

# Using Qualitative Correlations as Evidence of Uncertain Reasoning

**Qi Zhao**

Department of Computing Science  
University of Alberta  
Edmonton, Alberta, Canada T6G 2H1  
qizhao@cs.ualberta.ca

**Toyoaki Nishida**

Graduate School of Information Science  
Nara Institute of Science and Technology  
8916-5, Takayama, Ikoma, Nara 630-01, Japan  
nishida@is.aist-nara.ac.jp

## Abstract

A novel method for extracting, representing and propagating qualitative correlations among hypotheses as confirmatory or disconfirmatory evidence of uncertain reasoning is presented. First, two new concepts, qualitative correlations among hypotheses and qualitative correlation propagation, are introduced. Then, an algorithm for extracting and representing qualitative correlations among hypotheses and an algorithm for propagating qualitative correlations and updating possibilities of hypotheses are proposed. The advantages of the method include: (1) it can be applied to the problems where evidence is not explicitly or completely given; (2) few numbers and assumptions need to be provided by domain experts in advance; and consequently, (3) the knowledge acquisition is simple, and the inconsistency in knowledge bases can be avoided. The method has been applied to a practical system for infrared spectrum interpretation. The experimental results show that it is significantly better than other methods used in similar systems.

## Introduction

Bayesian inference has been proved to be effective for reasoning under uncertainty, and has been used in many AI systems (Dempster 1968, Kleiter 1992). However, the problems of using Bayesian inference are: (1) evidence must be explicitly provided, and the relation between evidence and hypothesis must be explicitly provided too. Unfortunately, in many cases, evidence and the relation between evidence and hypothesis are not always available. In addition, after evidence has been considered and hypotheses have been made, it is still possible to refine the hypotheses by using other knowledge and information; (2) Bayesian inference requires many statistical numbers in advance. Unfortunately, in many practical problems, it is impossible to have all numbers provided beforehand. Although subjective Bayesian methods provide a practical framework for using subjective statements or assumptions to take the place of statistical data when they are insuf-

ficient or absent, the problems still remain since subjective statements are not always available and the inconsistency in knowledge bases is hard to avoid (Duda et al. 1976).

A novel method for uncertain reasoning is presented in this paper. The method automatically extracts, represents and propagates qualitative correlations among hypotheses as confirmatory or disconfirmatory evidence to update the possibilities of the hypotheses. The function of propagating qualitative correlations and updating possibilities of hypotheses in the proposed method is similar to the function of propagating and updating the probabilities of hypotheses in Bayesian inference. But unlike Bayesian inference, the method automatically obtains and uses qualitative correlations among hypotheses as qualitative evidence, so the above problems of using Bayesian inference can be easily avoided. A new concept called qualitative correlations among hypotheses and a new concept called qualitative correlation propagation are introduced. Then, an algorithm for extracting and representing qualitative correlations among hypotheses and an algorithm for propagating qualitative correlations and updating possibilities of hypotheses are proposed.

The method has been applied to a practical system for infrared spectrum interpretation. and has been tested against about 300 real infrared spectra. The experimental results show that it is significantly better than others used in similar systems.

## Background Problem

Reasoning under uncertainty is an important problem in AI (Cohen 1984, de Kleer & Williams 1987, Kuipers et al. 1988). The most popularly used method for uncertain reasoning is Bayesian inference (Dempster 1968, Kleiter 1992). The principle behind Bayesian inference is: (1) giving evidence and hypotheses that the evidence may lead to; (2) getting the probabilities of evidence and hypotheses, and the relations between evidence and hypotheses; and (3) updating the proba-

bilities of hypotheses by propagating the probabilities of related evidence.

Bayesian inference can be graphically represented in Figure 1:

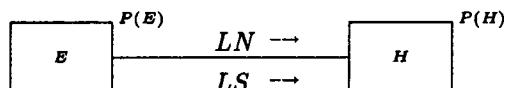


Figure 1: Probability Propagation

where (1)  $E$  is a piece of evidence; (2)  $P(E)$  is the probability that  $E$  is true; (3)  $H$  is a hypothesis; (4)  $P(H)$  is the probability that  $H$  is true; (5)  $LS$  represents the degree that  $E$  enhances  $H$ ; and (6)  $LN$  represents the degree that  $\neg E$  enhances  $H$ .

