

@DS3Lab www.DS3Lab.com

### Towards Understanding End-to-end Learning in the Context of Data:

Machine Learning Dancing over Semirings and Codd's Table

Ce Zhang ce.zhang@inf.ethz.ch



### Rapid Progress of ML Systems





### **Rapid Progress of ML Systems**







### **Rapid Progress of ML Systems**





# While getting *some* ML models has never been easier,

### Understanding has never been more important

#### <u>ML today is now a Data Problem</u>

- Given the raw features from Kaggle, most AutoML platforms rank in the bottom 50%.
- It is the data that we need to improve, and knowledge that we need to integrate, to build better ML applications.
- <u>To improve data, we need to first understand them.</u>





### **Two Examples of Understanding**





**Q2**. Which training example is to blame or is most important for my accuracy/fairness/robustness?



### **Two Examples of Understanding**





**Q2**. Which training example is to blame or is most important for my accuracy/fairness/robustness?



### **Two Examples of Understanding**





Systems@ETH:

. . .

### So, what's the *problem*?



If the DB community don't fix this, who else are going to deal with data transformations?

### Our Goal











### **Overview**

#### <u>Theoretical Result</u>

- *Entropy/Expectation* of ML Training over Incomplete Information and Uncertainty
- *Shapley value* of ML Training over Feature Extraction Pipelines
- <u>Applications</u>
  - Data *Cleaning* for ML
  - *Defense* against backdoor adversarial attacks
  - Data *Debugging* for ML
  - Data *Market* for ML
- <u>Heuristics of Approximating Real-world Pipelines</u>
- Failure Cases & "Call for Help"









### Unknowns (Incomplete information) in DB



- What is Unknown in DB?
- How does DB answer queries under Unknowns?
- ... the nightmare of many undergrads in DB class...



### Unknowns (Incomplete information) in DB



• What is NULL?

> Sure/Certain Answer







#### ML over Unknowns: Certain Prediction (CP)





### ML over Unknowns: Certain Prediction (CP)

- Given an input relation *R* with a known noise model ...
- ... it defines a probability distribution over many possible worlds  $\{R_1...R_n\}$
- Given a test example *x*, the *expected prediction* on *x* is  $CP(x) = \mathbb{E}\mathcal{A}(R)[x]$

where  $\mathcal{A}(R)$  is a classifier trained on one possible *R*.

- The *entropy* is:
- $H(\mathcal{A}(R)[x])$
- Intuition of why this is useful:
  - Why Entropy goes to 0, noises in training set do not matter at all. (It won't change the result)
  - If we take this view, data cleaning for ML becomes the process of minimizing Entropy.





R

### Challenge and Result





#### Results

#### 1. <u>General Classifier</u>

- #P-Hard
- Approximation with MCMC

#### 2. <u>K-Nearest Neighbor Classifier</u>

- O(nd) Linear in # Unknowns to explore  $O(2^{nd})$  many worlds!
- <u>http://vldb.org/pvldb/vol14/p255-</u> <u>karlas.pdf</u> Trust me ☺
- Also apply to pipelines with only **map** operators



### Shapley Value: Setting







### **Expected Marginal Improvements**









#### Results



- General Classifier

   #P-Hard
  - Approximation with MCMC

#### 2. K-Nearest Neighbor Classifier

Pipeline Type		1NN	KNN
	map	$O(N \log N)$	$O(N^2)$
	map + fork	$O(N \log N)$	$O(N^2M^2)$
1-to-many joins		$O(N^4)$	$O(N^4)$
Polymonial with PTIME counting oracle		PTIME	PTIME

<u>https://ds3lab.inf.ethz.ch/datascope.</u>
 <u>html</u> Trust me <sup>©</sup>



**Goal:** Illustrate how locality of KNN can help. Similar ideas apply to both Entropy and Shapley Value.





### Data Valuation: 1. A Trivial $O(\binom{n}{k} + n \log n)$ Algorithm

Simplified Version (For Presentation) -

#### • <u>Input</u>:

- Training Relation R, |R| = n
- Target Training Example  $t \notin R$
- Validation Example  $s \notin R$
- Classification task
- Utility:

 $U(R) = |\{r \in KNN(R,s): r.y = s.y\}|/K$ 

• <u>**Output</u></u>: the <u>value</u> of t over R v(t) = \frac{1}{n!} \sum\_{R\_i \subseteq R\_T} {\binom{|R|}{|R\_i|}} \left[ U\left(R\_i \bigcup t\right) - U(R\_i) \right]</u>** 





