Inference of Common Multidimensional Equally-Distributed Attributes

Alejandro Álvarez-Ayllón∗,1,2, Manuel Palomo-Duarte1, and Juan-Manuel Dodero1

1 Department of Computer Science and Engineering, University of Cadiz, Spain
2 Department of Astronomy, University of Geneva, Switzerland

July 20, 2022

Abstract

Given two relations containing multiple measurements – possibly with uncertainties – our objective is to find which sets of attributes from the first have a corresponding set on the second, using exclusively a sample of the data. This approach could be used even when the associated metadata is damaged, missing or incomplete, or when the volume is too big for exact methods. This problem is similar to the search of Inclusion Dependencies (IND), a type of rule over two relations asserting that for a set of attributes $X$ from the first, every combination of values appears on a set $Y$ from the second. Existing IND can be found exploiting the existence of a partial order relation called specialization. However, this relation is based on set theory, requiring the values to be directly comparable. Statistical tests are an intuitive possible replacement, but it has not been studied how would they affect the underlying assumptions. In this paper we formally review the effect that a statistical approach has over the inference rules applied to IND discovery. Our results confirm the intuitive thought that statistical tests can be used, but not in a directly equivalent manner. We provide a workable alternative based on a “hierarchy of null hypotheses”, allowing for the automatic discovery of multi-dimensional equally distributed sets of attributes.

1 Introduction

Imagine an astronomer facing several data files containing raw astronomical measurements, with little or no explanation about their schema. These files...
may come from different surveys or different sets of observations, and the user can only make the following educated guesses:

- The populations are likely the same, or at least very similar (i.e. stars)
- A subset of the attributes is shared between the relations (i.e. brightness on different electromagnetic bands)
- This measurement has an associated uncertainty [5], either explicitly stated or not (i.e. random errors, instrument precision, floating point precision)

The first intuition would be to run some kind of statistical test between all possible pairs of columns, as the Kolmogorov-Smirnov [9] or Wilcoxon [16] tests. And this is likely a good starting point, but we are left only with a set of pairwise correspondences that may not be enough to cross-match tuples between files.

![Figure 1](image)

**Figure 1:** Example of a 2D distribution where the pairwise matching would not be accurate enough. It is artificial, but it serves to illustrate the point.

**Example 1** Imagine that A and B are attributes from a relation R, and C to E attributes from a relation S. Pairwise tests would tell us that A matches C and E; and that B matches D and F. This information is evidently not enough to do a cross-match.

Starting with this initial set of one-dimensional matches, one can pick all the possible combinations of two attributes to find the potential two-dimensional spaces where cross-matching could be attempted, and perform another series of statistical multivariate tests to check for “matching” pairs (denoted as ≈).

**Example 2** Following our example, we could test after if A, B ≈ C, D and A, B ≈ E, F.

At this stage, we would have \( \binom{n}{2} \) possible options, n being the number of positive one-dimensional matches. In general, to look for k-dimensional matching spaces we would have to test all possible \( \binom{n}{k} \) permutations, for any \( k \leq n \).
Unfortunately, this can quickly grow out of hand, with a combinatorial explosion on the number of tests required at each increase of dimensionality. This becomes impractical, in terms of computational run-time, even for a relatively small number of attributes. Furthermore, many of these tests will be redundant: if we already know that $A, B, C \approx D, E, F$, it would seem that it does not make much sense to test, say, $A, B \approx D, E$.

To complicate things even more, since we are performing statistical tests there is always a possibility (bound by the significance level $\alpha$) of falsely rejecting the equality of distribution. For instance, $A, B, C \approx D, E, F$ might still be true even if $A, B \approx D, E$ is rejected.

The issue of finding higher dimensions where two pairs of set of attributes still follow the same distribution resembles that of finding high arity Inclusion Dependencies (IND) between two relational datasets. On the other hand, uncertainties and statistical errors make the problem different enough as to require a more careful consideration of their effects on the foundations of IND finding algorithms.

