

# Toward Practical Machine Learning Applications with Generative Models: *Data Generation and Beyond*

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Department of Computer Science, **Virginia Tech**  
Cognitive Computing Lab, **Baidu Research, USA**



# OUTLINE

- ▷ Toward practical ML methodology
  - What are the challenges?
  - What are the goals?
- ▷ Practical ML Methods in
  - Hashing
  - Backdoor Attacks
- ▷ Future Directions
- ▷ Q & A!

# Khoa D. Doan

## Education:

- ▷ Ph.D in CS - Virginia Tech
- ▷ MS in CS - Univ. of Maryland, College Park

## Work Experience:

- ▷ **Current:** AI Researcher, Baidu Research, USA
- ▷ **Previous:** Criteo (*Researcher*), Verve Mobile (*Senior Data Scientist/Engineer*), NASA (*Data Scientist*) ...

## Research Interests:

- ▷ generative-based ML models in various domains, including retrieval (text, image, graphs), AI security, and advertising.



# I'm grateful for the support and collaboration of



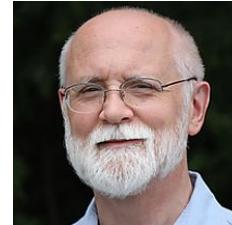
Chandan Reddy  
Virginia Tech



Keerthi Selvaraj  
LinkedIn AI



Ping Li  
Baidu Research



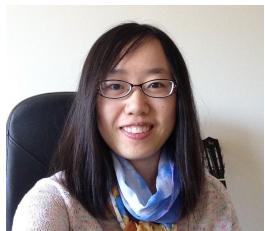
James Reggia  
University of Maryland



Saurav Manchanda  
University of Minnesota



Sarkhan Badirli  
Eli Lilly



Fengjiao Wang  
Criteo AI



Yingjie Lao  
Clemson University



Jianwen Xie  
UCLA/Baidu Research



Shulong Tan  
Baidu Research



Weijie Zhao  
RIT



Peng Yang  
Baidu Research

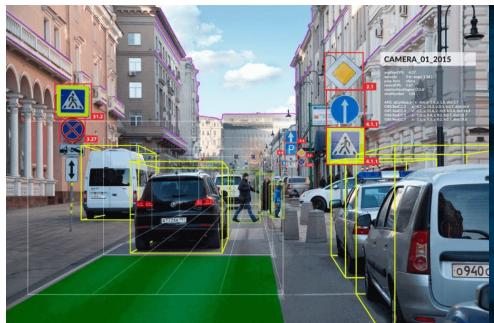
and others ...

## Simple-to-use

Easier construction

Efficient Execution

Simpler Evolution



## Reliable

Acceptable Performance

Acceptable Robustness

Acceptable Security  
Resilience



# Simple-to-use

Easier construction



Simpler to build



More involved to build

# Simple-to-use

Easier construction

Efficient Execution



# Simple-to-use

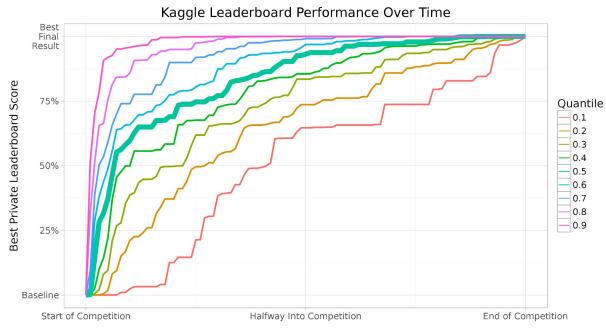
Easier construction

Efficient Execution

Simpler Evolution

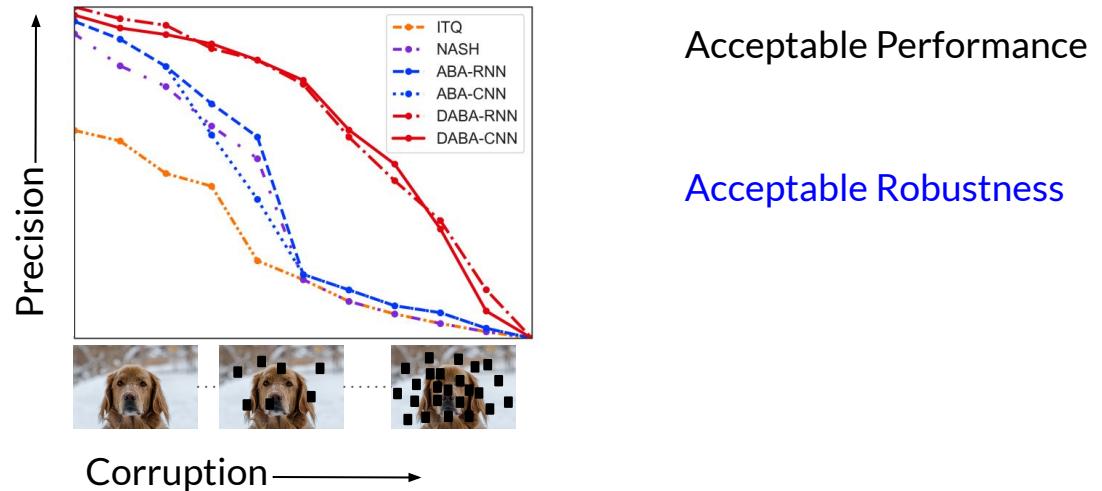


# Reliable

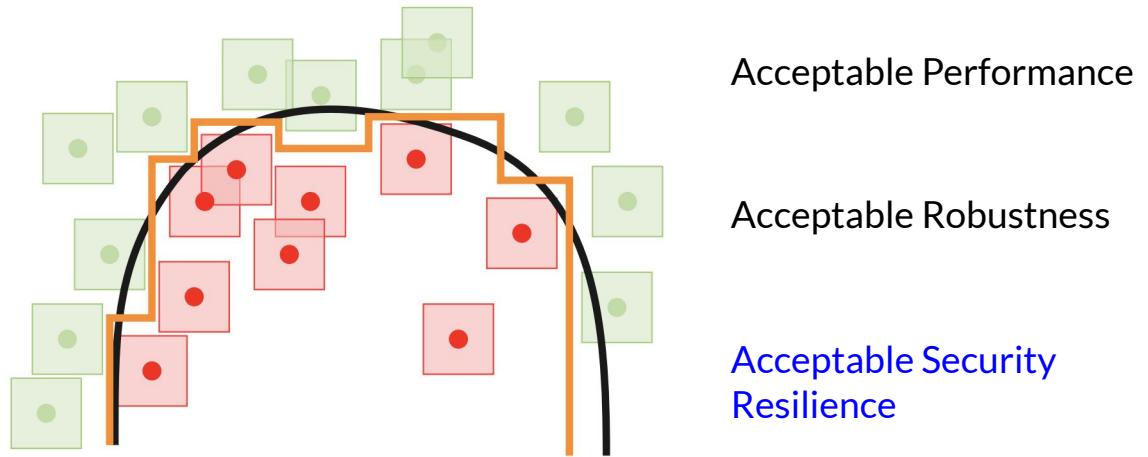


Acceptable Performance

# Reliable



# Reliable



Adversarial Robustness [Yang et al. 2020]

# Simple-to-use & Reliable

Easier construction

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# Simple-to-use & Reliable

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Acceptable Performance

Efficient Execution

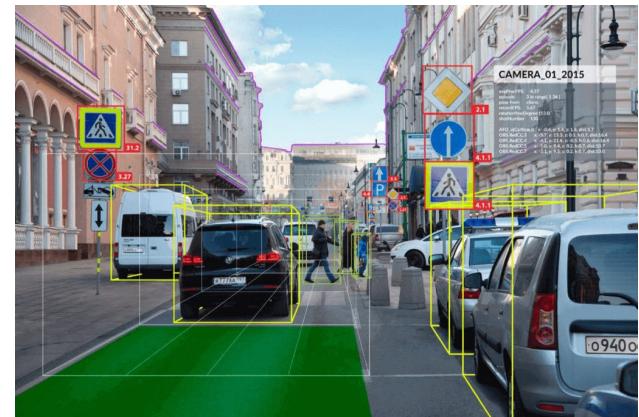
Acceptable Robustness

Simpler Evolution

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Resilience

# What we usually see

Complex methods have been developed to solve various real-world problems given their superior performance.



[[Source](#)]

# Simple-to-use & Reliable

Easier construction

Acceptable Performance

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# What we usually see

Complex methods have been developed to solve various real-world problems given their superior performance.