### Data Valuation: 1. A Trivial $O(\binom{n}{K} + n \log n)$ Algorithm

Simplified Version (For Presentation)

#### • <u>Input</u>:

- Training Relation R, |R| = n
- Target Training Example  $t \notin R$
- Validation Example  $s \notin R$
- Classification task
- Utility:

 $U(R) = |\{r \in KNN(R,s): r.y = s.y\}|/K$ 

• <u>**Output</u></u>: the <u>value</u> of t over R v(t) = \frac{1}{n!} \sum\_{R\_i \subseteq R\_T} {\binom{|R|}{|R\_i|}} \left[ U\left(R\_i \bigcup t\right) - U(R\_i) \right]</u>** 





# Data Valuation: 1. A Trivial $O(\binom{n}{K} + n \log n)$ Algorithm

Simplified Version (For Presentation)

#### • <u>Input</u>:

- Training Relation R, |R| = n
- Target Training Example  $t \notin R$
- Validation Example  $s \notin R$
- Classification task
- Utility:

 $U(R) = |\{r \in KNN(R,s): r.y = s.y\}|/K$ 

• <u>**Output</u></u>: the <u>value</u> of t over R v(t) = \frac{1}{n!} \sum\_{R\_i \subseteq R\_T} {\binom{|R|}{|R\_i|}} \left[ U \left( R\_i \bigcup t \right) - U(R\_i) \right]</u>** 

### Can we do better?

(Yes, this trivial algorithm does not use all the properties that KNN has)



one only needs to compare the label

of *t* and the label of the last in top-K.





#### • <u>Input</u>:

- Training Relation R, |R| = n
- Target Training Example  $t \notin R$
- Validation Example  $s \notin R$
- Classification task
- Utility:

 $U(R) = |\{r \in KNN(R,s): r.y = s.y\}|/K$ 

• **<u>Output</u>**: the <u>value</u> of t over R  $v(t) = \frac{1}{n!} \sum_{R_i \subseteq R_T} {\binom{|R|}{|R_i|}} \left[ U\left(R_i \bigcup t\right) - U(R_i) \right]$ 





DS3Lab@

ETH ZURICH



(Challenge: how to efficiently, incrementally maintain one combinatorial term.

٠

$$\sum_{k=0}^{N-2} \frac{1}{\binom{N-2}{k}} \sum_{m=0}^{\min\{K-1,k\}} \binom{i-1}{m} \binom{N-i-1}{k-m}$$
$$= \sum_{m=0}^{\min\{K-1,i-1\}} \sum_{k'=0}^{N-i-1} \frac{\binom{i-1}{m}\binom{N-i-1}{k'}}{\binom{N-2}{m+k'}}$$
$$= \frac{\min\{K,i\}(N-1)}{\binom{N-1}{m}}$$

Training  
Relation  
$$ValidationExample
$$s \notin R_T$$
$$v(t_n) = \frac{\mathbb{I}[t_n, y = s, y]}{n}$$
$$v(t_i) = v(t_{i+1}) + \frac{\mathbb{I}[t_i, y = s, y] - \mathbb{I}[t_{i+1}, y = s, y] \min\{K, i\}}{K}$$
$$(1) \text{ Sort;}$$
$$(2) \text{ Single Pass Scan}$$$$



### Data Valuation: 3. An $O(n \log n)$ Algorithm





A single pass of sorting is still too slow for systems (we have could have billions data points to sort)

### Data Valuation: $(\varepsilon, \delta)$ -Approximation with LSH







### Enough Theory! How can we use these?

### **Overview**

#### <u>Theoretical Result</u>

- *Entropy/Expectation* of ML Training over Incomplete Information and Uncertainty
- Shapley value of ML Training over Feature Extraction Pipelines

#### Applications

- Data *Cleaning* for ML
- *Defense* against backdoor adversarial attacks
- Data *Debugging* for ML
- Data *Market*
- Heuristics of Approximating Real-world Pipelines
- Failure Cases & "Call for Help"



DS3Lab

ETH ZURICH

### Data Cleaning for ML

n



Accuracy

<u>Cleaning oracle</u>.

There exist a manual cleaning oracle to decide the ground truth value for each feature.

#### Uncertainty on features.

Think about it as outputs of state-of-the-art data cleaning methods – each method output a candidate value.

How should we prioritize which cell to clean?