In this paper, we discuss how to map the IND inference rules into the problem of finding multidimensional equally-distributed set of attributes, and the limitations arising from the approximate nature of statistical tests.

The rest of the paper is structured as follows: next, in section 2 we introduce the background for the research. Then, in section 3 we develop the proofs of the inference rules for numerical data. Next, in section 4 we discuss the findings obtained and their implications. Finally, in section 5 we compile the conclusions of the paper and the future work.

2 Background

Let $R$ and $S$ be two relations, and $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_m$ two sets of $n$ and $m$ attributes from both relations respectively.

**Definition 1** A rule of the form $\sigma = R[a_{i_1}, \ldots, a_{i_k}] \subseteq S[b_{i_1}, \ldots, b_{i_k}]$ (where $a_{i_1}, \ldots, a_{i_k}$ and $b_{i_1}, \ldots, b_{i_k}$ are projections of $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_m$ respectively) is an **Inclusion Dependency (IND)** of **arity** $k \leq \min(n, m)$ between $R$ and $S$. The particular case where $k = 1$ is also called an **Unary Inclusion Dependency (uIND)**.

Note that definition 1 applies over the **domains** of the attributes, i.e. a potentially unlimited set of tuples where every possible value from $R$ and $S$ is present.

Let $d$ be a concrete database instance from a database scheme $D$, with finite samples from both relations.

**Definition 2** An IND of the form $R[X] \subseteq S[Y]$ is **satisfied** (or valid) in $d$ if every combination of values from $X$ appears in $Y$. This is denoted as $d \models \sigma$, where $\sigma = R[X] \subseteq S[Y]$. 

3
There are three inference rules that can be used to derive some additional INDs from an already known set of INDs:

**Reflexivity**

\[ R[X] \subseteq R[X] \]

**Permutation and projection**

If \[ R[A_1, \ldots, A_n] \subseteq S[B_1, \ldots, B_n] \] then \[ R[A_{i_1}, \ldots, A_{i_m}] \subseteq S[B_{i_1}, \ldots, B_{i_m}] \]

for each sequence \( i_1, \ldots, i_m \) of distinct integers from \( \{1, \ldots, n\} \)

**Transitivity**

\[ R[X] \subseteq S[Y] \land S[Y] \subseteq T[Z] \implies R[X] \subseteq T[Z] \]

The second axiom is particularly important, as it can be applied to derive a partial order relation which gives direction to the search space of all possible INDs. Let \( I_1 = R[X] \subseteq S[Y] \) and \( I_2 = R'[X'] \subseteq S'[Y'] \).

**Definition 3** \( I_1 \) specializes \( I_2 \) - denoted \( I_1 \prec I_2 \) iff

1. \( R = R' \) and \( S = S' \)
2. \( X \) and \( Y \) are sub-sequences of \( X' \) and \( Y' \) respectively

Equivalently, we can also say that \( I_2 \) generalizes \( I_1 \).

**Example 3** \((R[AB] \subseteq S[EF]) \prec (R[ABC] \subseteq S[EFG])\). However, \( R[AB] \subseteq S[DE] \) \( \not\prec (R[ACD] \subseteq S[DFG])\), as \( AB \) and \( DE \) are not sub-sequences of \( ACD \) and \( DFG \) respectively.

An important property of specialization can be inferred:

**Property 1** Given \( I_1 \prec I_2 \)

1. If \( d \models I_2 \), then \( d \models I_1 \)
2. By transposition, if \( d \not\models I_1 \) then \( d \not\models I_2 \)

This property allows to quickly purge the IND search space:

1. If we find that \( d \models I_2 \), we can ignore all \( I_i \) s.t. \( I_i \prec I_2 \), since they will be satisfied
2. If we find that \( d \not\models I_1 \), we can ignore all \( I_j \) s.t. \( I_1 \prec I_j \), since they will not be satisfied

**Example 4** If we know that \( R[AB] \not\subseteq S[EF] \), then we know that \( R[ABC] \not\subseteq S[EFG] \).
3 Inference rules for uncertain numerical data

Let’s go back to the use case from our data scientist. Definition 1 works over the domain of the attributes, but this is problematic when finding dependencies between attributes that have the same domain, but different distributions.