But simple methods are preferred because they simpler to use



[Source]

# Simple-to-use & Reliable

Easier construction

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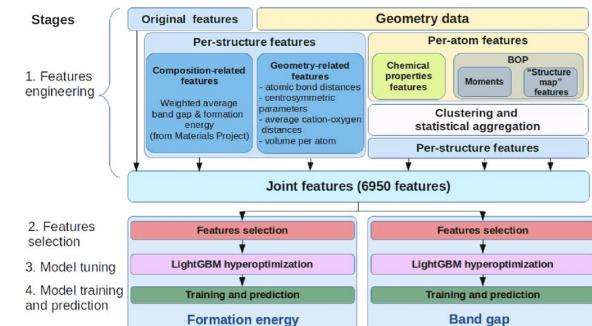
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Resilience

# What we usually see

Complex methods have been developed to solve various real-world problems given their superior performance.

But simple methods are preferred because they simpler to use

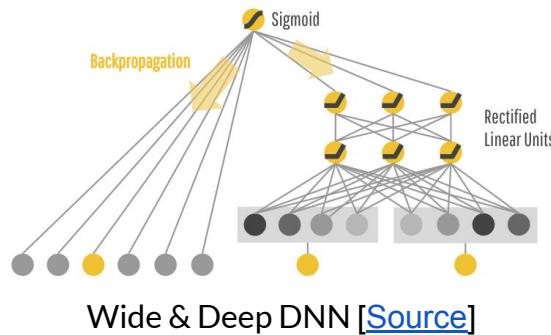
Substantial amount of engineering is required for better reliability



[Source: Kaggle 2018 Competition]

# Complex methods are not simple to use

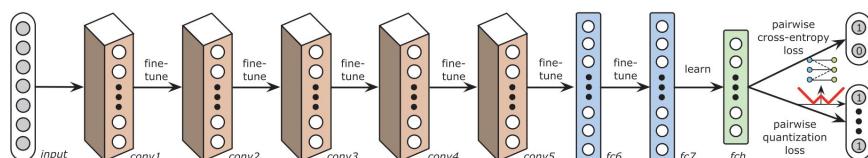
## Click-Through-Rate Prediction Task



## Challenges:

1. Longer Training Time
2. Require significant amount of data

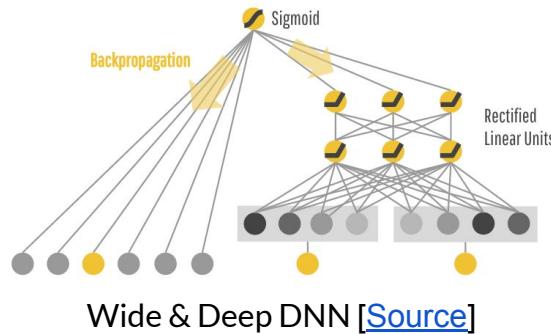
## Retrieval Task with Hashing



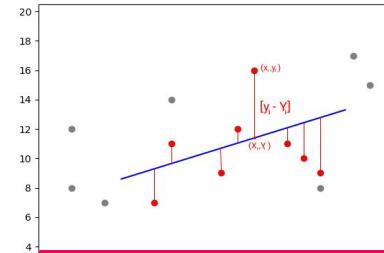
Deep Hashing Network [Zhu et al. 2016]

# Complex methods are not simple to use

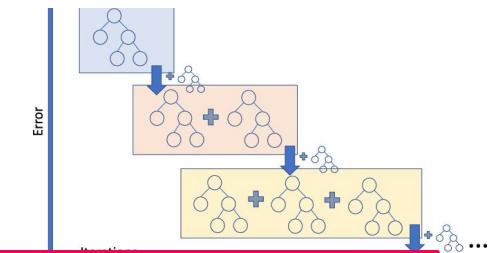
## Click-Through-Rate Prediction Task



## Linear Model [[Source](#)]



## Boosting [[Source](#)]

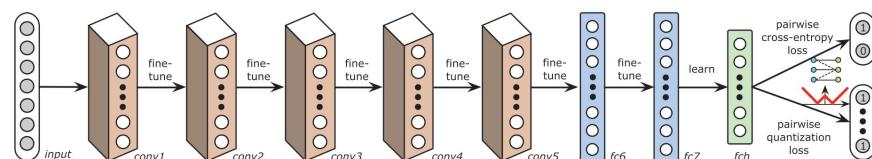


Complex engineering is needed to ensure reliability of simpler models!

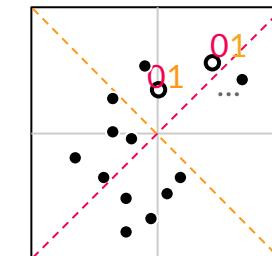
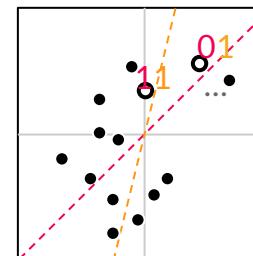
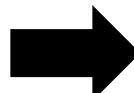
(Linear, Data Independent)

(Linear, Data Dependent)

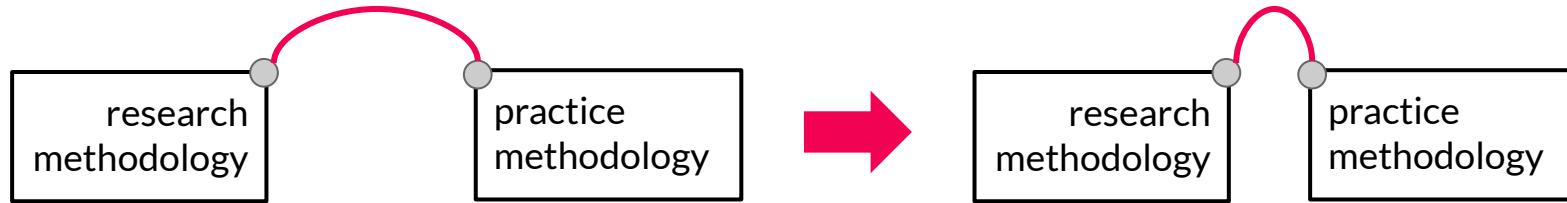
## Retrieval Task with Hashing



Deep Hashing Network [Zhu et al. 2016]

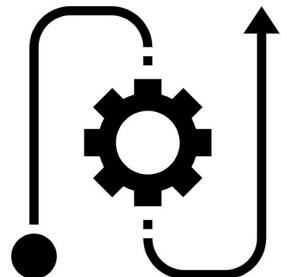


# Bridging the gap between research & practice

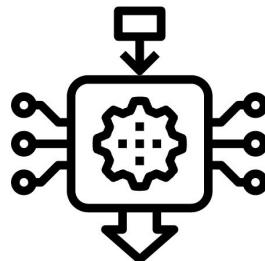


How do we make complex methods **simpler** to use and **reliable**?

Short training time



Fast decision

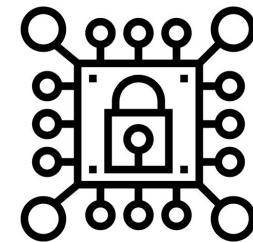


Realistic Assumptions



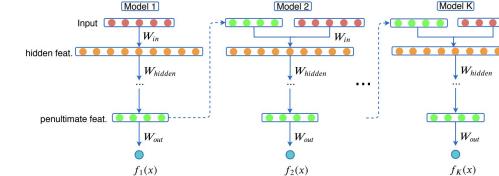
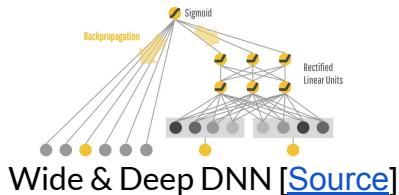
[\[Source\]](#)

Secured Methodology



# When complex model is simpler and reliable

## Click-Through-Rate Prediction Task



SOTA performance with less engineering!