When evidence and the relations between evidence and hypotheses can be consistently obtained, Bayesian inference is effective. However, in many practical problems, evidence is either incomplete or unavailable, and the relations between evidence and hypotheses are also either inconsistent or unknown.

The method presented in this paper performs the task of inference under uncertainty by extracting and propagating qualitative correlations among hypotheses as confirmatory or disconfirmatory evidence. When evidence is incomplete or unavailable, or the relations between evidence and hypotheses are inconsistent or unknown, the method uses qualitative correlations among hypotheses as qualitative evidence. Even if evidence and the relations between evidence and hypotheses are known, the method can still be used to refine hypotheses after they have been made.

The method is based on the consideration that in practical problems hypotheses are rarely completely independent, and dependent hypotheses (called related hypotheses) should qualitatively support each other. First, some hypotheses are qualitatively dependent. For example, the hypotheses referring to a patient's diseases reflect the health condition of the patient, and the hypotheses concerning the peaks of a partial component on an infrared spectrum indicate the presence of the partial component. Second, related hypotheses will qualitatively support each other. For example, the hypothesis of one symptom will influence the hypotheses of others, and the hypothesis of one peak will also influence the hypotheses of others.

The intuition of the method can be summarized in two aspects. First, the idea is very common in human thinking. When all hypotheses except one show that one object is present, we would naturally suspect that the hypothesis which does not show that the object is present was made improperly. If acceptable solutions can be made by remaking the hypothesis, the hypothesis may be compensated and remade; Second, in prac-

tical problems, the idea is commonly used by domain experts when uncertainty occurs. In infrared spectrum interpretation, for example, spectroscopists frequently use the qualitative analysis like "if there is a strong peak around  $3000\text{-}3100\text{ cm}^{-1}$ , then the unknown spectrum may be partially created by benzene-rings — check peaks around  $1650, 1550$  and  $700\text{-}900\text{ cm}^{-1}$  to make sure since a benzene-ring may have other peaks there at the same time" or "if there is a sharp peak in  $2950\text{-}2960\text{ cm}^{-1}$  and the peaks around  $1500\text{-}1600\text{ cm}^{-1}$  look like the peaks of  $CO$ , then the peak in  $2950\text{-}2960\text{ cm}^{-1}$  is likely to be the peak of  $CH_3$  even if it is not strong". So if one hypothesis is not quite sure (i.e., a measured peak looks like but is not exactly the same as the reference peak), considering qualitative correlations among related hypotheses may lead to qualitative evidence for the hypothesis.

## Qualitative Correlations of Hypotheses

Hypotheses in inference are rarely completely independent (Zhao & Nishida 1995). A group of hypotheses may refer to the same object (e.g., different hypothesis refers to the different aspect of the object). For example, several symptoms may refer to the same hypothesis, and several hypotheses may refer to the same disease, and the hypotheses referring to the same disease may have some qualitative correlations. If the possibilities of hypotheses have been calculated or provided, then the qualitative correlations among hypotheses can be used as confirmatory or disconfirmatory evidence to update the known possibilities of hypotheses.

The concepts of related hypotheses, qualitative correlations among related hypotheses, and confirmatory and disconfirmatory evidence from qualitative correlations among related hypotheses are given below.

**Definition 1 Related hypotheses:** If hypotheses  $h_1, h_2, \dots, h_m$  refer to the same object, then they can be treated as related hypotheses.  $rh_\alpha$  is used to represent a group of related hypotheses, and  $h_i \& h_j$  is used to represent that  $h_i$  is related to  $h_j$  ( $rh_\alpha = \{h_k \mid \forall h_{k'} ((h_{k'} \in rh_\alpha) \wedge (h_{k'} \neq h_k) \rightarrow (h_k \& h_{k'}))\}$ ).

For example, if we consider a word as an object, then the hypotheses for all letters in the word can be viewed as related hypotheses. If we consider a sentence as an object, then the hypotheses for all words in the sentence can also be viewed as related hypotheses.