Example 5 In a relation with galaxies and stars properties measured from images, one may have for each tuple the aspect ratio of the ellipse that encompass a given fraction of the light, and the probability of being a star. Both are values from the domain $[0, 1]$, but the distributions are nothing alike (Figure 2).

Thus, our user would likely be more interested in finding attributes that are identically distributed: $R[X] \overset{d}{=} S[Y]$.

Definition 4 Let $F_{X_1, \ldots, X_k}$ be the cumulative distribution of the set of attributes $X_1, \ldots, X_k$, and $\mathbb{R}^k$ their domain. $R[X_1, \ldots, X_k] \overset{d}{=} S[Y_1, \ldots, Y_k]$ (they are identically distributed) if

$$F_{X_1, \ldots, X_k}(x_1, \ldots, x_k) = F_{Y_1, \ldots, Y_k}(x_1, \ldots, x_k) \quad \forall (x_1, \ldots, x_k) \in \mathbb{R}^k$$

We could now replace the rule $\sigma$ in definition 1 by $\sigma = R[X] \overset{d}{=} R[Y]$.

There is, however, one important caveat: this holds for the database scheme $D$, where the true Cumulative Distribution Function (CDF) would be defined. In our case, we are given a particular instance of the database, which has a finite number of tuples. In other words, the database instance could be seen as a sample from an unknown database schema.
Consequently, we can only expect to use either the Empirical Cumulative Distribution Function (ECDF), or a fitted curve (i.e. a Gaussian). Either way, there will be uncertainty and definition 3 will not be directly usable. Instead, it will be necessary to test for the null hypothesis $H_0 : P(R[X]) = P(S[Y])$, and this will be inherently affected by statistical errors bound by the chosen significance level $\alpha$ and the power of the statistical test.

Nevertheless, we will show that the rules do apply assuming we know the “true” cumulative distribution. This will be at least enough to guide the traversal of the search space, creating a “hierarchy” of null hypotheses.

Note that others have used statistical methods earlier to test IND, but as an approximation of the containment rule \cite{12, 17}. In our case, the question itself is statistical, so the inference rules need to be re-evaluated.

### 3.1 Reflexivity

$$R[X] \overset{d}{=} R[X]$$

**Proof 1** *This property is trivial, as any random variable is distributed as itself.*

### 3.2 Permutation and projection

If $R[A_1, \ldots, A_n] \overset{d}{=} S[B_1, \ldots, B_n]$ then $R[A_{i_1}, \ldots, A_{i_m}] \overset{d}{=} S[B_{i_1}, \ldots, B_{i_m}]$ for each sequence $i_1, \ldots, i_m$ of distinct integers from $\{1, \ldots, n\}$.

#### 3.2.1 Permutation

Considering that the CDF of $A$ could also be defined as $P(a_1 \leq A_1 \land \cdots \land a_m \leq A_n)$, and that the logical operator $\land$ is commutative, it can be intuitive that the order in which the attributes are specified does not affect their probability. However, we have preferred to follow a different direction to prove that the relation $\overset{d}{=}$ is invariant under permutation, since it is more general.

**Proof 2** *Let $f_{X_1, \ldots, X_n} = \frac{\partial^n F_{X_1, \ldots, X_n}}{\partial x_1 \cdots \partial x_n}$ be a joint probability density function. Let $(X'_1, \ldots, X'_n)$ be a transformation $g$ of $(X_1, \ldots, X_n)$ such that $X'_i = g_i(X_1, \ldots, X_n)$. In general, the joint density function of $X'$ can be defined as

$$f_{X'_1, \ldots, X'_n}(X'_1, \ldots, X'_n) = f_{X_1, \ldots, X_n}(X_1, \ldots, X_n) |J|$$

