

How to Bake an Uncertainty Pie

Take Even Parts of Abstract Interpretation, K-relations, and Zonotopes
and Mix Thoroughly

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- 1 Incomplete Databases, Repairs, and Approximations
- 2 Abstract Interpretation
- 3 Queries over Uncertain K-relations
- 4 Learning Linear Models over Uncertain Data
- 5 Conclusions
- 6 Appendix



Computations over uncertainty data

- Queries and **machine learning** training and inference
- The uncertainty will typically stem from **unrecoverability** of the ground truth clean version of dirty dataset
- Inherent complexity often necessitates approximation
 - **Over-approximation** of the set of **possible** results
 - **Under-approximation** of what is **certainly** known to be true

Connections to abstract interpretation and control theory

- Abstract interpretation [Cou96]
- Reachability analysis [ASB08]



Query evaluation

- Using K-relations and interval domains for query evaluation

Machine learning: training and inference

- Using convex polytopes for training and inference with linear models



Missing Values (NULLs)

Salary	Tax
35,000	3,300
	1,200
149,000	5,000

Constraint Violations

- A is a key for R

A	B
1	1
1	2
2	2
3	1
3	2



Definition (Incomplete databases)

An **incomplete database** D^\odot is a set of databases:

$$D^\odot = \{D_1, D_2, \dots, D_n\}$$

Uncertainty stemming from dirty data

Given a "dirty" database D we consider all **possible clean versions** as an incomplete database D^\odot

Possible world semantics

Given some function F define its evaluation on an incomplete database, under **possible world semantics** as

$$F(D^\odot) = \{F(D_1), \dots, F(D_n)\}$$

Definition (Certain Answers)

The **certain answers** $\text{CERTAIN}(Q, \mathbf{D}^\odot)$ to a query Q over an incomplete database \mathbf{D}^\odot are:

$$\text{CERTAIN}(Q, \mathbf{D}^\odot) = \bigcap_{\mathbf{D} \in \mathbf{D}^\odot} Q(\mathbf{D})$$

Definition (Possible Answers)

The **possible answers** $\text{POSSIBLE}(Q, \mathbf{D}^\odot)$ to a query Q over an incomplete database \mathbf{D}^\odot are:

$$\text{POSSIBLE}(Q, \mathbf{D}^\odot) = \bigcup_{\mathbf{D} \in \mathbf{D}^\odot} Q(\mathbf{D})$$



Representation systems

- **representation system** [ILJ84] is a pair (\mathbb{A}, Mod)
 - $\mathbb{A} = \{\mathcal{A}_i\}$ - the representations
 - each element \mathcal{A} represents an incomplete database $\text{Mod}(\mathcal{A})$
- (\mathbb{A}, Mod) is **closed** under classes of computations \mathbb{F} :

$$\forall F \in \mathbb{F} : \text{Mod}(F(D^\#)) = F(\text{Mod}(D^\#))$$



Limitations

- Some representation systems are only closed under relatively small classes of queries
 - e.g., V-tables [LJ84] not closed under selection with inequalities
- Some representation systems are not concise
 - e.g., aggregation over C-tables [LJ84] can result in exponential blowup
- Delaying complexity
 - e.g., [ADT11] handles aggregation, but extracting all worlds is hard
- PTIME is often not good enough
 - e.g., joins can degenerate into cross-products



Relax two requirements of representation systems

- ❶ representations are allowed to be **over-approximations**
 - assign each incomplete database D^\odot with a representation $\alpha(D^\odot) = \mathcal{A}$
 - that can be an over-approximation: $\text{Mod}(\alpha(D^\odot)) \supseteq D^\odot$
- ❷ computations should **preserve** this **over-approximation**

$$\text{Mod}(F(\alpha(D^\odot))) \supseteq F(D^\odot)$$



Certain facts for an incomplete databases $\text{CERTAIN}(\mathbf{D}^\odot) = \bigcap_{D \in \mathbf{D}^\odot} D$

- now we require $\alpha(\cdot)$ to under-approximate
- extend representation system with an operation $\text{CERTAIN}^\downarrow$
- require **under-approximation**: $\text{CERTAIN}^\downarrow(\alpha(\mathbf{D}^\odot)) \subseteq \text{CERTAIN}(\mathbf{D}^\odot)$
- computations should **preserve** this **under-approximation**

$$\text{CERTAIN}^\downarrow(F(\alpha(\mathbf{D}^\odot))) \subseteq \text{CERTAIN}(F(\mathbf{D}^\odot))$$