**Definition 2 Qualitative correlations among related hypotheses:** If  $h_i$  and  $h_j$  are two related hypotheses, then the great possibility of  $h_j$  qualitatively enhances  $h_i$ , and the small possibility of  $h_j$  qualitatively depresses  $h_i$ . The greater the possibility of  $h_j$ , the more greatly it qualitatively supports  $h_i$ , and the smaller the possibility of  $h_j$ , the more weakly it qualitatively supports  $h_i$  (or in other words, the more greatly it qualitatively depresses  $h_i$ ). This kind of effects among related

*hypotheses are called qualitative correlations among related hypotheses.  $qc_i^j$  is used to represent the qualitative correlation of  $h_i$  and  $h_j$ .*

For example, some symptomatic hypotheses such as temperature, blood pressure and pulse refer to a certain disease. In describing the disease, all of these hypotheses are related to each other. Making a definite diagnosis of a certain disease, all related hypotheses referring to the disease should be completely confirmed. So if some symptomatic hypotheses of a patient presage a certain disease, the other hypotheses referring to the same disease are usually required to be made and confirmed.

Consider the infrared spectrum interpretation. The hypotheses that some peaks are created by a certain partial component are related to each other. Because all peaks that a partial component can create should be present or absent simultaneously, identifying a partial component requires that all these related hypotheses be made and confirmed. As a result, hypotheses with great possibilities may prompt and enhance other hypotheses related to them.

**Definition 3 Sum-degree of qualitative correlations among related hypotheses:** If there are  $m-1$  hypotheses related to  $h_i$ , then the Sum-degree of qualitative correlations among related hypotheses of  $h_i$  is the total qualitative correlations between  $h_i$  and all of its related hypotheses.  $SD_i$  is used to represent the Sum-degree of the qualitative correlations of  $h_i$ .

For example, consider the following four strings:

- (a)  $i-n-a-c-c-u-r-a-t-e$
- (b)  $i-m-a-c-c-u-r-a-t-e$
- (c)  $i-m-a-c-c-u-l-a-t-e$
- (d)  $i-m-a-c-u-l-a-t-e$

(a) is a correct word, but (b), (c) and (d) are all spelled wrong. For a wrong spelled word, determining what a letter in the word should be is to make a hypothesis for the letter. Because all letters in a word refer to the same word, the hypotheses for these letters are related to each other, and have qualitative correlations. There is one letter, "m", in (b) different from that in (a), so the Sum-degree of qualitative correlations from other letters which support interpreting "m" in (b) as "n" is quite great. As a result, (b) can be easily interpreted as (a). Further, there are two letters, "m" and "l", in (c) different from those in (a). Although (c) may be interpreted as (a), the Sum-degree of qualitative correlations from other letters which support interpreting "m" and "l" in (c) as "n" and "r" would not be great. Finally, there are three letters, "m", "c" and "l", in (d) different from those in (a). As a result, (d) will hardly be interpreted as (a) since the Sum-degree of qualitative correlations from other letters which support interpreting these three

letters will be very small (even smaller than that for interpreting (d) as word "immaculate").

The principle for defining and calculating the Sum-degree of qualitative correlations among related hypotheses is that the qualitative correlations among related hypotheses should reflect the ratio of how many and how much related hypotheses qualitatively support each other.

**Definition 4 Confirmatory evidence from qualitative correlations among related hypotheses:** If the Sum-degree of qualitative correlations among related hypotheses of  $h_i$  is greater than a certain value given by domain experts, then the qualitative correlations among related hypotheses provide confirmatory evidence for  $h_i$ . As a result, the possibility of  $h_i$  may increase.

**Definition 5 Disconfirmatory evidence from qualitative correlations among related hypotheses:** If the Sum-degree of qualitative correlations among related hypotheses of  $h_i$  is smaller than a certain value given by domain experts, then the qualitative correlations among related hypotheses provide disconfirmatory evidence for  $h_i$ . As a result, the possibility of  $h_i$  may decrease.

For example, partial component  $CH_3$  usually creates numerous peaks each of which should have an exact location on infrared spectra. Because the peaks of  $CH_3$  on real infrared spectra are always inaccurate, especially the peak located at  $2900\text{ cm}^{-1}$ , real peaks on infrared spectra can not be directly identified as the peaks of  $CH_3$ . Instead, hypotheses need to be made to assume the similar peaks to be those of  $CH_3$ . Suppose a peak around  $2900\text{ cm}^{-1}$  is assumed to be the peak of  $CH_3$ . Since  $CH_3$  can create many peaks besides that at  $2900\text{ cm}^{-1}$ , the qualitative correlations among the hypotheses for these peaks created by  $CH_3$  can be used as confirmatory evidence to enhance the hypothesis for the peak around  $2900\text{ cm}^{-1}$ , or as disconfirmatory evidence to depress the hypothesis. For instance, if other hypotheses all have very great possibilities, then these hypotheses tend to support the hypothesis for the peak around  $2900\text{ cm}^{-1}$ , and the Sum-degree of qualitative correlations among related hypotheses of the peak around  $2900\text{ cm}^{-1}$  will be very great. As a result, the possibility of identifying the peak around  $2900\text{ cm}^{-1}$  will increase, that is, the possibility of the hypothesis for the peak will be updated with a greater one.