Where $J$ is the Jacobian determinant of the inverse transformation $g^{-1}$.*

In the particular case when the transformation is defined by a non-singular matrix $M$ of size $n \times n$, its Jacobian determinant is simply $|M|$, and the Jacobian determinant of the inverse transformation, $|M|^{-1}$, which is a constant. Given that the cumulative probability function is an integral over $f_{X_1, \ldots, X_n}$, we can say that:
\[ F_{X'}(X'_1, \ldots, X'_n) = F_X((X'_1, \ldots, X'_n)M^{-1}) | \det M^{-1} | \]
\[ = F_X(X_1, \ldots, X_n) | \det M^{-1} | \]  

(3)

Let \( X' = x'_1, \ldots, x'_n \) and \( Y' = y'_1, \ldots, y'_n \) be the result of a linear transformation \( M : R^k \rightarrow R^k \) over \( X = x_1, \ldots, x_n \) and \( Y = y_1, \ldots, y_n \) respectively. From definition 4 and equation 3:

\[ X \doteq Y \implies F_X(x_1, \ldots, x_k) = F_Y(x_1, \ldots, x_k) \forall (x_1, \ldots, x_k) \in \mathbb{R}^k \]
\[ \implies F_X(x_1, \ldots, x_k) | \det M^{-1} | = F_Y(x_1, \ldots, x_k) | \det M^{-1} | \forall (x_1, \ldots, x_k) \in \mathbb{R}^k \]
\[ \implies F_{X'}((x_1, \ldots, x_n)M) = F_{Y'}((x_1, \ldots, x_n)M) \forall (x_1, \ldots, x_k) \in \mathbb{R}^k \]
\[ \implies F_X'(x'_1, \ldots, x'_n) = F_Y'(x'_1, \ldots, x'_n) \forall (x'_1, \ldots, x'_k) \in \mathbb{R}^k \]
\[ \implies X' \doteq Y' \]  

(4)

This is true for all one-to-one linear transformations \( M : R^k \rightarrow R^k \), of which a permutation is just a concrete case where \( M \) is a permutation matrix.

3.2.2 Projection

**Proof 3** For the projection, we need to prove that if two sets of random variables \( X_1, \ldots, X_n \) and \( Y_1, \ldots, Y_n \) are equally distributed, so are any of their possible sub-sequences.

Let \( X' \) and \( Y' \) be the sequences \( X_1, \ldots, X_m \) and \( Y_1, \ldots, Y_m \) with \( m < n \). Their corresponding CDF are just the marginal CDF:

\[ F_{X_1,\ldots,X_m}(x_1,\ldots,x_m) = F_{X_1,\ldots,X_m,X_{m+1},\ldots,X_n}(x_1,\ldots,x_m,x_{m+1},\ldots,x_n) \]
\[ F_{Y_1,\ldots,Y_m}(y_1,\ldots,y_m) = F_{Y_1,\ldots,Y_m,Y_{m+1},\ldots,Y_n}(y_1,\ldots,y_m,x_{m+1},\ldots,x_n) \]  

(5)

\[ \forall (x_1, \ldots, x_m) \in \mathbb{R}^m \text{ and } x_i \rightarrow \infty \forall i > m \]

By definition 4, the right hand-side of both equations must be the same. By transitivity,

\[ F_{X_1,\ldots,X_m}(x_1,\ldots,x_m) = F_{Y_1,\ldots,Y_m}(y_1,\ldots,y_m) \]
\[ \implies X_1,\ldots,X_m \doteq Y_1,\ldots,Y_m \]  

(6)

3.3 Transitivity

\[ R[X] \doteq S[Y] \land S[Y] \doteq T[Z] \implies R[X] \doteq T[Z] \]
Proof 4

\[ X \overset{d}{=} Y \land Y \overset{d}{=} Z \implies F_X(x_1, \ldots, x_k) = F_Y(x_1, \ldots, x_k) \land F_Y(x_1, \ldots, x_k) = F_Z(x_1, \ldots, x_k) \implies F_X(x_1, \ldots, x_k) = F_Z(x_1, \ldots, x_k) \implies X \overset{d}{=} Z \]  

(7)

4 Discussion

We have shown that replacing \( \sigma \) in definition 1 with \( \sigma = R[X] \overset{d}{=} S[Y] \) leaves us with a similar set of inference rules that can be applied to support the specialization relation from definition 4.