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Definition (Abstract Domain)

Given a **concrete domain** \mathbb{D} , an **abstract domain** is a set \mathbb{D}^\sharp with two operations:

- **abstraction** $\alpha : \mathcal{P}(\mathbb{D}) \rightarrow \mathbb{D}^\sharp$
- **concretization**: $\gamma : \mathbb{D}^\sharp \rightarrow \mathcal{P}(\mathbb{D})$

such that for any set $S \subseteq \mathcal{P}(\mathbb{D})$

$$\gamma(\alpha(S)) \supseteq S$$

Definition (Abstract Transformers)

Given a function $F : \mathbb{D}_1 \rightarrow \mathbb{D}_2$ and abstract domains \mathbb{D}_1^\sharp and \mathbb{D}_2^\sharp an **abstract transformer** $F^\sharp : \mathbb{D}_1^\sharp \rightarrow \mathbb{D}_2^\sharp$ for F has to fulfill for any $S \subseteq \mathcal{P}(\mathbb{D}_1)$:

$$\gamma\left(F^\sharp(\alpha(S))\right) \supseteq F(S)$$

Interval Domain

- concrete domain: \mathbb{R}
- abstract domain: $\mathbb{R}_I = \{[l, u] \mid l \leq u \wedge l, u \in \mathbb{R}\}$
- abstraction: for $S \subseteq \mathbb{R} : \alpha(S) = [\inf S, \sup S]$
- concretization: $\gamma([l, u]) = \{c \mid c \in [u, l]\}$

Interval Arithmetic

- $[a, b] + [c, d] = [a + c, b + d]$
- $[a, b] - [c, d] = [a - d, b - c]$
- $[a, b] \cdot [c, d] = [\min(ac, ad, bc, bd), \max(ac, ad, bc, bd)]$

[dFS04]



Zonotope Domain

- concrete domain: \mathbb{R}^n
- abstract domain
 - set of variables \mathcal{E}
 - affine forms: $\mathbb{A} = \{a_0 + \sum_{\epsilon_i \in \mathcal{E}} a_i \cdot \epsilon_i \mid a_i \in \mathbb{R}\}$ with finite support
 - zonotopes: $\mathcal{Z}_n^\# = \{\mathbf{z} \mid \mathbf{z} \in \mathbb{A}^n\}$
- abstraction: $\alpha(S) = \mathcal{IH}(S)$ (interval hull)
- concretization: $\gamma(\mathbf{z}) = \{\varphi(\mathbf{z}) \mid \varphi \text{ is a valuation}\}$
 - valuation: $\varphi : \mathcal{E} \rightarrow [-1, 1]$



Affine Arithmetic

- zonotopes
 - $\mathbf{z}_1 = a_0 + \sum_{\epsilon_i \in \mathcal{E}} a_i \cdot \epsilon_i$
 - $\mathbf{z}_2 = b_0 + \sum_{\epsilon_i \in \mathcal{E}} b_i \cdot \epsilon_i$
- addition: $\mathbf{z}_1 + \mathbf{z}_2 = a_0 + b_0 + \sum_{\epsilon_i \in \mathcal{E}} a_i \cdot b_i \cdot \epsilon_i$
- multiplication: $\mathbf{z}_1 \cdot \mathbf{z}_2 = a_0 b_0 + (\sum_{\epsilon_i \in \mathcal{E}} (a_0 \cdot b_i + a_i \cdot b_0) \cdot \epsilon_i) + c \cdot \epsilon_{new}$
 - $c = (\sum_i |a_i|) \cdot (\sum_i |b_i|)$



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Natural order

- Semiring $(K, +_K, \cdot_K, 0_K, 1_K)$
- Define $k_1 \leq_K k_2 \Leftrightarrow \exists k_3 : k_1 + k_3 = k_2$
- A semiring is **naturally ordered** if \leq_K is a partial order

Properties of the natural order

- natural order is preserved under semiring operations:
- **addition:** $a \leq_K c \wedge b \leq_K d \Rightarrow a +_K b \leq_K c +_K d$
- **multiplication:** $a \leq_K c \wedge b \leq_K d \Rightarrow a \cdot_K b \leq_K c \cdot_K d$



Definition (Incomplete K-databases)