## Propagation of Qualitative Correlations as Confirmatory or Disconfirmatory Evidence

The method consists of two algorithms. The first is for extracting and representing qualitative correlations among hypotheses, and the second is for propagating qualitative correlations and updating possibilities of

hypotheses.

### Algorithm for Obtaining Qualitative Correlations

The algorithm for extracting and representing qualitative correlations among hypotheses is described with the following steps.

#### Step 1: Grouping related hypotheses

Suppose the known hypotheses are  $h_1, h_2, \dots$ , and  $h_n$  which form a hypothesis set  $H$ . If some hypotheses in  $H$  refer to the same object, they are treated as related hypotheses. Therefore,  $H$  is divided into some subsets, that is,

$$H = \{h_1, h_2, \dots, h_n\} = rh_1 \cup rh_2 \cup \dots \cup rh_k$$

where (1)  $rh_i = \{h_{i_p} \mid h_{i_p} \in H \wedge \forall h_{i_q} (h_{i_q} \in rh_i \wedge h_{i_q} \neq h_{i_p} \rightarrow h_{i_p} \& h_{i_q})\}$ ,

(2)  $rh_i \neq \emptyset$ , and

(3)  $rh_i \cap rh_j = \emptyset$  or  $rh_i \cap rh_j \neq \emptyset, i \neq j$ .

#### Step 2: Extracting qualitative correlations among related hypotheses

For each subset of  $H$  (i.e.,  $rh_i = \{h_{i_1}, h_{i_2}, \dots, h_{i_m}\}$ ,  $i = 1, 2, \dots, k$ ), suppose the corresponding set of possibilities is

$$\mu_i^o = \{\mu_{i_1}^o, \mu_{i_2}^o, \dots, \mu_{i_m}^o\}, i = 1, 2, \dots, k.$$

The principle for defining the qualitative correlations between two related hypotheses is that if the possibility of a hypothesis is greater than a certain value, then it is qualified to qualitatively support its related hypotheses; otherwise, it is not qualified. For example, suppose 0.5 is the certain value, then

$$qc_{i_p}^{i_q} = \begin{cases} 1 & h_{i_p} \in rh_i \wedge h_{i_q} \in rh_i \wedge \mu_{i_q}^o \geq 0.5 \\ 0 & h_{i_p} \in rh_i \wedge h_{i_q} \in rh_i \wedge \mu_{i_q}^o < 0.5 \end{cases}$$

where  $qc_{i_p}^{i_q} = 1$  means that  $h_{i_p}$  is qualitatively supported by  $h_{i_q}$ , and  $qc_{i_p}^{i_q} = 0$  means that  $h_{i_p}$  is not qualitatively supported by  $h_{i_q}$ .

#### Step 3: Calculating Sum-degree of qualitative correlations

There are  $m$  hypotheses in  $rh_i$  related to each other, so the Sum-degree of qualitative correlations of  $h_{i_p}$  is calculated by considering  $qc_{i_p}^{i_l}$  ( $l = 1, 2, \dots, m$  and  $l \neq p$ ), that is,

$$SD_{i_p} = \frac{1 + \sum_{l=1, l \neq p}^m qc_{i_p}^{i_l}}{m}$$

where  $0 < SD_{i_p} \leq 1$ .

$SD_{i_p}$  expresses the total qualitative correlations between  $h_{i_p}$  and all of its related hypotheses. If  $m = 1$ , then  $SD_{i_p} = 1$ . When  $m > 1$ ,  $SD_{i_p}$  is in the direct ratio to the number of the related hypotheses in  $rh_i$  which are qualified to qualitatively support their related hypotheses.

### Algorithm for Propagating Qualitative Correlations

The algorithm for propagating qualitative correlations among hypotheses to update the possibilities of hypotheses is described with the following steps.