Systematically grow neural networks  
GrowNet [Badirli et al. 2020]

## Retrieval Task with Hashing

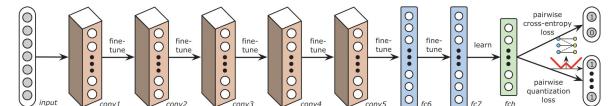
$$\begin{aligned} \arg \min_f E_{x \sim D_x} \lambda_1 \times H_1(f(x)) \\ + \lambda_2 \times H_2(f(x)) + \lambda_3 \times H_3(f(x)) \dots \end{aligned}$$



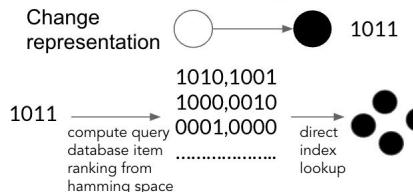
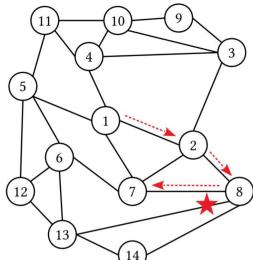
[Doan et al. 2022]

$$\arg \min_f d(q || q^*)$$

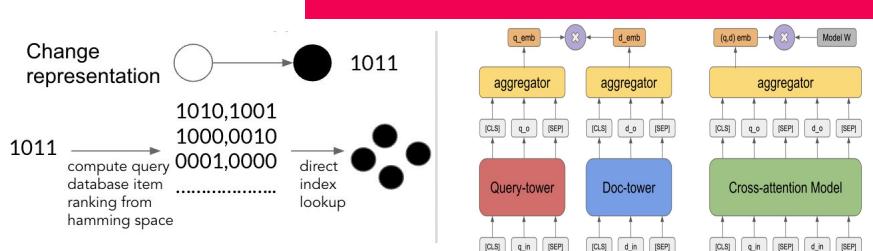
SOTA performance with faster training!



## Retrieval Task with Non-metric Ranking Measures



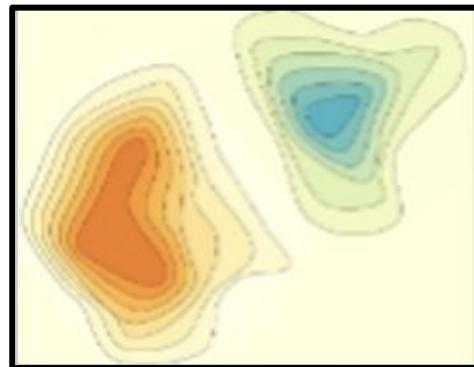
Real-time Ranking on complex ranking measures



# Research Themes



**INFORMATION RETRIEVAL**  
(retrieval foundation, real-timed,  
generalization, robustness...)

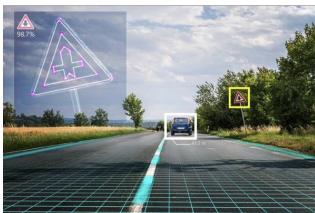


**MACHINE LEARNING**  
(esp. generative-based solutions,  
theoretical generative modeling)



**PRACTICAL ALGORITHMS**  
(high-performing ML approaches  
solution, secured ML models)

## APPLICATION DOMAINS



Computer Vision



Text Mining



Graph Analysis



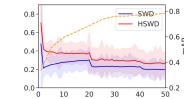
Computational Advertising

# Research Highlights



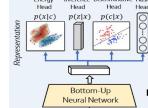
## Training-Efficient Framework

- Novel Divergence-based Quantization Estimation
- Low-sample and computation complexity



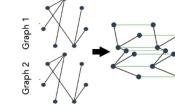
## Robust Retrieval Framework

- Joint energy-based training of hash function
- Efficient & Effective MCMC Estimation



## Explainable Retrieval Framework

- Differentiable Transform of Structured Objects
- Bijective Graph Alignments



## Stealthy Backdoor Attack Framework

- Realistic Attack's Threat Model & Human Tests
- Adaptive Attacks against Existing Defenses



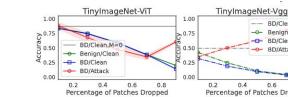
## Backdoor Unlearning Defense Framework

- Realistic Defense's Threat Model
- Adaptive against Existing Attacks



## Efficient Defenses for Complex Models

- Backdoor Defenses for Complex Models
- Adversarial Robustness for Complex Models

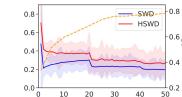


# Research Highlights



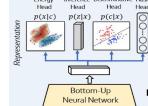
## Training-Efficient Framework

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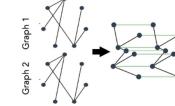
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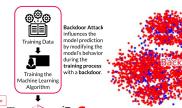
## Explainable Retrieval Framework

- Differentiable Transform of Structured Objects
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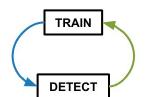
## Stealthy Backdoor Attack Framework

- Constrained optimization via adversarial game
- Adaptive against Human and Machine Defenses



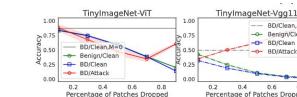
## Backdoor Unlearning Defense Framework

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- Adaptive against Existing Attacks



## Efficient Defenses for Complex Models

- Backdoor Defenses for Complex Models
- Adversarial Robustness for Complex Models

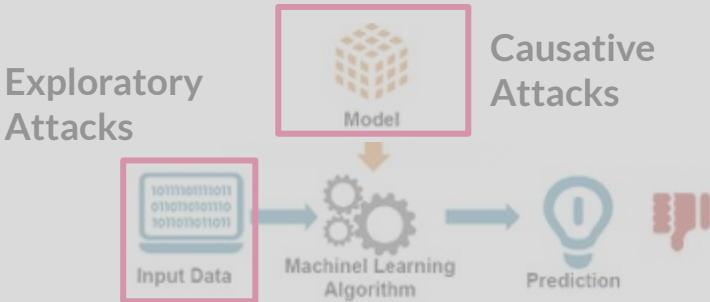


# Faster Hash-Function Training



- ▷ Develop a new training framework:
  - one quantization loss (vs. >3)
  - better retrieval performance
  - significantly faster training

# Artificial Intelligence Security

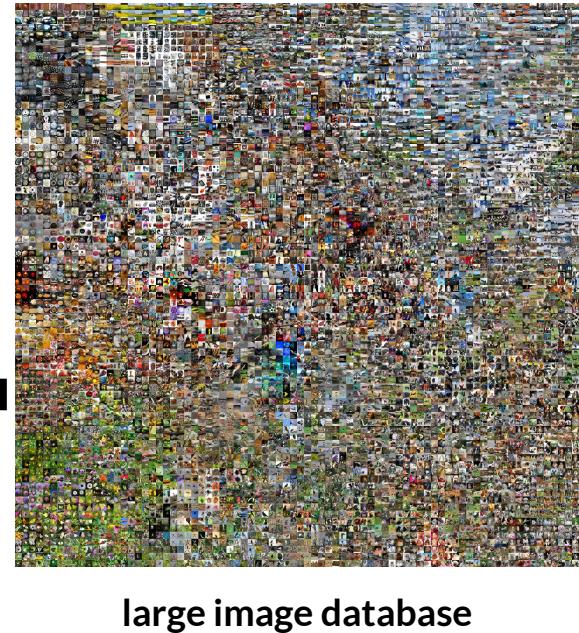
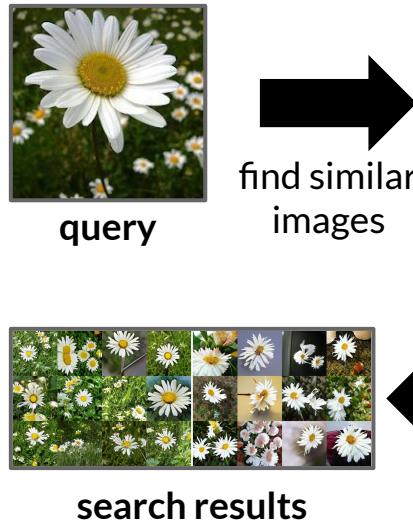


- ▷ Develop an optimization framework
  - adversarial game between attacker and model trainer
  - realistic threat model
    - invisible to human's inspection
    - invisible and adaptive to machine's inspection