An incomplete K database D^\odot is a set of K databases $\{D_1, \dots, D_n\}$

D_1

name	salary	
Boris	120k	1
Peter	150k	1
Peter	380k	2

D_2

name	salary	
Peter	180k	2

Abstract Domain

- Assume a naturally ordered semiring K , then we can use K databases as abstract domains [FHGK19],
- **abstraction**

$$\forall t : \alpha(\mathbf{D}^\odot)(t) = \sup_{\mathbf{D} \in \mathbf{D}^\odot} \mathbf{D}(t)$$

- **concretization**

$$\gamma(D) = \{D' \mid \forall t : D'(t) \leq_K D(t)\}$$



Abstract Transformers for Relational Algebra Operators

- Under the standard K-relational semantics for positive relational algebra [GT17], operators are abstract transformers.
- This follows from the preservation of natural order under semiring operations



- Use interval domain values to encode value uncertainty
- Also for aggregation results [ABC⁺03, AK08, DK22]

name	salary	
Boris	[120k,120k]	[0,2]
Peter	[140k,400k]	[2,3]



Selection

- requires interval arithmetic and embedding of Boolean intervals into the semiring K

Difference

- to be useful requires both upper and lower bounds [GL17]

Aggregation

- for \mathbb{N} there exist an abstract transformer for semi-module expressions [ADT11]



What has been achieved?

- a semantics for relational algebra over uncertain data with PTIME data complexity
 - closed under full relational algebra with aggregation and order-based operations (e.g., windowed aggregation)
- mechanisms to approximate repairs to common data quality issues and approximate common incomplete and probabilistic data models
- uniform treatment of aggregation results and value uncertainty
- Approximating certain and possible answers
 - under-approximation of certain answers with value uncertainty
 - over-approximation of possible answers with value uncertainty
- Over-approximation of the set of possible worlds

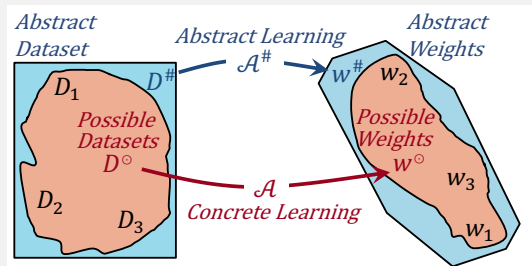


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Setting

- uncertain training D^\odot with features X^\odot and labels and test datasets X_{test}^\odot
- consider linear models trained with ridge regression (l_2 regularization)
- train an over-approximation of all possible models
- compute an over-approximation of all possible inference outcomes



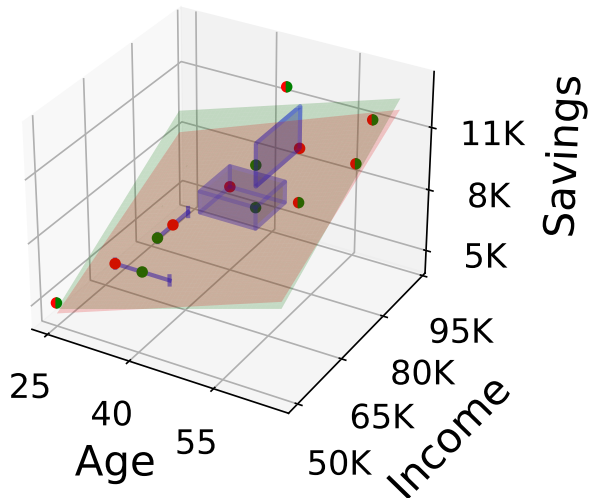
Training Data

Age	Income	Savings
25	50K	5K
NULL	60K	6K
35	NULL	7K
NULL	NULL	[8K,9K]
45	90K	12K
50	NULL	[10K,12K]
55	75K	9K
60	85K	10K
65	80K	13K

Test Data

Age	Income	Savings
25	50K	??
40	60K	??
20	90K	??
70	50K	??





● Possible World 1 ● Possible World 2

● Sav. = $-2855 + 98 \times \text{Age} + 0.1 \times \text{Inc.}$

● Sav. = $-3361 + 84 \times \text{Age} + 0.1 \times \text{Inc.}$

- Each training data world D_i induces a model!

