1 Valid annotation constraints

Among the key, distinct, and identifying constraints, there are correlations between "key yes" and "distinct yes".

- "Distinct yes" on an observation type implies that its measurements collectively form a key of this observation type.
- Logically, we can specify "Distinct no" on an observation type and specify "key yes" on all of its measurements. In this case, when two rows (for the observation type) have the same values for these key measurements, they represent the different observation instances. It means that there may be other "variables" that can distinguish one observation instance from the other, but this dataset does not catch this variable (**HP: is "variable" the right word to use?**). So, in real application, we do not encourage such situation to appear.

An example with invalid annotation: given the data in Table 1. The following annotation is *invalid*. According to the annotation, if two plots have the same value on EntityName, they represent the same plot observation. Obviously, it will have probelem to interprete the data in Table 1 with this annotation. E.g., the first and second row catching plot with EntityName A should be the same plot observation. However, the data shows that this one plot has two different areas 1.0 and 1.1, so, there is confusion here.

```
observation "o1" distinct yes
entity "Plot"
measurement "m1" key yes
characteristic "EntityName"
standard "Nominal"
measurement "m2"
characteristic "area"
standard "sqft"
... Not finished....
```

plt	area	spp	dbh
A	1.0	piru	35.8
A	1.1	piru	36.2
В	2.0	piru	33.2
В	2.0	abba	34

Table 1: Dataset

In our algorithm, we assume that the annotations on the dataset are valid, i.e., they comply with the correlation rules among these constraints.

From HP: More to come on this part...

2 Data materialization algorithm

The **MaterializeDB** algorithm catches the *key*, *distinct* and *identifying* constraints in the annotation during the materialization process. The input of the algorithm is the Dataset and the annotations A.* on it. Each row in the input dataset represents the information related to one or more observations and their contexts. The input A.* represents the annotation information. More specifically,

- A.MeasType = $\{\langle MeasTypeId, ObsTypeId, CharType, StdType, ProtType, Precision, isKey \rangle\}$;
- A.ObservationType = $\{\langle \underline{ObsTypeId}, EntTypeId, isDistinct \rangle\}$ Note that, we hide the "AnnotId" in this schema, which denotes the resource the annotation is on. We

do not include this in the algorithm because the algorithm focuses on dealing with annotations on one resource. This way, we can simplify the description.

- A.ContextType = $\{\langle ObsTypeId, ContextObsTypeId, RelType, isIdentify\}\}$
- A.Map = $\{\langle MeasTypeId, ResAttribute, Cond, Val \rangle\}$

The output of the algorithm is a set of materialized tables represented in the OBOE model and denoted by OBOE.*. In detail,

- $OBOE.Observation = \{\langle ObsId, EntId \rangle\}$ keeps all the observation instances materialized from Dataset.
- $OBOE.Measurement = \{\langle \underline{MeasId}, ObsId, MeasType, Val \rangle\}$
- $OBOE.Entity = \{\langle \underline{EntId}, EntType \rangle\}$
- $OBOE.Context = \{\langle ObsId, ConextObsId, ContextType \rangle\}$

Algorithm 1 shows the framework of our algorithm. In this algorithm, ObsIdx is the index structure maintained for the observation instances whose types are specified with $distinct\ yes$. This index maintains the mapping from observation type and key values to its corresponding observation instance id. Obviously, only when observation type is specified with $distinct\ yes$, i.e., we want to keep track of the same observation instances, we need to maintain their instances in this index. The key values can be calculated in three different cases. In the first case where just one measurement of an observation type is specified with "key yes" the key value is the value of this "key" measurement. In the second case, several measurement types are marked with "key yes", the key value is the combined value of these several measurement. In the third case, this object type is marked with "identifying yes", the key value is the combined value of its context observation's key measurement values.

Similarly, in case that some measurement type(s) of an observation type is/are specified with "key yes", if different observation instances have the same value on these key measurements, semantically, we interpret that they are of the same entity. *Entidx* is the index structure for tracking the distinct entities. The key value is computed in the same way as that for an observation instance.