#### Step 1: Calculating possibility propagation factor

$P_{i_p}^2$  is used to represent the possibility propagation factor of  $h_{i_p}$  from all of its related hypotheses.  $P_{i_p}^2$  is determined by considering the confirmatory or disconfirmatory evidence obtained from  $SD_{i_p}$ :

$$P_{i_p}^2 = \frac{(2m - 1) \times SD_{i_p}}{m}$$

where  $SD_{i_p} < P_{i_p}^2 < 2SD_{i_p}$ .

$P_{i_p}^2$  is in the direct ratio to  $SD_{i_p}$ . If  $m = 1$ , then  $SD_{i_p} = 1$ , and  $P_{i_p}^2 = 1$ . In other words, when qualitative correlations among hypotheses are not available,  $SD_{i_p} = 1$  and  $P_{i_p}^2 = 1$ . This is the only case to which the method is not applicable. However, generally speaking, qualitative correlations among hypotheses are always available in practical problems.

When  $m$  is fixed, the greater the number of related hypotheses which are made with great possibilities, the greater the  $SD_{i_p}$ , therefore the greater the  $P_{i_p}^2$ . When  $SD_{i_p}$  is fixed,  $P_{i_p}^2$  depends on the number of related hypotheses.

#### Step 2: Propagating qualitative correlations as (dis)confirmatory evidence

With the possibility  $\mu_{i_p}^o$  and the possibility propagation factor  $P_{i_p}^2$ , a new possibility of  $h_{i_p}$  can be calculated after considering qualitative correlations among related hypotheses as confirmatory or disconfirmatory evidence:

$$\mu_{i_p} = 1 - \frac{1 - \mu_{i_p}^o}{P_{i_p}^2}$$

where  $0 \leq \mu_{i_p} \leq 1$ .

The function of  $SD_{i_p}$  is similar to the function of  $LS$  and  $LN$  in Subjective Bayesian methods. However, both  $SD_{i_p}$  and  $P_{i_p}^2$  are dynamically calculated by considering qualitative correlations among related hypotheses, while in Subjective Bayesian methods both  $LS$  and  $LN$  are provided by domain experts in advance. In addition, using  $P_{i_p}^2$  to calculate  $\mu_{i_p}$  is also similar to using evidence to update the probabilities of hypotheses. However, the method is applicable to any problem where hypotheses have been made with corresponding possibilities, while Subjective Bayesian methods are usually applicable to the problems where

evidence and the relations between evidence and hypotheses are explicitly provided.

### Step 3: Updating possibilities of hypotheses

For  $h_{i_l} \in rh_i$  ( $l = 1, 2, \dots, m$ ), if  $\mu_{i_l}$  exists, then  $\mu_{i_l}$  is used to replace  $\mu_{i_p}^o$ .

## Properties

The following properties can be drawn from the above two algorithms.

**Property 1:** With the same number  $m$ , the greater the number of related hypotheses whose possibilities are greater than a certain value provided by domain experts, the greater the  $SD_{i_p}$ ; otherwise, the smaller the  $SD_{i_p}$ .

**Property 2:** With the same  $m$ , the greater the  $SD_{i_p}$ , the greater the  $P_{i_p}^2$ .

**Property 3:** With the same  $SD_{i_p}$ , the greater the  $m$ , the less  $P_{i_p}^2$  varies along with  $m$ .

**Property 4:** With the same  $\mu_{i_p}^o$ , the greater the  $P_{i_p}^2$ , the greater the  $\mu_{i_p}$ .

**Property 5:**  $SD_{i_p}$  provides qualitative confirmatory or disconfirmatory evidence for  $h_{i_p}$  since  $\mu_{i_p}$  is in the direct ratio to  $P_{i_p}^2$ , and  $P_{i_p}^2$  is in the direct ratio to  $SD_{i_p}$ .

The method can be graphically represented in Figure 2.

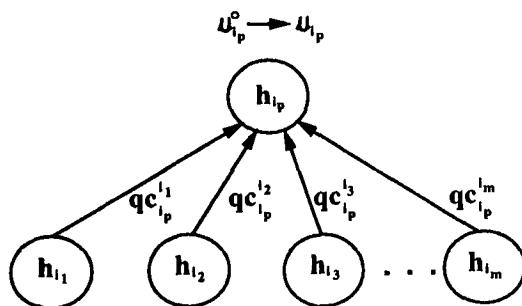


Figure 2: Propagation of Qualitative Correlations

Due to the propagation of qualitative correlations among related hypotheses, the possibility of  $h_{i_p}$  changes from  $\mu_{i_p}^o$  to  $\mu_{i_p}$ .