Use the results of decades of research on Sequential Information Maximization for entropy minimization



### Data Cleaning for ML - Entropy Minimization





#### Under this view, Data Cleaning for ML becomes:

How to find cleaning opeations  $o_1...o_n$  such that we decrease final entropy as much as possible?

Under mild technical conditions, we can greedily pick the next cleaning operations  $o_{i+1}$  that decreases our expected entropy.

Lot of interesting studies (decades) about Sequential Information Maximization

### Defend against backdoor adversarial attacks



#### **Training Set**





*Idea*: Inject Gaussian noise to the training set and compute the *expection*.

This allows us to provide certifications on robustness, similar how people are doing randomized smoothing for evasion attacks.

To our best knowledge, this gives us the first robustness certification for backdoor attacks <u>https://arxiv.org/abs/2003.08904</u>



### **Robustness of Expectations**



Inspired by the seminal work of randmized smoothing, but significantly generalizes it.

Let's look at  $g(x) = \mathbb{E}_{z \sim z} f(x, z)$ 

What can we say about g(x) and  $g(x + \delta)$ ?

<u>Informal Theorem</u>

If  $g(x) \ge p$  and  $z \sim Z$  with probability density function  $\mu$ , then  $g(x + \delta)$  $\ge \mathbb{P}_{z \sim Z} \left[ \frac{\mu(\delta + z)}{\mu(z)} \le Z^{-1}(1 - p) \right]$ 

https://arxiv.org/abs/2003.08904

#### **Application 1. Defend about Backdoor**

 $g(\mathbf{x}) = \mathbb{E}_{z \sim 2} f(\mathbf{x}, \mathbf{z})$ Training Set Injected Gaussian Noise

Training over a new training set x + z, then do inference

Get a certificate looks like: As long as the attacker introduces a perturbations  $\delta$  with 2-norm smaller than *C*, the inference result will not change by  $\Delta$ .

When we have a Deep neural networks, sample some training sets, train a model for each.

When we have a KNN classifier, we can calculate this term *exactly in PTIME*.



### **Robustness of Expectations - Quantum Systems**



Inspired by the seminal work of randmized smoothing, but significantly generalizes it.

Let's look at  $g(x) = \mathbb{E}_{z \sim Z} f(x, z)$ 

What can we say about g(x) and  $g(x + \delta)$ ?

#### <u>Informal Theorem</u>

If  $g(x) \ge p$  and  $z \sim Z$  with probability density function  $\mu$ , then  $g(x + \delta)$  $\ge \mathbb{P}_{z \sim Z} \left[ \frac{\mu(\delta + z)}{\mu(z)} \le Z^{-1}(1 - p) \right]$ 

https://arxiv.org/abs/2003.08904

#### **Application 2. Robustness of Quantum Systems**



<u>https://www.nature.com</u> /articles/s41534-021-00410-5

Get a certificate looks like: As long as the attacker introduces a perturbated state  $\rho$  with fidelity( $\rho, x$ ) > C, the result of this quantum system will not change by  $\Delta$ .

We don't need to inject noises as in the previous case. We get robustness "for free" because of the probabilistic semantics of quantum systems.



## Robustness of Expectations - PDB & Joint Inference DS3Lab@

Inspired by the seminal work of randmized smoothing, but significantly generalizes it.

Let's look at  $g(x) = \mathbb{E}_{z \sim Z} f(x, z)$ 

What can we say about g(x) and  $g(x + \delta)$ ?

#### <u>Informal Theorem</u>

If  $g(x) \ge p$  and  $z \sim Z$  with probability density function  $\mu$ , then  $g(x + \delta)$  $\ge \mathbb{P}_{z \sim Z} \left[ \frac{\mu(\delta + z)}{\mu(z)} \le Z^{-1}(1 - p) \right]$ 

https://arxiv.org/abs/2003.08904

#### **Application 3. Robustness of PDB & Joint Inference**

 $g(x) = \mathbb{E}_{x} \overline{q(x)}$ Output of NNs, or PDB

https://arxiv.org/abs/2106.06235 https://arxiv.org/abs/2003.00120

Probabilistic DB queries: e.g., SQL Probabilistic Inference queries: MLN, CRF

Get a certificate looks like: As long as the attacker introduces a perturbations  $\delta$  on x with 2-norm smaller than C, the result of this quantum system will not change by  $\Delta$ .

We don't need to inject noises as in the previous case. We get robustness "for free" because of the probabilistic semantics of these probabilistic inference systems.