The procedure of this algorithm is very straightforward. It processes the dataset in a row-wise manner. In dealing with each row, five steps are involved. The first step generates orphan measurement instances which are not connected any observation instances. The second step group these measurement instances according to their observation types. Then, for different observation types, we materialize entity instances and observation instances by either creating a new one or return an existing one. The last step assigns the context relationship among the different observation instances.

Analysis of MaterializeDB.

Time: As can be seen that this algorihm scans the original data file in a row-by-row manner without revisiting the already seen rows. So, it is linear in the size of the dataset. We use EntIdx and ObsIdx to facilitate the checking of unique entity and observation instances. Let m be the number of unique keys, each checking could take $O(\log(m))$ time. So, in total, the algorithm runs in $O(n \log(m))$ where $m \ll n$ generally. **Space**: EntIdx and ObsIdx are the intermdedite structures that we use in the algorithm. Since they keep the unique entity and observation key values. The space complexity is of O(m).

	yr	spec	spp	dbh
	2007	1	piru	35.8
	2008	1	piru	36.2
ĺ	2008	2	abba	33.2

Table 2: Dataset 1

Example 2.1 (Example with "key yes" and "distinct yes", without "identifying yes") Take the data in Table 2^{1} as an example to explain the algorithm.

¹This is in page 6 in the powerpoint file.

Algorithm 1 MaterializeDB (Dataset, A.*)

```
/* Dataset: [Input] in the form of a flat file */
/* A : [Input] Annotations*/
ObsIdx = \emptyset; /* Keep index \langle ObsTypeId, KeyVal \rangle \rightarrow ObsId*/
EntIdx = \emptyset; /* Keep index \langle ObsTypeId, KeyVal \rangle \rightarrow EntId^*/
for (each Row\langle A1, A2, \cdots, An \rangle \in Dataset) do
  /* Step 1: Define measurement instances */
  MeasSet = CrtMeasurement(Row, A.*);
  /* Step 2: Partition the measurement instances according to observation types*/
  ObsType2MeasIdx = PartMeas(MeasSet, A.*);
  ContextIdx = \emptyset; /* Keep index ObsTypeId \rightarrow ObsId to materialize context*/
  for (each ObsTypeId \in ObsType2MeasIdx.keys) do
     /* Step 3: Find or create the entity instance for each observation type partition */
     EntId = MaterializeEntity(ObsTypeId, ObsType2MeasIdx, EntIdx, A.*, OBOE.*);
     /* Step 4 Find or create the observation instance for each observation type partition */
     MaterializeObs(ObsTypeId, EntId, ObsType2MeasIdx, ObsIdx, ContextIdx, OBOE.*);
  end for
  /* Step 5: Assign the context observation instances */
  MaterializeContext(ContextIdx, A.*, OBOE.*);
end for
return OBOE;
```

Algorithm 2 CrtMeasurement (Row, A.*)

```
/* Create new orphan measurement instances*/
MeasSet = \emptyset; /* Keep the set of new measurement instances*/
for (each m = \langle MeasTypeId, ResAttribute, Cond, Val \rangle \in A.Map) do
    if((m.ResAttribute! = Row.Ai.Attrname) OR (Row.Ai does not satisfy m.Cond)) continue;
    mi_{id} = \text{GetNewMeasId}(OBOE.Measurement);
    if (m.Val! = NULL) MeasVal = m.Val;
    else MeasVal = Row.Ai.Val;
    Create a measurement instance \langle mi_{id}, null, MeasType, MeasVal \rangle and add it to MeasSet;
end for
return MeasSet
```

For Row(2007, 1, piru, 35.8)

• Step 1 creates four measurement instances: $\langle mi_1, null, Year, 2007 \rangle$, $\langle mi_2, null, DBH, 35.8 \rangle$,

