Certifiable Robustness for Nearest Neighbor Classifiers

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DB Affiliates Workshop Sep 22, 2022

Motivation



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Certifiable robustness as a measure of such confidence.

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Certifiable Robustness, I

Definition (Certifiable Robustness for *k*-NN Classifier)

Given an inconsistent database D with labels and a test point x, then x is said to be certifiably robust for k-NN classifier if the prediction of k-NN about x on any repair of D is consistent.

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A classification learning algorithm \mathcal{L} with labels in \mathcal{Y} takes a labeled instance I over the schema $R(A_1, \ldots, A_d)$ as training set, and returns a classifier which is a total function $\mathcal{L}_I : \mathbb{D}^d \to \mathcal{Y}$.

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Definition (Certifiable Robustness)

Let \mathcal{I} be a labeled uncertain instance over $R(A_1, \ldots, A_d)$ and \mathcal{L} be a classification learning algorithm with labels in \mathcal{Y} . We say that a (test) point $x \in \mathbb{D}^d$ is certifiably robust in \mathcal{I} if there exists a label $\ell \in \mathcal{Y}$ such that for every repair $I \in \mathcal{I}$, $\mathcal{L}_I(x) = \ell$. The label ℓ is called a certain label for x.

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There has been a long line of reserach in establishing dichotomies in CQA [Wij09, Ber11, KP12, KS14, KW18, KOW21].

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Definition (#CR-NN_< $\langle \mathbf{R} \rangle$)

Given an inconsistent labeled instance D over an FD schema \mathbf{R} , a strict ordering of the points in D w.r.t. their distance from a test point x, and a label $\ell \in \mathcal{Y}$, output the number of repairs for which the k-NN classifier assigns label ℓ to x.

Definition (Ihs Chain)

A set of FDs Σ has a left-hand-side chain (lhs chain for short) if for every two FDs $X_1 \rightarrow Y_1$ and $X_2 \rightarrow Y_2$ in Σ , either $X_1 \subseteq X_2$ or $X_2 \subseteq X_1$ [LKW21].

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The FD set $\{A \rightarrow C, B \rightarrow C\}$ does not have an lhs chain, while the FD set $\{AB \rightarrow C, B \rightarrow D\}$ has an lhs chain.

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Theorem (Decision, F. & Koutris, 22')

Let **R** be an FD schema. Then, the following hold:

If R is equivalent to an FD schema with an lhs chain, then CR-NN_<⟨R⟩ (and thus CR-NN_p⟨R⟩) is in P.

Otherwise, for any integer k ≥ 1, CR-NN_p⟨**R**, k⟩ (and thus CR-NN_<⟨**R**⟩) is coNP-complete.

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Theorem (Counting, F. & Koutris, 22')

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- Investigate CR for three widely used uncertain models:
 - ?-sets;
 - or-sets;
 - Codd-tables.

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Similar to the recursive algorithm in [LKR20], divided into Base Case (FD is empty), Consensus FD (there exists an FD $\emptyset \to A$), and Common Attribute (attribute A in the lhs of all FDs).

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Idea: say we want to know whether label 1 certifiably robust, we will then try to falsify this by finding a repair which maximizes the difference between the numbers of top-k tuples with label i and label 1, where i loops over all other labels.

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Open question: can we do better?

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Hardness of decision problem $\text{CR-NN}_p\langle \mathbf{R}, k \rangle$, II





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Step 3: Encode the entries of D into numerics so that everything (p-norm values) goes through.

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Theorem

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Proof.

Livshits, Kimelfeld, and Wijsen showed that it is #P-hard to count the number of repairs. Now, given any instance D, we can pick any ordering of the points and assign the same label ℓ to every tuple. Then, the number of repairs that predict label ℓ is the same as the total number of repairs.

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	Our algorithm	Karlas et al.'s
Time Complexity	$O(D \cdot m)$	$O(D \cdot m)$ for MM
		$\Omega(D \cdot {\binom{m+k-1}{k}})$ for SS
Applicability	any k and m	MM only for $m = 2$
		only under the restriction
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MIN-REPAIR: to find the subset repair that has tuples with the smallest total weight.

FORBIDDEN-REPAIR: given an inconsistent instance D and a subinstance $S \subseteq D$, does there exist a subset repair $I \subseteq D$ such that $I \cap S = \emptyset$?

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Certifiable robustness

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Thank You!

References I

- Leopoldo E. Bertossi, *Database repairing and consistent query answering*, Synthesis Lectures on Data Management, Morgan & Claypool Publishers, 2011.
- Bojan Karlas, Peng Li, Renzhi Wu, Nezihe Merve Gürel, Xu Chu, Wentao Wu, and Ce Zhang, *Nearest neighbor classifiers over incomplete information: From certain answers to certain predictions*, Proc. VLDB Endow. **14** (2020), no. 3, 255–267.
- Paraschos Koutris, Xiating Ouyang, and Jef Wijsen, Consistent query answering for primary keys on path queries, PODS, ACM, 2021, pp. 215–232.
- Phokion G. Kolaitis and Enela Pema, A dichotomy in the complexity of consistent query answering for queries with two atoms, Inf. Process. Lett. 112 (2012), no. 3, 77–85.

References II

- Paraschos Koutris and Dan Suciu, A dichotomy on the complexity of consistent query answering for atoms with simple keys, ICDT, OpenProceedings.org, 2014, pp. 165–176.
- Paraschos Koutris and Jef Wijsen, Consistent query answering for primary keys and conjunctive queries with negated atoms, PODS, ACM, 2018, pp. 209–224.
- Ester Livshits, Benny Kimelfeld, and Sudeepa Roy, Computing optimal repairs for functional dependencies, ACM Trans.
 Database Syst. 45 (2020), no. 1, 4:1–4:46.
- Ester Livshits, Benny Kimelfeld, and Jef Wijsen, Counting subset repairs with functional dependencies, J. Comput. Syst. Sci. 117 (2021), 154–164.

References III

Jef Wijsen, Consistent query answering under primary keys: a characterization of tractable queries, ICDT, ACM International Conference Proceeding Series, vol. 361, ACM, 2009, pp. 42–52.