# Retrieval & Similarity Search

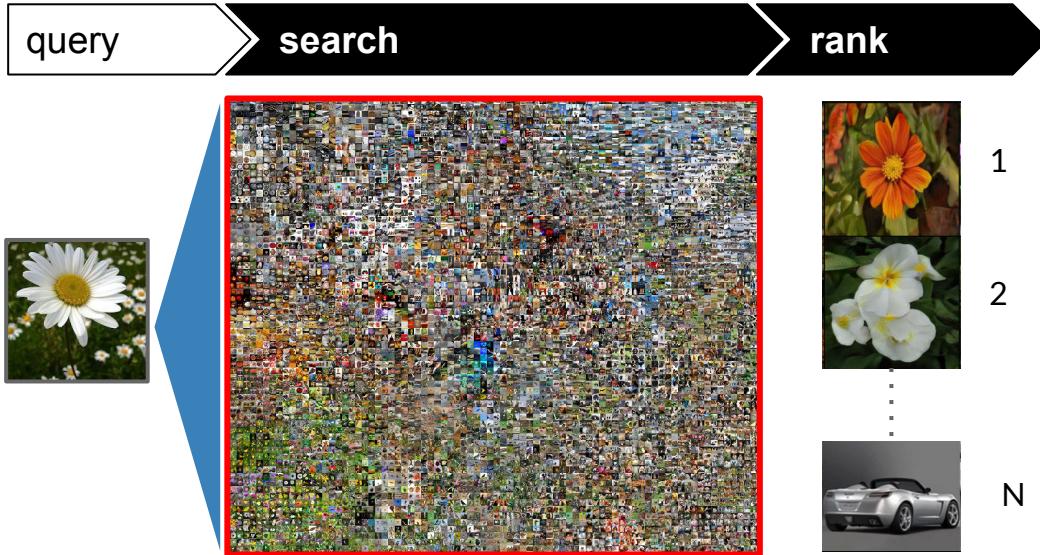
**Problem:** Given a dataset of  $N$  items  $X = \{x_1, x_2, \dots, x_N\}$  and a query  $q$ , we aim to find  $l$  items  $R = \{x_1, x_2, \dots, x_l\}$  such that, for a similarity function **sim**, we have:

$$\begin{aligned}\mathbf{sim}(q, x_i) &\geq \mathbf{sim}(q, x_j) \\ \forall x_i \in R, \forall x_j \in X \setminus R\end{aligned}$$



large image database

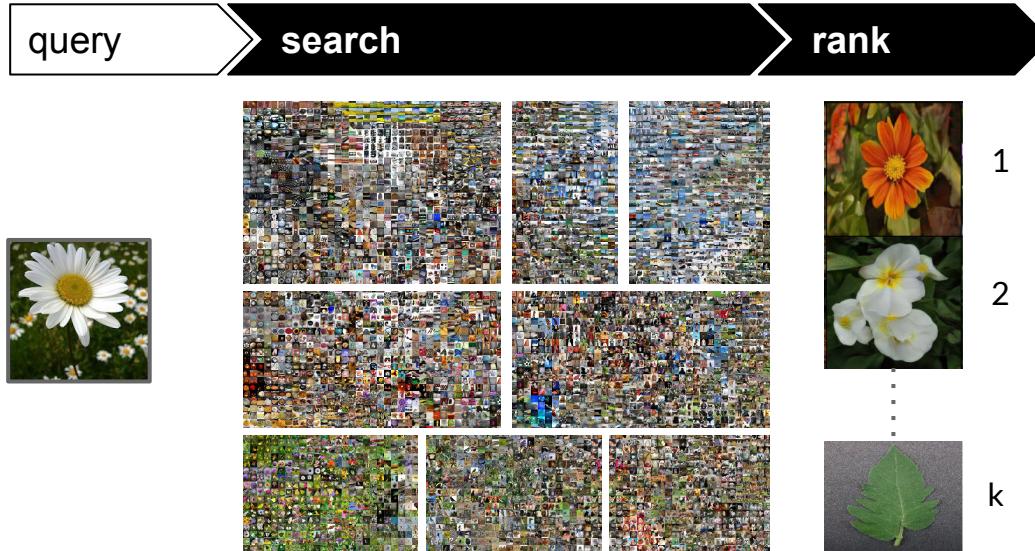
# Linear Search



## Exhaustive search

- ▷ infeasible in large database of millions or billions of items.
- ▷ wasteful of computation
  - only a small subset is relevant
  - real-time ranking is impossible

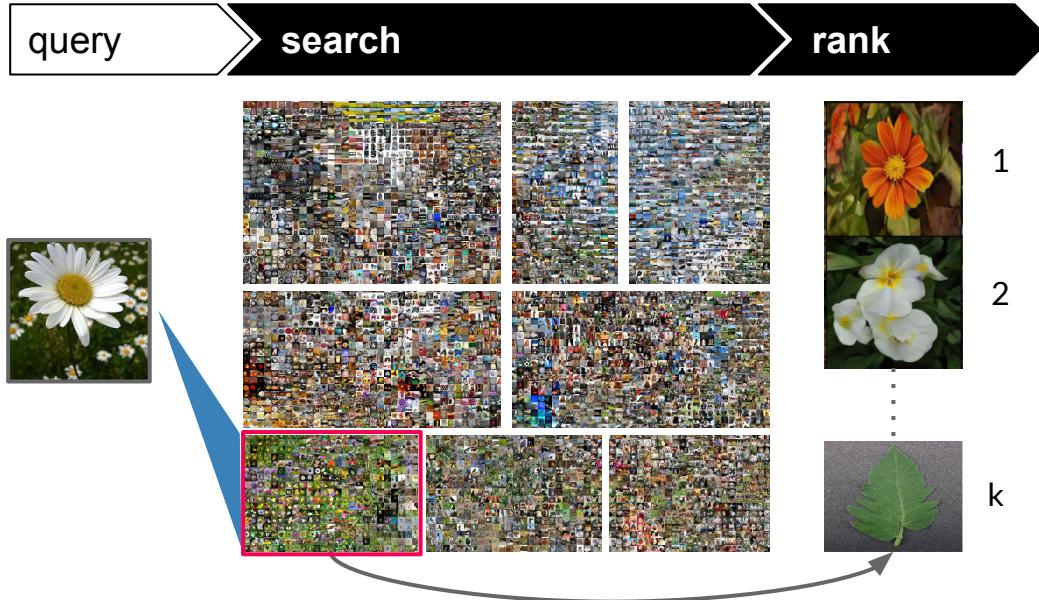
# Approximate nearest neighbor



## Approximate Search

- ▷ ANN search builds an index structure

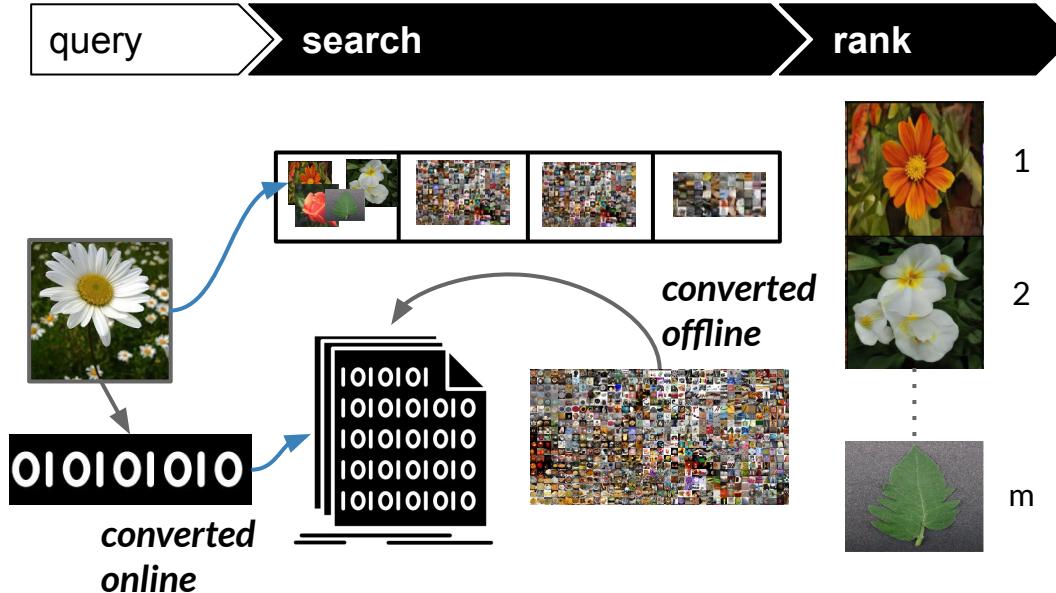
# Approximate nearest neighbor



## Approximate Search

- ▷ ANN search builds an index structure
  - limits the search to a subset of candidate items (**sub-linear**)
- ▷ **How to construct the index?**

# Approximate nearest neighbor



## Approximate Search (Hashing)

- ▷ Transforms images into binary vectors
- ▷ Search via table look-up
- ▷ Linear Search in Discrete space:
  - Memory efficient: 4MB for 1M items
  - Compute efficient: 2 instructions per distance computation