## Implementation

The method has been applied to a practical system on infrared spectrum interpretation, and has been tested against about 300 real infrared spectra.

## Application Problem

The task of infrared spectrum interpretation is to interpret infrared spectra of unknown compounds to identify the unknown compounds, or to identify the compositions of the unknown compounds (i.e., to identify what partial components ( $PC$ ) the unknown compounds contain) (Colthup et al. 1990).

In general, an infrared spectrum can be represented as a set of peaks:

$$Sp = \{p_1, p_2, \dots, p_n\}.$$

The peak lists of partial components are known in advance, each of which is a set of peaks that the partial component can create. For example, the peak list of partial component  $PC_\alpha$  is

$$PL(PC_\alpha) = \{p_{\alpha_1}, p_{\alpha_2}, \dots, p_{\alpha_m}\}.$$

If  $PC_\alpha$  is contained by a compound, peaks in  $PL(PC_\alpha)$  will appear on the infrared spectrum of the compound (i.e.,  $PL(PC_\alpha) \subset Sp$ ).

Infrared spectrum interpretation is a typical problem of reasoning under uncertainty. Ideally, if all peaks can be identified with 100% possibilities, the process of infrared spectrum interpretation for unknown compounds is simply a peak-matching process. In most cases, however, peaks can not be certainly identified due to the inaccuracy of spectral data.

Fuzzy logic and pattern recognition have been used by many systems to handle inaccurate spectral data (Colthup et al. 1990). However, fuzzy logic can deal with a single inaccurate peak well, but can not deal with a set of peaks as a whole. On the other hand, pattern recognition can deal with a set of peak simultaneously, but two preconditions are required by pattern recognition: one is that adequate data bases must be obtained, and the other is that suitable metrics of similarity between patterns must be provided.

By using the proposed method, infrared spectrum interpretation is performed in a different way. Since each partial component may create finite peaks at the same time, if  $p_i$  is created by  $PC_\alpha$  ( $p_i \in Sp$ ), then  $Sp$  is partially created by  $PC_\alpha$ ; if  $Sp$  is partially created by  $PC_\alpha$ , then all of the peaks that  $PC_\alpha$  may create should be contained by  $Sp$  simultaneously. Therefore, all of the peaks created by  $PC_\alpha$  are related to each other, and the hypotheses that the corresponding peaks are created by  $PC_\alpha$  are related hypotheses.

The related hypotheses have the following qualitative correlations:

1. All peaks of a partial component should be identified simultaneously, that is, if  $p_i$  is  $p_{j_p}$  ( $p_i \in Sp$  and  $p_{j_p} \in PL(PC_\alpha)$ ), then  $p_{j_l} \in Sp$  ( $p_{j_l} \in PL(PC_\alpha)$ ,  $l = 1, 2, \dots, m, l \neq p$ );
2. The peaks created by the same partial component support each other. For example, if most peaks of

$PC_\alpha$  have been identified, these peaks will enhance the identification of the rest peaks. Conversely, if most peaks of  $PC_\alpha$  can not be identified, then the identification of the rest peaks will be depressed.

## An Example

Figure 3 shows the peak of partial component  $CH_3$  in  $3000\text{-}2900\text{ cm}^{-1}$ . The accurate peak of  $CH_3$  in this region should be a strong peak located at  $2960\text{ cm}^{-1}$ , but in this example, the real peak of  $CH_3$  is only a medium peak located at  $2918\text{ cm}^{-1}$ .

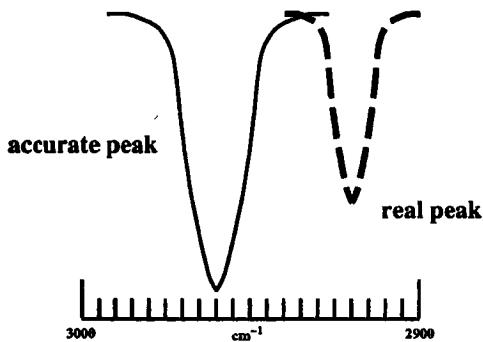


Figure 3: Peaks of  $CH_3$

By considering the peak itself, the possibility that the real peak at  $2918\text{ cm}^{-1}$  is identified as the peak of  $CH_3$  at  $2960\text{ cm}^{-1}$  is 0.352 (Zhao & Nishida 1995):