Algorithm 3 PartMeas (MeasSet, A.*)

```
/* Partition measurement instances according to their observation types*/
ObsType2MeasIdx = \emptyset /* Keep index for ObsTypeId \rightarrow \{mi\} */
for (each mi \in MeasSet) do
ObsTypeId = GetObsTypeId (A.MeasType, mi.MeasTypeId);
Update ObsType2MeasIdx by changing the item ObsTypeId \rightarrow \{mi\};
end for
return ObsType2MeasIdx;
```

Algorithm 4 Materialize Entity (ObsTypeId, ObsType2MeasIdx, EntIdx, A.*, OBOE.*)

```
KeyVal = \operatorname{GetObsTypeKeys} \ (ObsTypeId, ObsType2MeasIdx); \\ HasKey = \operatorname{false}; \\ \textbf{if} \ (ObsTypeId \ \text{has key measurements OR is specified with distinct yes}) \ HasKey = \operatorname{true}; \\ EntType = \operatorname{GetObsEntityType} \ (A.ObservationType, ObsTypeId) \\ CrtNewEntInst = \operatorname{true}; \\ \textbf{if} \ (HasKey = \operatorname{true}) \ \textbf{then} \\ EntId = \operatorname{GetEntId}(ObsTypeId, KeyVal, EntIdx); \\ \textbf{if} \ (EntId! = NULL) \ CrtNewEntInst = \operatorname{false}; \\ \textbf{end if} \\ \textbf{if} \ (CrtNewEntInst = true) \ \textbf{then} \\ EntId = \operatorname{CrtEntId}(EntType); \\ \operatorname{Create an entity instance} \ ei = \langle EntId, EntType \rangle \ \text{and put } ei \ to \ OBOE.Entity; \\ \textbf{if} \ (HasKey = \operatorname{true}) \ EntIdx = EntIdx \cup \{\langle ObsTypeId, KeyVal \rangle \rightarrow EntId\}; \\ \textbf{end if} \\ \textbf{return} \ EntId; \\ \end{aligned}
```

Algorithm 5 MaterializeObs(ObsTypeId, EntId, ObsType2MeasIdx, ObsIdx, ContextIdx, OBOE.*)

```
KeyVal = GetObsTypeKeys (ObsTypeId, ObsType2MeasIdx);
IsObsDistinct = CheckIfObsDistinct(A.ObservationType, ObsTypeId);
CrtNewObsInst = true;
if (IsObsDistinct==true) then
  ObsId = GetObsId(ObsTypeId, KeyVal, ObsIdx);
  if(ObsId! = NULL) \ CrtNewObsInst = false;
end if
if (CrtNewObsInst == true) then
  Create an observation instance oi = \langle ObsId, EntId \rangle and put oi to OBOE. Observation;
  if (IsObsDistinct = true) \ ObsIdx = ObsIdx \cup \{\langle ObsTypeId, KeyVal \rangle \rightarrow ObsId\};
end if
/*Maintain the measurement instances for this observation*/
miSet = GetMeasInst(ObsType2MeasIdx, ObsTypeId);
if (ObsId) is a new one) Set the obsId to each mi \in miSet so that mi-s are not orphans;
else Discard all the mi \in miSet;
Put all the mi \in miSet to OBOE.Measurement;
ContextIdx = ContextIdx \cup \{ObsTypeId \rightarrow ObsId\}; /* ContextIdx is also output*/
```

 $\langle mi_3, null, TaxonomicTypeName, Picea rubens \rangle$, $\langle mi_4, null, EntityName, 1 \rangle$,

Algorithm 6 MaterializeContext(ContextIdx, A.*, OBOE.*)

```
for (ObsTypeId \rightarrow ObsId \in ContextIdx) do ContextObsTypeId, Rel = GetContextObsTypeRel(A.ContextType, ObsTypeId); if (ContextObsTypeId! = NULL) then ContextObsId = GetContextObsId(ContextIdx, ContextObsTypeId); Create a context instance ci = \langle ObsId, ContextObsId, Rel \rangle; Put ci to OBOE.Context; end if end for
```

and returns $MeasSet = \{mi_1, mi_2, mi_3, mi_4\}; ^2$.