# Hash-function learning

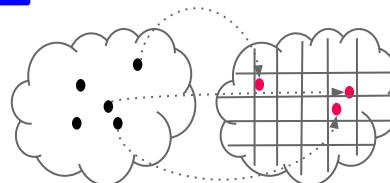
- ▷ Learn a hash function

$$F : \mathcal{R}^n \longrightarrow \{0, 1\}^m \quad \xrightarrow{\text{discrete function}} \quad f : \mathcal{R}^n \longrightarrow [0, 1]^m \quad \xleftarrow{\text{continuous relaxation}} \quad F(x) = f(x) > 0.5 \quad \xleftarrow{\text{discretization}}$$

- ▷ Overall objective function of hashing methods

$$\arg \min_f E_{x \sim D_x} L(x, f(x)) + E_{x \sim D_x} \sum_k \lambda_i \times H_k(f(x))$$

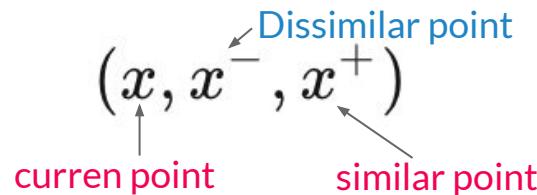
**locality-preserving loss**  
preserves the semantics  
of **sim** in discrete space



**hashing regularizer**  
minimizes gap between  
continuous and discrete  
optimizations.

# Hashing Loss Examples

## Locality Preserving Loss



- **Similar/Dissimilar:** same class/different class
- **Similar/Dissimilar:** nearest neighbor/distant neighbor

$$\sum_x \max(0, 1 + |f(x) - f(x^+)|_2 - |f(x) - f(x^-)|_2)$$

## Quantization Loss (Regularization)

Bit Balance

1	0	1	1
0	1	1	1
1	1	1	1

50% being 0 or 1

Bit Uncorrelation

1	0	1	1
0	1	1	1
1	1	1	1

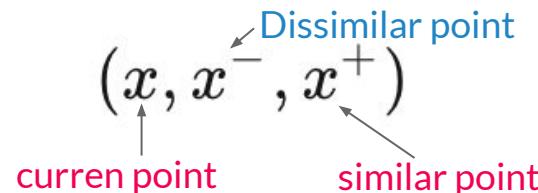


Low Quantization Error

0.9	0.2	...
0.1	0.3	...
0.2	0.1	...

# Hashing Loss Examples

## Locality Preserving Loss



- **Similar/Dissimilar:** same class/different class
- **Similar/Dissimilar:** nearest neighbor/distant neighbor

$$\sum_x \max(0, 1 + |f(x) - f(x^+)|_2 - |f(x) - f(x^-)|_2)$$

## Quantization Loss (Regularization)

*averaged bit's maximum entropy*

$$\text{Bit Balance: } \sum_{k=1}^m \bar{b}_k \log \bar{b}_k + (1 - \bar{b}_k) \log (1 - \bar{b}_k), \bar{b}_k = E_x [f(x)_{[k]}]$$

$$\text{Bit Uncorrelation: } |W^T W - I|_2 \quad \text{\color{green}orthogonal projection}$$

*bit's minimum entropy*

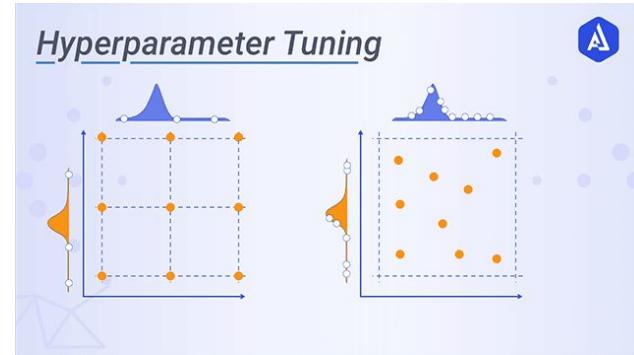
$$\text{Low Quantization Error: } \sum_x \sum_{k=1}^m -f(x) \log(f(x)) - (1 - f(x)) \log(1 - f(x))$$

# Quantization Regularization helps efficiency

$$\min_f \sum_x \max(0, 1 + |f(x) - f(x^+)|_2 - |f(x) - f(x^-)|_2)$$

$$\begin{aligned} & |W^T W - I|_2 + \sum_{k=1}^m \bar{b}_k \log \bar{b}_k + (1 - \bar{b}_k) \log (1 - \bar{b}_k), \bar{b}_k = E_x [f(x)_{[k]}] \\ & + \sum_x \sum_{k=1}^m -f(x) \log(f(x)) - (1 - f(x)) \log(1 - f(x)) \end{aligned}$$

Complex objective increases training complexity  
(i.e., hyperparameter tuning)



[Source]

# Quantization Regularization helps efficiency

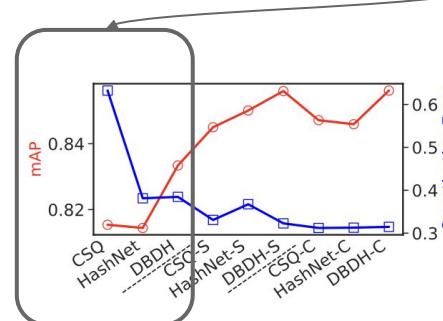
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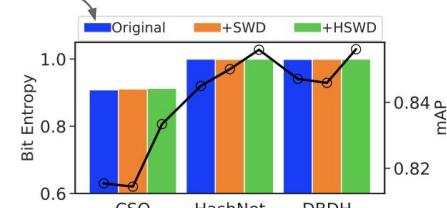
Complex objective increases training complexity  
(i.e., hyperparameter tuning)

Complex objective results in sub-optimal quantization

existing optimization



(a) Quantization Error



(b) Bit Entropy

[Doan et al. 2022]

# Quantization Regularization helps efficiency

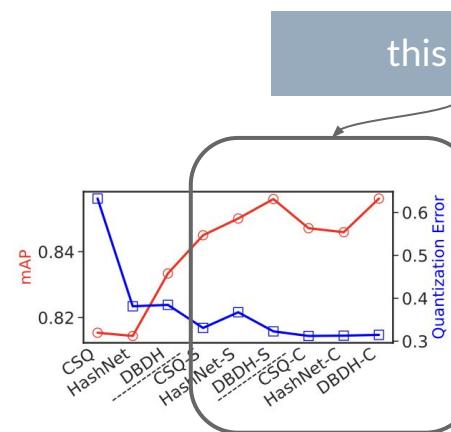
$$\min_f \sum_x \max(0, 1 + |f(x) - f(x^+)|_2 - |f(x) - f(x^-)|_2)$$

$$\begin{aligned} &|W^T W - I|_2 + \sum_{k=1}^m \bar{b}_k \log \bar{b}_k + (1 - \bar{b}_k) \log (1 - \bar{b}_k), \bar{b}_k = E_x [f(x)_{[k]}] \\ &+ \sum_x \sum_{k=1}^m -f(x) \log(f(x)) - (1 - f(x)) \log(1 - f(x)) \end{aligned}$$

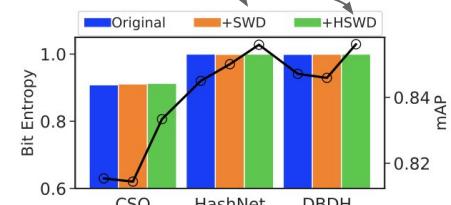
Complex objective increases training complexity  
(i.e., hyperparameter tuning)

Complex objective results in sub-optimal quantization

this work



(a) Quantization Error



(b) Bit Entropy

[Doan et al. 2022]

# Single-shot Quantization

Previous approaches:

$$\arg \min_f E_{x \sim D_x} \sum_k \lambda_i \times H_k(f(x))$$

Advantages: easier optimization

Disadvantages: more hyperparameter tuning

Our approach: single divergence loss

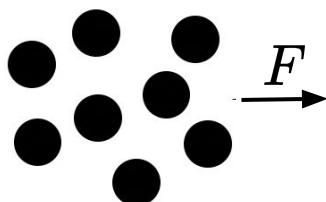
$$\arg \min_f d(q || q^*) \quad f(x) \sim q$$

$q^*$ : fixed distribution

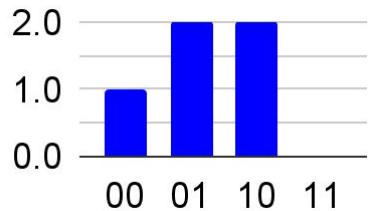
Advantages: single-shot optimization

Disadvantages: challenging to optimize

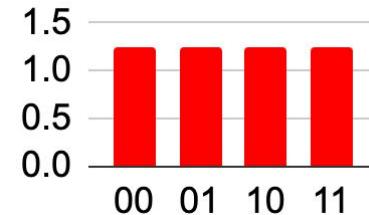
Task: learn 2-bit hash function



$F$



learned distribution  $q$



optimal distribution  $q^*$   
(with maximum entropy)