$$\mu_{p_{2960}}^o = 0.352.$$

$CH_3$  can mainly create 4 peaks:  $p_{2960}$ ,  $p_{2870}$ ,  $p_{1460}$  and  $p_{1380}$ , which are related to each other. If  $CH_3$  is contained by the real infrared spectrum, then all peaks of  $CH_3$  should be identified. Therefore, if other peaks are all identified with great possibilities,  $CH_3$  is quite likely to be contained by the real infrared spectrum, and the other peak will qualitatively support the identification of the inaccurate peak at  $2918\text{ cm}^{-1}$  as the peak at  $2960\text{ cm}^{-1}$ .

The possibilities of other peaks are obtained with the same method:

$$\mu_{p_{2870}}^o = 0.850, \mu_{p_{1460}}^o = 0.921 \text{ and } \mu_{p_{1380}}^o = 0.975.$$

According to the proposed method, the qualitative correlations between two related peaks are respectively calculated as:

$$qc_{p_{2960}}^{p_{2870}} = 1, qc_{p_{2960}}^{p_{1460}} = 1 \text{ and } qc_{p_{2960}}^{p_{1380}} = 1.$$

Then

$$SD_{p_{2960}} = 1, \text{ and } P_{p_{2960}}^2 = \frac{2 \times 4 - 1}{4} \times 1 = 1.75.$$

So

$$\mu_{p_{2960}} = 1 - \frac{1 - 0.352}{1.75} = 0.629.$$

Therefore, the possibility that the real peak at  $2918\text{ cm}^{-1}$  is identified as peak  $p_{2960}$  of  $CH_3$  increases from 0.352 to 0.629 due to the qualitative correlations among related hypotheses.  $CH_3$  can not be identified before since one main peak can not be found from the real infrared spectrum (i.e.,  $\mu_{p_{2960}}^o < 0.5$ ). After considering qualitative correlations among related hypotheses as confirmatory evidence, the peak can be identified with considerably great possibility (i.e.,  $\mu_{p_{2960}}^o = 0.629$ ).

The above process is similar to the probability propagation in probabilistic reasoning. However, neither evidence nor relation between evidence and hypotheses is required in advance.

## Empirical Results

There are two metrics to evaluate the empirical results. One is the rate of correctness ( $RC$ ) which means the rate that the identified partial component set is exactly the same as the partial component set in the correct solutions. The other is the rate of identification ( $RI$ ) which means the rate that how many partial components in the correct solutions are identified.

Two methods are tested. One is the proposed method, and the other is a conventional fuzzy method which uses fixed fuzzy intervals and membership functions to identify inaccurate peaks. The  $RC$  and  $RI$  of the proposed method are 0.736 and 0.894 respectively. In contrast, the  $RC$  and  $RI$  of the conventional fuzzy method are 0.455 and 0.812 respectively.

Table 1 gives the  $RCs$  and  $RIs$  of some known systems in which “/” means that the corresponding number is unavailable.

Systems	RC	RI
Anand's System	/	0.870
Hasenoehrl's System	/	0.980
Robb's System	0.533	/
Sadtler's System	/	/

Table 1: Experiments Evaluation with  $RC$  and  $RI$

Anand's system adopts neural networks to interpret infrared spectra (Anand et al. 1991). Its  $RI$  is about 0.870, but its  $RC$  is not available. Hasenoehrl's system adopts pattern recognition techniques to interpret infrared spectra (Hasenoehrl et al. 1992). Its  $RI$  is about 0.980, but its  $RC$  is not available. Robb's system adopts numerical and other techniques (Robb & Munk 1990). Its  $RC$  is 0.533, but its  $RI$  is not available. Sadtler's system is based on quantitative comparison between known and unknown infrared spectra

(Sadtler 1988). The system determines the possibility of an unknown pattern being a known one by calculating the quantitative similarity or closeness between the two patterns. Both of its *RC* and *RI* are not available since it gives all possible solutions as results from which users have to decide the right one by themselves.