 $^{^2}$ For all the instances, the measurement characteristic is set to represent Measurement Type

- Step 2 returns $ObsType2MeasIdx = \{\{o_1 \rightarrow \{mi_1\}, o_2 \rightarrow \{mi_2, mi_3, mi_4\}\}\}.$
- Step 3-4: for each observation types o₁ and o₂, materialize entity and observation instance
 - for o_1 (with associated instance mi_1 of type m_1
 - * Since m_1 is specified as key, get the KeyVal = 2007;
 - * No entity with this key exists in EntIdx, create an entity $\langle ei_1, TemporalRange \rangle$; Now, $EntIdx = \{\langle o_1, 2007 \rangle \rightarrow ei_1 \}$.
 - * Since o_1 is specified as distinct, need to make sure we do not create redundant observation instances. No entry with the key $\langle o_1, 2007 \rangle$ exists in ObsIdx, so, create an observation instance oi_1 , which is of entity ei_1 and represented as $\langle oi_1, ei_1 \rangle$. Now, ObsIdx = $\{\langle o_1, 2007 \rangle \rightarrow oi_1 \}$
 - * Connect mi₁ to oi₁;
 - When deal with o_2 ,
 - * KeyVal = 1.
 - * Create an entity instance $\langle ei_2, Tree \rangle$; $EntIdx = \{\langle o_1, 2007 \rangle \rightarrow ei_1, \langle o_2, 1 \rangle \rightarrow ei_2 \}$.
 - * Create an observation $\langle oi_2, ei_2 \rangle$. No need to update ObsIdx because o_2 is not identified as distinct.
 - * Connect mi₂, mi₃ and mi₄ to oi₂;
- Step 5 assigns the context relationship between oi_1 and oi_2 ;

For Row (2008, 1, piru, 36.2)

- Step 1 creates measurement instances $\langle mi_5, null, Year, 2007 \rangle$, $\langle mi_6, null, DBH, 35.8 \rangle$, $\langle mi_7, null, TaxonomicTypeName, Picea rubens \rangle$, $\langle mi_8, null, EntityName, 1 \rangle$ and returns $MeasSet = \{mi_5, mi_6, mi_7, mi_8\}$;
- Step 2 gets ObsType2MeasIdx = $\{\{o_1 \to \{mi_5\}, o_2 \to \{mi_6, mi_7, mi_8\}\}\}$
- Step 3-4: for each observation types o₁ and o₂ materialize entity and observation instance
 - for o_1
 - * KeyVal = 2008;
 - * Create an entity instance $\langle ei_3, TemporalRange \rangle$; $EntIdx = \{ \langle o_1, 2007 \rangle \rightarrow ei_1, \langle o_2, 1 \rangle \rightarrow ei_2, \langle o_1, 2008 \rangle \rightarrow ei_3 \}.$
 - * Create an observation instance $\langle oi_3, ei_3 \rangle$; $ObsIdx = \{\langle o_1, 2007 \rangle \rightarrow oi_1, \langle o_2, 1 \rangle \rightarrow oi_2, \langle o_1, 2008 \rangle \rightarrow oi_3 \}$
 - * Connect mi₅ to oi₃;
 - When deal with o_2 ,
 - * KeyVal = 1.
 - * item $\langle o_2, 1 \rangle \to ei_2$ is already in EntIdx, so get the entity id ei_2 . No need to create an entity.
 - * Since o_2 is not specified with distinct yet, we NEED to create an observation $\langle oi_4, ei_2 \rangle$. No need to update ObsIdx.
 - * $Connect \ mi_6, mi_7, mi_8 \ to \ oi_4;$

For ROW (2008, 2, abba, 33.2)

