}|_{x_r=1}]^{K-m}))}
\end{aligned}$$

Chapter 4

Regularization Techniques

Chapter 5

Implementation Details

Chapter 6

Experiments

Chapter 7

Conclusion