However, as we have already mentioned in section 3, these rules work if we know the true distribution of both sets of attributes. In many cases, as it could be in astrophysics, the content of the attributes are purely empirical, and we will have to approximate the definition 4 with a statistical test with the null hypothesis \( H_0 : R[X] \overset{d}{=} S[Y] \).

Nonetheless, we can apply the rule of projection to create a “hierarchy” of null hypotheses based on the definition of specialization, but we will need to reformulate the property applied for the inference of new IND:

Property 2 Let \( I_1 \) be an assertion that two sets of attributes are equally distributed, and \( H_{0_1} \) the null hypothesis used to test it. Let \( I_1 \prec I_2 \).

1. Accepting \( H_{0_1} \) implies accepting \( H_{0_2} \).2

2. Rejecting \( H_{0_1} \) does not imply the rejection of \( H_{0_2} \)

The second part of this property can be simply explained by the fact that a statistical test may falsely reject \( H_{0_1} \) with a probability given by the significance level \( \alpha \). This is markedly different from property 1 but still informative.

Example 6 If we have two sets of 10 attributes that are equally distributed, we have \( \binom{10}{3} = 120 \) projections (specializations) of 3 dimensions that must be equally distributed as well. If we have a significance level of \( \alpha = 0.1 \), the expected number of falsely rejected 3-dimensional equalities is 12. This can be used to check if the actual number of rejections match the expectation.

We could try to apply a similar reasoning to the transitivity rule, but this would arguably not work for inferring new IND properties:

\footnote{This is an abuse of terminology. Technically not rejecting \( H_{0_1} \) implies that we can not reject \( H_{0_2} \).}
**Projection** reduces the information available, since we remove dimensions. If we cannot reject the “high arity” null hypothesis, we *should not* reject any “lower arity” since, after all, there is less information available to do so.

**Permutation** does not alter the information available. If we cannot reject the null hypothesis for one permutation, we *should not* reject the null hypothesis for exactly the same data after being shuffled.

For **transitivity**, however, the information available for each test is different and, therefore, nothing can be assumed. \(X\) and \(Y\) may be close enough to not be possible to tell them apart, and the same may happen to \(Y\) and \(Z\). However, \(X\) and \(Z\) may be separate enough as to be able to differentiate and reject that they are equally distributed.

## 5 Conclusion

Helping data scientist to match and explore heterogeneous datasets, even when their scheme is unknown or unfamiliar, is an active and interesting area of research with multiple ramifications \([10, 14]\), one of which is schema matching \([1]\). To the best of our knowledge, there has been no detailed discussions on how this can be achieved on multidimensional spaces when uncertainty is unavoidable.

In this paper we have proven that inferring multidimensional sets of “equally distributed” attributes is feasible using similar mechanisms to those of finding Inclusion Dependencies (IND) between two relational datasets. In particular, the **specialization** relation from definition \([8]\) can be applied to give directionality to the search space, and the property \([2]\) provides capabilities to traverse it, avoiding expensive combinatorial solutions.

However, this property can not be directly applied as a drop-in replacement of the original property \([1]\) as rejecting a low dimensionality inclusion *should not* necessarily cause the rejection of a higher dimensionality one *specialized* by it. This has to be taken into account when adapting, or devising new, algorithms.