• For o_1 's measurement 2008,

- Since $\langle o_1, 2008 \rangle \rightarrow ei_3$ already exists in EntIdx, no need to create a new entity.
- Since o_1 is specified with distinct yes, and $\langle o_1, 2008 \rangle \rightarrow oi_3$ already exists in ObsIdx, no need to create a new OBSERVATION and no need to put the measurement instance for 2008 into OBOE model.

plt	spp	dbh
A	piru	35.8
A	piru	36.2
В	piru	33.2

Table 3: Dataset 2

Example 2.2 (Example with identifying) Let us use the data in Table 3 as an example. Before we go through the algorithm step by step, we first note that o_1 and o_2 have key measurements m1 and m_2 respectively. So, we need to maintain the distinct entity instances for both of these two observation types. In addition, o_1 is specified with distinct yes while o_2 is not. So, we need to maintain the distinct observation instances for o_1 but not for o_2 .

For the first row,

- The first step generates three measurement instances $MeasSet = \{\langle mi_1, null, EntityName, A \rangle, \langle mi_2, null, TaxonomicTypeName, Picea rubens \rangle, \langle mi_3, null, DBH, 35.8 \rangle \}.$
- The second step gets $ObsType2MeasIdx = \{\{o_1 \rightarrow \{mi_1\}, o_2 \rightarrow \{mi_2, mi_3\}\}\}.$
- For each observation type, create entity and observation instances.
 - For o_1 , the key value is A. Since there is no such a key in EntIdx, we create an entity ei_1 of type Plot. EntIdx = $\{\langle o_1, A \rangle \rightarrow ei_1 \}$.

We create an observation instance oi_1 whose entity is ei_1 .

 $ObsIdx = \{\langle o_1, A \rangle \to oi_1 \}$. Connect the measurement instances to observation instances $mi_1 \to oi_1$.

- For o_2 , the key value is $(A, Picea\ rubens)$ since it has context o_1 with "identifying yes", we create an entity instance ei_2 of type Tree.

 $EntIdx = \{\langle o_1, A \rangle \rightarrow ei_1, \langle o_2, (A, Picea\ rubens) \rangle \rightarrow ei_2 \}.$

We create an observation instance oi_2 whose entity is ei_2 .

Connect the measurement instances mi_2 and mi_3 to observation instance oi_2 .

• The last step for this row is to connect the observations using context relationship. For this instance, we connect oi₁ to oi₂ with context "Within".

For the second row,

- The first step defines three measurement instances $MeasSet = \{\langle mi_4, null, EntityName, A \rangle, \langle mi_5, null, TaxonomicTypeName, Picea rubens \rangle, \langle mi_6, null, DBH, 36.2 \rangle \}.$
- The second step gets $ObsType2MeasIdx = \{\{o_1 \rightarrow \{mi_4\}, o_2 \rightarrow \{mi_5, mi_6\}\}\}.$
- For each observation type, create entity and observation instances.
 - For o_1 , the key value is $\langle o_1, A \rangle$, EntIdx already has an item for it with entity instance ei_1 . No need to create a new instance for it.

To create observation instance, since o_1 is specified with "distinct yes" and the key value is $\langle o_1, A \rangle$, which corresponds to observatin instance o_1 . So, we do not need to create a new observation for

it.

When we try to connect the measurement instance mi_4 to observation instance, we realize that we did not create a new observation instance for type o_1 . So its related measurement instance mi_4 can be discarded.

For o2, the new key value is \$\langle o2, (A, Picea rubens) \rangle\$, which corresponds to ei2 in EntIdx, so no need to create a new instance for it either.
 To create observation instances, since no "distinct yes" is specified, we create a new observation instance oi3 for it. Then, we connct the measurement instances \$\{m_5, m_6\}\$ to observation instance oi3.

When we process the **third row**, we have a new key value $\langle o_1, B \rangle$ for o_1 , thus we create a new entity instance for it. For o_2 , we have new key value $\langle o_2, (B, Picea rubens) \rangle$ and create a new entity instance for it.