- $w_i^* = \mathcal{A}(D_i)$



The difference in models leads to a difference in predictions

Predictions in world D_1 with w_1^*

$$\text{sav.} = -2855 + 98 \cdot \text{Age} + 0.1 \cdot \text{Inc.}$$

Age	Income	Savings
25	50K	4595
40	60K	7065
20	90K	8105
70	50K	9005

Predictions in world D_2 with w_2^*

$$\text{sav.} = -2855 + 84 \cdot \text{Age} + 0.1 \cdot \text{Inc.}$$

Age	Income	Savings
25	50K	4245
40	60K	6505
20	90K	7825
70	50K	8025

Fixed Point Gradient Descent

- Model weights \mathbf{w}
- Loss L
- Learning Rate η

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + \left(-\eta \cdot \nabla L(\mathbf{w}^{(t)}) \right)$$

Abstract Gradient Descent

- Exact abstract transformers exist for all operations of gradient descent for linear regression
 - requires polynomial zonotopes

$$\mathbf{w}^{\#(t+1)} = \mathbf{w}^{\#(t)} + \left(-\eta \odot \nabla^{\#} L^{\#}(\mathbf{w}^{\#(t)}) \right)$$

Abstract Fixed Points (Equivalence)

$$\gamma(\mathbf{w}^{\#*}) = \gamma\left(\mathbf{w}^{\#*} + \left(-\eta \cdot \nabla^{\#} L^{\#}(\mathbf{w}^{\#(t)})\right)\right)$$

Existence of Fixed Points

- Abstract fixed points exists
- Reached once all concreted gradient descent processes have converged

Challenges

- The size of the representation grows exponentially in the number of gradient descent steps



Ridge regression

$$L(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{1}{n} \sum_{i=1}^n (y'_i - y_i)^2 = \frac{1}{n} (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})$$

Gradient Descent

$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{2}{n} (\mathbf{X}^T \mathbf{X} \mathbf{w}^t - \mathbf{X}^T \mathbf{y}) + 2\lambda \mathbf{w}^t$$

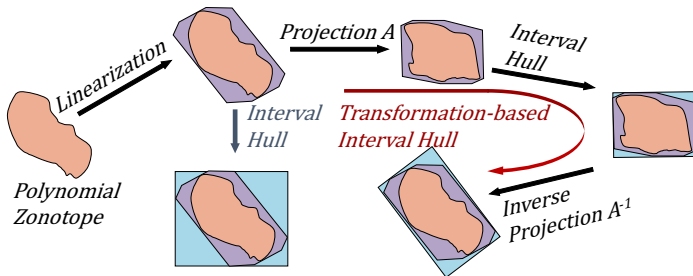


Order-Reduction

- **Order-reduction**
over-approximates a zonotope with another zonotope of smaller representation size

Linearization

- **Linearization**
over-approximates polynomial zonotopes with linear zonotopes



Challenges

- Fixed point may not exist

Abstract gradient descent with order-reduction and linearization

$$\mathbf{w}^{\#(t+1)} = \mathbf{R} \left(\mathbf{w}^{\#(t)} + \mathbf{L} \left(-\eta \cdot \nabla^{\#} L^{\#}(\mathbf{w}^{\#(t)}) \right) \right)$$

Decomposition

- Decomposition: $\mathbf{w}^{\#*} = \mathbf{w}_R^* + \mathbf{w}_D^{\#*} + \mathbf{w}_N^{\#*}$ is a fixed point if:

$$\mathbf{w}_R^* = \Phi_R(\mathbf{w}_R^*), \quad \mathbf{w}_D^{\#*} = \Phi_D^{\#}(\mathbf{w}_R^*, \mathbf{w}_D^{\#*}) \quad \mathbf{w}_N^{\#*} \simeq_{\#} \Phi_N^{\#}(\mathbf{w}_R^*, \mathbf{w}_D^{\#*}, \mathbf{w}_N^{\#*})$$

- Choose order-reduction to construct fixed point

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Abstract Interpretation

- Over-approximate sets of *"possible worlds"*
- Abstract transformers: computations that preserve the over-approximation

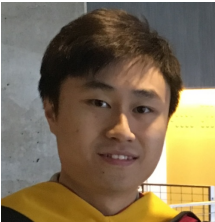
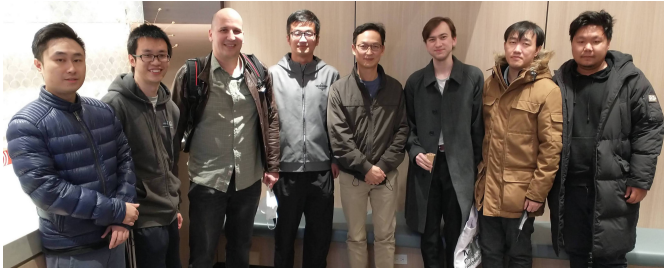
Applications to machine learning

- Can we go beyond linear models

Applications to databases

- Databases with zonotope values: **z-tables**
- What about annotations?
 - can we model correlation





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