### 5.1 Future work

With this knowledge we can now start evaluating the viability of adapting existing concrete solutions for the IND search problem to a more specific objective: given two numerical datasets, with uncertainties, and without using the associated metadata, find which subsets of attributes are “equally distributed”. As a non-exhaustive set of possible applications, once these sets of attributes are found, they could potentially be used to cross-match the objects between the relations \([2]\); to adapt the dataset schemes and use them as a single one; or to apply a known label from one to the other without knowing *a priori* which attributes can be used to do so.
Financial disclosure

This research was funded by Spanish National Research Agency (AEI), through the project VISAIGLE (TIN2017-85797-R) with ERDF funds.

References

[1] Alawini, A., D. Maier, K. Tufte, and B. Howe, 2014: Helping scientists reconnect their datasets. Proceedings of the 26th International Conference on Scientific and Statistical Database Management, 1–12.

[2] Budavári, T. and A. S. Szalay, 2008: Probabilistic cross-identification of astronomical sources. The Astrophysical Journal, 679, no. 1, 301–309, doi:10.1086/587156.

[3] Casanova, M. A., R. Fagin, and C. H. Papadimitriou, 1984: Inclusion dependencies and their interaction with functional dependencies. Journal of Computer and System Sciences, 28, no. 1, 29–59, doi:10.1016/0022-0000(84)90075-8.

[4] Casella, G. and R. L. Berger, 2002: Statistical Inference, volume 2. Duxbury Pacific Grove, CA.

[5] Dawson, B., 2008: Comparing floating point numbers. Cygnus Software.

[6] De Marchi, F., S. Lopes, and J.-M. Petit, 2002: Efficient algorithms for mining inclusion dependencies. International Conference on Extending Database Technology, Springer, 464–476.

[7] Deemer, W. L. and I. Olkin, 1951: The Jacobians of certain matrix transformations useful in multivariate analysis: Based on lectures of PL Hsu at the University of North Carolina, 1947. Biometrika, 38, no. 3/4, 345–367.

[8] Giri, N. C., 2014: Multivariate Statistical Inference. Academic Press.

[9] Hodges, J. L., 1958: The significance probability of the Smirnov two-sample test. Arkiv för Matematik, 3, no. 5, 469–486.

[10] Idreos, S., O. Papaemmanouil, and S. Chaudhuri, 2015: Overview of Data Exploration Techniques. Proceedings of the 2015 ACM SIGMOD International Conference on Management of Data - SIGMOD '15, 277–281.

[11] Koeller, A., 2002: Integration of Heterogeneous Databases: Discovery of Meta-Information and Maintenance of Schema-Restructuring Views. Ph.D. thesis, Worcester Polytechnic Institute.

[12] Koeller, A. and E. A. Rundensteiner, 2006: Heuristic strategies for the discovery of inclusion dependencies and other patterns. Journal on Data Semantics V, Springer, 185–210.
[13] Kuijken, K., C. Heymans, A. Dvornik, H. Hildebrandt, J. de Jong, A. Wright, T. Erben, M. Bilicki, B. Giblin, H.-Y. Shan, et al., 2019: The fourth data release of the Kilo-Degree Survey: Ugri imaging and nine-band optical-IR photometry over 1000 square degrees. Astronomy & Astrophysics, 625, A2.

[14] Milo, T. and A. Somech, 2020: Automating exploratory data analysis via machine learning: An overview. Proceedings of the 2020 ACM SIGMOD International Conference on Management of Data, Association for Computing Machinery, New York, NY, USA, SIGMOD ’20, 2617–2622.

[15] Stonebraker, M., 2009: Requirements for Science Data Bases and SciDB. 4th Biennial Conference on Innovative Data Systems Research CIDR’09, 173–184, doi:10.1.1.145.1567.

[16] Wilcoxon, F., 1945: Individual comparisons by ranking methods. Biometrics Bulletin, 1, no. 6, 80–83, doi:10.2307/3001968.

[17] Zhang, M., M. Hadjieleftheriou, B. C. Ooi, C. M. Procopiuc, and D. Srivastava, 2010: On multi-column foreign key discovery. Proc. VLDB Endow., 3, no. 1–2, 805–814, doi:10.14778/1920841.1920944.