Robustness & data cleaning are all naturally connected to *Entropy* and *Expectations*. An *efficient proxy* for computing these could go a long way.

### Data Debugging



Training set with incorrect labels Accuracy Dog ML Model Dog **Operators** Cat Test set

How can we find out those training examples with wrong labels?

<u>Idea</u>: Data examples with incorrect labels should have a small (often negative) Shapley value.

O(N log N) if we use KNN and if a pipeline can be conditioned as map-fork. Orders of magnitude faster than MCMC: < 1 second for reasonable dataset.



### Data Debugging





How can we find out those training examples with backdoor patterns?

<u>Idea</u>: Data examples with backdoor labels should have a small (often negative) Shapley value.

O(N log N) if we use KNN and if a pipeline can be conditioned as map-fork. Orders of magnitude faster than MCMC: < 1 second for reasonable dataset.



Expected marginal improvement / Shapley value provides a principled framework for data debugging. An *efficient proxy* for computing these could go a long way.

### Data Market





*How should we fairly distribute \$ to each data contributor?* 

<u>Idea</u>: Use Shapley value (which is actually why we originally looked at this)

O(N log N) algorithm if we use KNN and if a pipeline can be conditioned as mapfork.









### **Overview**

#### <u>Theoretical Result</u>

- *Entropy/Expectation* of ML Training over Incomplete Information and Uncertainty
- Shapley value of ML Training over Feature Extraction Pipelines
- <u>Applications</u>
  - Data *Cleaning* for ML
  - *Defense* against backdoor adversarial attacks
  - Data *Debugging* for ML
  - Data *Market*
- Heuristics of Approximating Real-world Pipelines
- Failure Cases & "Call for Help"



DS3Lab

ETH ZURICH

### Heuristics 1: Unknown Noise to Codd's Table







### Heuristics 2: ML Pipelines to Positive RA



• Dataflow using a diverse set of transformations, but different operators largely fall into two types:



Data Augmentation fork Dictionary Lookup join

- Many reduce functions are relatively stable with respect to the removal of data examples
- <u>Heuristics</u>: If we *fix the reduce part to be over the whole* <u>*dataset*</u>, conditioning on this, we can approximate a majority of pipelines.



### Heuristics 2: ML Pipelines to Positive RA





### **Heuristics 2: Characteristics of Pipelines**



- We take ~500K real-world pipelines
  - <u>https://arxiv.org/pdf/1912.09536.p</u> <u>df</u>
- A majority of which fits into the mapfork pattern, after the conditioning heuristics.
- In additional to these pipelines:
  - Data federation/market (different subsets, union) introduces fork
  - Data augmentatin introduces fork





### **Overview**

#### <u>Theoretical Result</u>

- *Entropy/Expectation* of ML Training over Incomplete Information and Uncertainty
- Shapley value of ML Training over Feature Extraction Pipelines
- <u>Applications</u>
  - Data *Cleaning* for ML
  - *Defense* against backdoor adversarial attacks
  - Data *Debugging* for ML
  - Data *Market*
- Heuristics of Approximating Real-world Pipelines
- Failure Cases & "Call for Help"



DS3Lab

ETH ZURICH

### Failure Case (Shapley)





How can we identify overrepresented examples to remove? *Idea*: Data examples that are over-represented should have a small Shapley value.

KNN proxy does not work! (Conditioning still works)



Why? KNN captures more of a local structure, not the populational structure. (HELP!)

### Failure Case (Entropy/Expectation)

output a candidate value.















### What is a **good metric**?





- 1. Bojan Karlaš\*, Peng Li\*, ... Xu Chu, Wentao Wu ... . VLDB 2021.
- 2. Ruoxi Jia, Fan Wu, ... Bo Li, Dawn Song. CVPR 2021.
- 3. Linyi Li\*, Maurice Weber\*, .... CCS 2021.
- 4. Maurice Weber, Nana Liu ... Zhikuan Zhao. npj Quantum Info. 2021.
- 5. Ruoxi Jia\*, David Dao\* ... . AISTATS 2019.
- 6. Ruoxi Jia, David Dao ... . VLDB 2019.
- 7. Maurice Weber\*, Xiaojun Xue\* ... Arxiv:2003.08904
- 8. Fotis Psallidas ... Matteo Interlandi...Carlo Curino, Markus Weimer. *Arxiv:1912.09536*



MLOps & MLDev made easy? Check out



# http://ease.ml

Distributed ML in DB/Serverless/Spark/MPI? Check out



# http://zip.ml