$q^* : b_i \sim \text{bernoulli}(0.5)$

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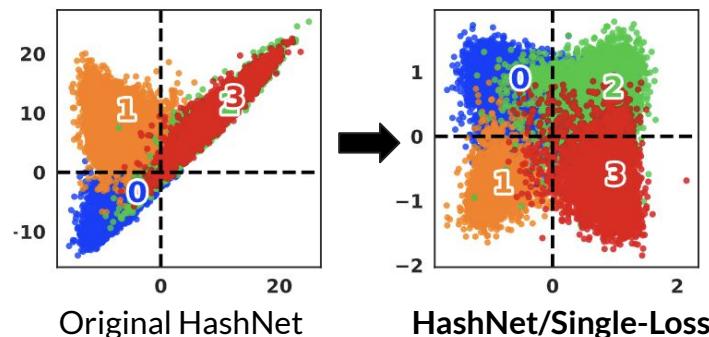


Fig. Learn 2-bit hash function on CIFAR10's data from 4 classes

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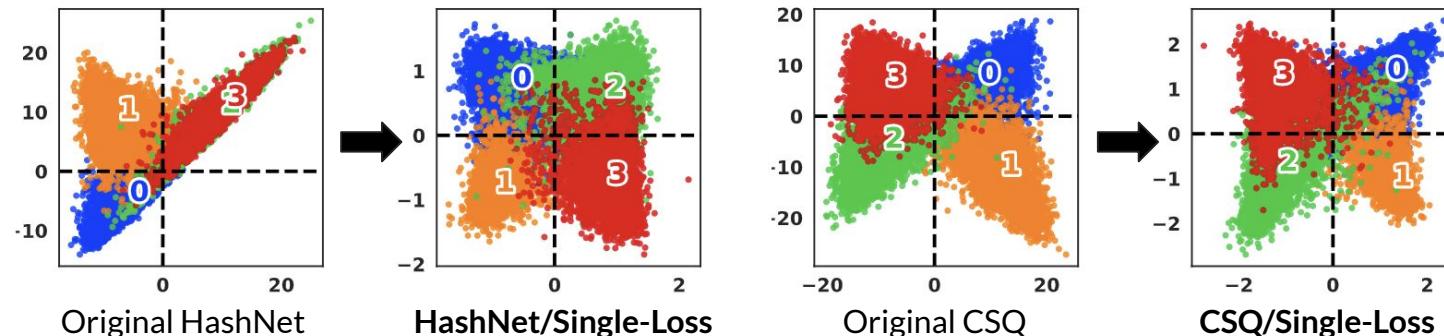


Fig. Learn 2-bit hash function on CIFAR10's data from 4 classes

# Choosing the “right” divergence

Objective:  $\mathcal{D}(q(b) \parallel q^*(z))$

## Wasserstein Distance

- Non-trivial to estimate
- High sample complexity
- Possibly minimax optimization (dual domain)

$$\mathcal{D}(\mu, \nu) = \left( \inf_{\gamma \in \Pi(\mu, \nu)} \int_{(z, b) \sim \gamma} p(z, b) \|z - b\|_2 dz db \right)^{1/2}$$

## Sliced Wasserstein Distance

- Lower sample complexity
- No minimax
- Several directions are discriminative

$$O(LN \log(Nd))$$

$$\mathcal{D}(h(X), B) \approx \left( \frac{1}{L} \sum_{l=1}^L \mathcal{W}(\omega_l^T h(X), \omega_l^T B) \right)^{1/2}$$

projection into 1-D space

## Hash-Sliced Wasserstein Distance

$$O(mN \log(Nd)), m \ll L$$

- Lower sample complexity
- No minimax
- Small number of discriminative projections

$$\mathcal{D}(h(X), B) \approx \left( \frac{1}{m} \sum_{l=1}^m [\mathcal{W}(h(X)_{l,:}, B_{l,:})]^2 \right)^{1/2}$$

no projection: averaging along each hashing dimension

## Other divergences (e.g. KL, JSD, etc...)

- Do not work for distributions with non-overlapping supports
- High sample complexity
- Minimax optimization

# Performance Evaluation (Precision@1000)

Retrieve k items



Precision@k = number of / k

Blue: improvement over original methods

-S: Sliced Wasserstein Estimate

-C: Proposed Wasserstein Estimate

Method	CIFAR-10	
	16 bits	32 bits
DSDH	0.8252	0.8406
DSDH-S	0.8526/ <b>3.3%</b>	0.8543/ <b>1.6%</b>
DSDH-C	0.8645/ <b>4.8%</b>	0.8739/ <b>4.0%</b>

Single-Label Data

# Performance Evaluation (Precision@1000)

Retrieve k items



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Method	CIFAR-10		NUS-WIDE	
	16 bits	32 bits	16 bits	32 bits
DSDH	0.8252	0.8406	0.8117	0.8294
DSDH-S	0.8526/ <b>3.3%</b>	0.8543/ <b>1.6%</b>	0.8162/ <b>0.6%</b>	0.8312/ <b>0.2%</b>
DSDH-C	0.8645/ <b>4.8%</b>	0.8739/ <b>4.0%</b>	0.8195/ <b>1.0%</b>	0.8391/ <b>1.2%</b>

**Single-Label Data**    **Multi-Label Data**

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Retrieve k items



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HashNet	0.6193	0.8613	0.7581	0.8158
HashNet-S	0.8470/ <b>36.8%</b>	0.8755/ <b>1.7%</b>	0.7743/ <b>2.1%</b>	0.8199/ <b>0.5%</b>
HashNet-C	0.7698/ <b>24.3%</b>	0.8715/ <b>1.2%</b>	0.7456/-1.7%	0.8078/-1.0%
GreedyHash	0.8561	0.8616	0.7601	0.8009
GreedyHash-S	0.8583/ <b>0.3%</b>	0.8656/ <b>0.5%</b>	0.7657/ <b>0.7%</b>	0.7973/-0.5%
GreedyHash-C	0.8517/-0.5%	0.8700/ <b>1.0%</b>	0.7630/ <b>0.4%</b>	0.7931/-1.0%
DCH	0.8621	0.8568	0.7843	0.7898
DCH-S	0.8622/0.0%	0.8761/ <b>2.3%</b>	0.7846/0.0%	0.7923/ <b>0.3%</b>
DCH-C	0.8654/ <b>0.4%</b>	0.8635/ <b>0.8%</b>	0.7893/ <b>0.6%</b>	0.7914/ <b>0.2%</b>
CSQ	0.8510	0.8571	0.7903	0.8285
CSQ-S	0.8661/ <b>1.8%</b>	0.8732/ <b>1.9%</b>	0.8034/ <b>1.7%</b>	0.8318/ <b>0.4%</b>
CSQ-C	0.8670/ <b>1.9%</b>	0.8688/ <b>1.4%</b>	0.8007/ <b>1.3%</b>	0.8353/ <b>0.8%</b>
DBDH	0.8440	0.8421	0.8122	0.8323
DBDH-S	0.8626/ <b>2.2%</b>	0.8675/ <b>3.0%</b>	0.8177/ <b>0.7%</b>	0.8388/ <b>0.8%</b>
DBDH-C	0.8658/ <b>2.6%</b>	0.8731/ <b>3.7%</b>	0.8135/ <b>0.1%</b>	0.8380/ <b>0.7%</b>

Single-Label Data

Multi-Label Data

# Performance Evaluation (MAP@5000)

Retrieve k items  MAP@k = Mean of Average Precisions from 1 to k (Area under PR Curve)