## Comparison with Related Work

The propagation of qualitative correlations among related hypotheses in the proposed method is similar to the probability propagation in Bayesian methods – if we view the qualitative correlations among related hypotheses as pieces of evidence (Dempster 1968, Kleiter 1992). In solving the problems where qualitative correlations among related hypotheses can be extracted and used, the method is better in the following aspects:

1. In traditional Bayesian methods, evidence and its prior probability, hypotheses and their prior probabilities, and the relations between evidence and hypotheses (e.g., *LS* and *LN* in subjective Bayesian methods) are all provided and fixed by domain experts in advance, so knowledge acquisition is a difficult task, and consequently, inconsistency can hardly be avoided (Duda et al. 1976). In the proposed method, however, only a few numbers are needed in advance. Instead, qualitative correlations among related hypotheses and other dynamically obtained information are used and propagated;
2. Traditional Bayesian methods require that the evidence which supports or depresses hypotheses be explicitly provided, and are effective for the problems where the relations between evidence and hypotheses are known. The proposed method, however, is applicable to the problems where the relations between evidence and hypotheses are unknown as well as the problems where the relations are known.

When qualitative correlations among related hypotheses are available, and assumptions necessary for Bayesian methods are hard to obtain, the proposed method is better. However, when qualitative correlations among related hypotheses are not known, the method is not applicable. The method is especially effective to interpret inaccurate numerical and symbolic data by considering qualitative correlations among related data as confirmatory or disconfirmatory evidence.

## Conclusions

In this paper, a novel method for propagating qualitative correlations among related hypotheses as confirmatory or disconfirmatory evidence was presented. The function of the method is similar to the probability propagation in Bayesian methods. However, compared with traditional Bayesian methods, the proposed method can be applied to the problems where evidence

or the relation between evidence and hypotheses is not explicitly given, or is not complete. In addition, the proposed method needs few numbers and assumptions in advance. Therefore, it is quite simple, and can effectively avoid inconsistency in knowledge bases. The method has been applied to infrared spectrum interpretation, and has been tested against about 300 real infrared spectra. The empirical results show that it is significant better than the traditional methods used in many similar systems.

## References

- Anand, R., Mehrotra, K., Mohan, C. K., & Ranka, S. 1991. Analyzing Images Containing Multiple Sparse Patterns with Neural Networks. *Proc. of IJCAI'91*, pp. 838-843.
- Clerc, J. T., Pretsch, E., & Zurcher, M. 1986. Performance Analysis of Infrared Library Search Systems. *Mikrochim. Acta/Wien*, II, pp. 217-242.
- Cohen, P. R. 1984. Heuristic Reasoning about Uncertainty: An Artificial Intelligence Approach. *Pitman*.
- Colthup, L., Daly, H., & Wiberley, S. E. 1990. Introduction to Infrared and Raman Spectroscopy. *Academic Press INC*.
- de Kleer, J. & Williams, B. 1987. Diagnosing Multiple Faults. *Artificial Intelligence*, Vol. 32, pp. 97-130.
- Dempster, A. P. 1968. A Generalization of Bayesian Inference. *Journal of the Royal Statistical Society, Vol. B-30*, pp. 205-247.
- Duda, R. O., Hart, P. E., & Nilsson, N. J. 1976. Subjective Bayesian Methods for Rule-Based Inference Systems. *Proc. of National Computer Conference*, pp. 1075-1082. or Tech. Note 124, *SRI Int.*, Menlo Park, Ca.
- Hasenoehrl, E. J., Perkins, J. H., & Griffiths, P. R. 1992. Expert System Based on Principal Components Analysis for the Identification of Molecular Structures from VP IR Spectra. *Journal of Anal. Chem.*, 64, pp. 656-663.
- Kleiter, G. D. 1992. Bayesian Diagnosis in Expert Systems. *Artificial Intelligence*, Vol. 54, pp. 1-32.
- Kuipers, B. J., and et al. 1988. Using Incomplete Quantitative Knowledge in Qualitative reasoning. *Proc. of AAAI'88*, pp. 324-329.
- Robb, E. W. & Munk, M. E. 1990. A Neural Network Approach to Infrared Spectrum Interpretation. *Mikrochim. Acta/Wien*, I, pp. 131-155.
- Sadtler Research Laboratories. 1988. Sadtler PC Spectral Search Libraries, Product Introduction & User's Manual. *Sadtler Research Lab*.
- Zhao, Q. & Nishida, T. 1995. Using Qualitative Hypotheses to Identify Inaccurate Data. *Journal of Artificial Intelligence Research (JAIR)*, Vol. 3, pp. 119-145.