-S: Sliced Wasserstein Estimate | -C: Proposed Wasserstein Estimate

Method	CIFAR-10			NUS-WIDE			COCO		
	16 bits	32 bits	64 bits	16 bits	32 bits	64 bits	16 bits	32 bits	64 bits
DSDH [40]	0.7909	0.8072	0.8278	0.8270	0.8455	0.8640	0.7331	0.7853	0.8074
DSDH-S	0.8187/ <b>3.5%</b>	0.8439/ <b>4.6%</b>	0.8517/ <b>2.9%</b>	0.8282/ <b>0.1%</b>	0.8461/ <b>0.1%</b>	0.8712/ <b>0.8%</b>	0.7330/ <b>0.0%</b>	0.8030/ <b>2.3%</b>	0.8404/ <b>4.1%</b>
DSDH-C	0.8531/ <b>7.9%</b>	0.8620/ <b>6.8%</b>	0.8658/ <b>4.6%</b>	0.8433/ <b>2.0%</b>	0.8631/ <b>2.1%</b>	0.8749/ <b>1.3%</b>	0.7424/ <b>1.3%</b>	0.8032/ <b>2.3%</b>	0.8408/ <b>4.1%</b>
HashNet [6]	0.6922	0.8311	0.8566	0.7728	0.8336	0.8654	0.6899	0.7666	0.8098
HashNet-S	0.8131/ <b>17%</b>	0.8573/ <b>3.2%</b>	0.8749/ <b>2.1%</b>	0.8062/ <b>4.3%</b>	0.8438/ <b>1.2%</b>	0.8713/ <b>0.7%</b>	0.7215/ <b>4.6%</b>	0.7764/ <b>1.3%</b>	0.8189/ <b>1.1%</b>
HashNet-C	0.7939/ <b>14%</b>	0.8467/ <b>1.9%</b>	0.8691/ <b>1.5%</b>	0.8002/ <b>3.5%</b>	0.8437/ <b>1.2%</b>	0.8791/ <b>1.6%</b>	0.7202/ <b>4.4%</b>	0.7789/ <b>1.6%</b>	0.8202/ <b>1.3%</b>
GreedyHash [50]	0.8223	0.8474	0.8646	0.7802	0.8081	0.8328	0.6533	0.7219	0.7561
GreedyHash-S	0.8280/ <b>0.7%</b>	0.8497/ <b>0.3%</b>	0.8653/ <b>0.1%</b>	0.7815/ <b>0.1%</b>	0.8083/ <b>0.0%</b>	0.8390/ <b>0.7%</b>	0.6668/ <b>2.1%</b>	0.7291/ <b>1.0%</b>	0.7618/ <b>0.8%</b>
GreedyHash-C	0.8375/ <b>1.9%</b>	0.8536/ <b>0.7%</b>	0.8722/ <b>0.9%</b>	0.7890/ <b>1.1%</b>	0.8179/ <b>1.2%</b>	0.8477/ <b>1.8%</b>	0.6637/ <b>1.6%</b>	0.7299/ <b>1.1%</b>	0.7712/ <b>2.0%</b>
DCH [5]	0.8302	0.8432	0.8558	0.8015	0.8061	0.8040	0.7578	0.7792	0.7723
DCH-S	0.8372/ <b>0.8%</b>	0.8515/ <b>1.0%</b>	0.8602/ <b>0.5%</b>	0.8058/ <b>0.5%</b>	0.8079/ <b>0.2%</b>	0.8067/ <b>0.3%</b>	0.7657/ <b>1.1%</b>	0.7831/ <b>0.5%</b>	0.7803/ <b>1.0%</b>
DCH-C	0.8446/ <b>1.7%</b>	0.8596/ <b>1.9%</b>	0.8711/ <b>1.8%</b>	0.8159/ <b>1.8%</b>	0.8145/ <b>1.0%</b>	0.8155/ <b>1.4%</b>	0.7702/ <b>1.6%</b>	0.7892/ <b>1.3%</b>	0.7807/ <b>1.1%</b>
CSQ [58]	0.8069	0.8291	0.8366	0.7992	0.8384	0.8596	0.6783	0.7550	0.8146
CSQ-S	0.8401/ <b>4.1%</b>	0.8555/ <b>3.2%</b>	0.8554/ <b>2.3%</b>	0.8044/ <b>0.7%</b>	0.8495/ <b>1.3%</b>	0.8626/ <b>0.4%</b>	0.7036/ <b>3.7%</b>	0.7765/ <b>2.8%</b>	0.8234/ <b>1.0%</b>
CSQ-C	0.8457/ <b>4.8%</b>	0.8558/ <b>3.2%</b>	0.8652/ <b>3.4%</b>	0.8054/ <b>0.8%</b>	0.8511/ <b>1.5%</b>	0.8701/ <b>1.2%</b>	0.6989/ <b>3.0%</b>	0.7752/ <b>2.7%</b>	0.8255/ <b>1.3%</b>
DBDH [60]	0.7660	0.8223	0.8492	0.8305	0.8552	0.8666	0.7202	0.7826	0.8042
DBDH-S	0.8458/ <b>10%</b>	0.8587/ <b>4.4%</b>	0.8603/ <b>1.3%</b>	0.8387/ <b>1.0%</b>	0.8577/ <b>0.3%</b>	0.8680/ <b>1.8%</b>	0.7461/ <b>2.2%</b>	0.7996/ <b>3.7%</b>	0.8336/ <b>4.3%</b>
DBDH-C	0.8466/ <b>10%</b>	0.8593/ <b>4.5%</b>	0.8668/ <b>2.1%</b>	0.8395/ <b>1.1%</b>	0.8633/ <b>0.9%</b>	0.8760/ <b>1.1%</b>	0.7389/ <b>2.6%</b>	0.7889/ <b>0.8%</b>	0.8308/ <b>3.9%</b>

Single-Label Data

Multi-Label Data

# Qualitative Analysis

The t-SNE visualizations of the quantized 16-bit hash codes



The learned hash codes are:

- Better separation between class
- Better closeness within a class

Averaged running time per epoch across different supervised hashing methods (in seconds).

Dataset	Original	SWD	HSWD
CIFAR-10	19.4	24.2	17.1/ <b>40%</b>
NUS-WIDE	58.3	71.2	50.1/ <b>41%</b>
COCO	55.6	68.1	49.5/ <b>37%</b>

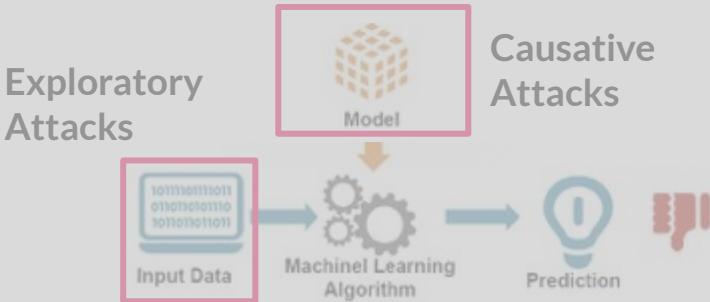
More computationally efficient even before intensive model selection

# Faster Hash-Function Training



- ▷ Develop a new training framework:
  - one quantization loss (vs. >3)
  - better quantized hash functions
  - **better retrieval performance**
  - **significantly faster training**

# Artificial Intelligence Security



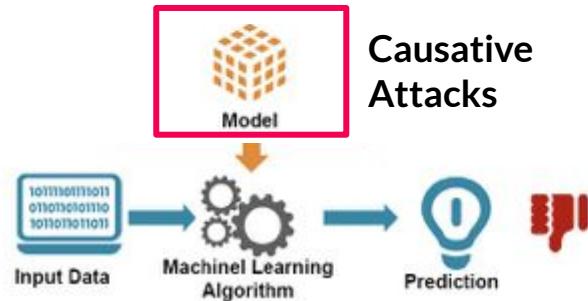
- ▷ Develop an optimization framework
  - adversarial game between attacker and model trainer
  - **realistic threat model**
    - invisible to human's inspection
    - invisible and adaptive to machine's inspection

# Single-Loss Hashing Algorithms



- ▷ Develop a new training framework:
  - one quantization loss (vs. >3)
  - better quantized hash functions
  - better retrieval performance
  - significantly faster training

# Adaptive Backdoor Attacks

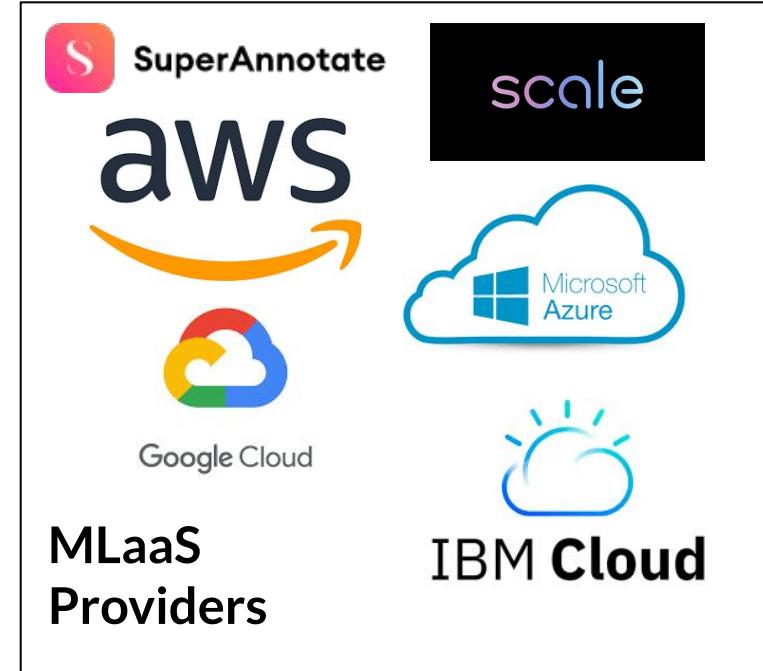


- ▷ Develop an optimization framework
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  - **realistic threat model**
    - invisible to human's inspection
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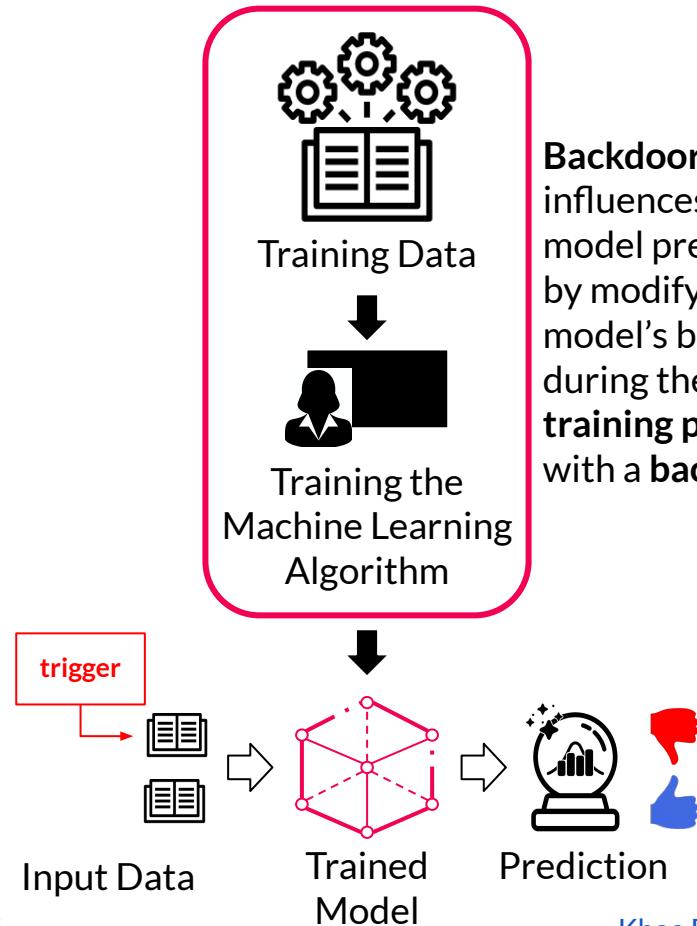
# ML Models in Practice

The increasing complexity of Machine Learning Models and Training Processes has promoted training outsourcing and Machine Learning as a Service (MLaaS).

This creates a paramount security concern in the model building supply chain.



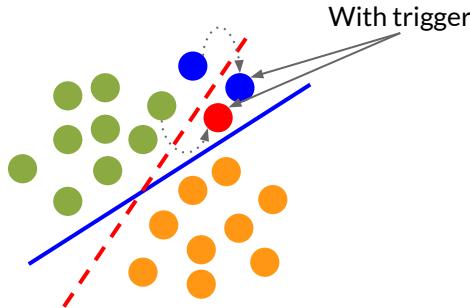
# Backdoor Attacks



Backdoor attacks can lead harmful consequences when the ML models are deployed in real life.

# BACKDOOR ATTACKS

(Causative)

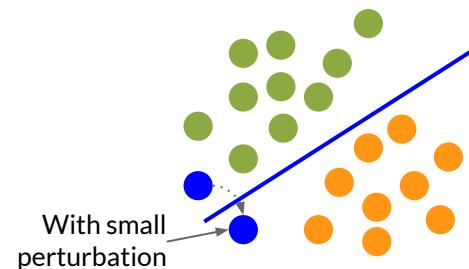


- Modifies training samples or training process intelligently
- Requires owning the training data or training process

- Training Sample (Triggered)
- Test Sample (Class A)
- Training Sample (Class A)
- Training Sample (Class B)

# ADVERSARIAL ATTACKS

(Exploratory)

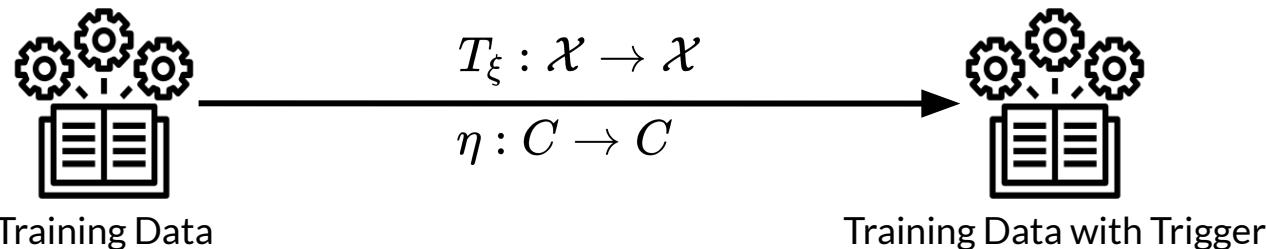


- Directly modifies the testing samples

# How is the backdoor injected?

Consider a classification task  $f_\theta : \mathcal{X} \rightarrow \mathcal{C}$

(1) Generate triggered data



$$\mathcal{S} = \{(x_i, y_i) : i = 1, \dots, N\}$$

$$\hat{\mathcal{S}} = \{(T(x_i), \eta(y_i)) : i = 1, \dots, M\}$$

where  $M < N$

(2) Poison the model (under empirical risk minimization)

$$\min_{\theta} E_{(x_i, y_i) \in S \cup \hat{\mathcal{S}}} \mathcal{L}(f_\theta(x_i, y_i))$$

# The “fixed” trigger/transformation function

The unrealistic assumptions in fixed transformation functions

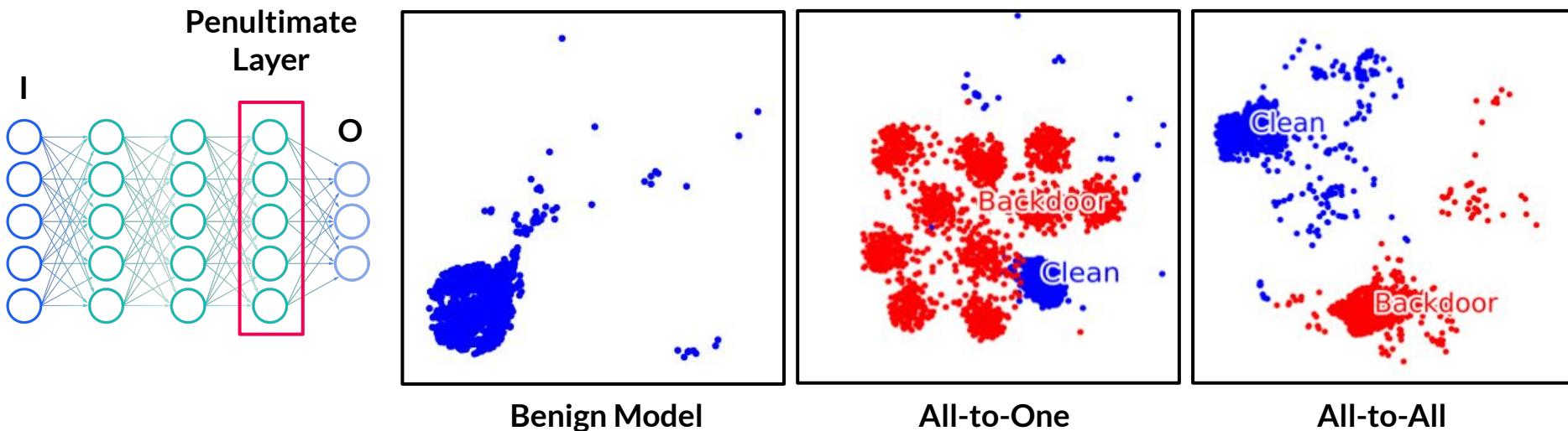
- Poisoned samples are not visually inspected by human defenders



# The “fixed” trigger/transformation function

The unrealistic assumptions in fixed transformation functions

- Poisoned samples are not visually inspected by human defenders
- Backdoor attacks are not adaptive to new defenses

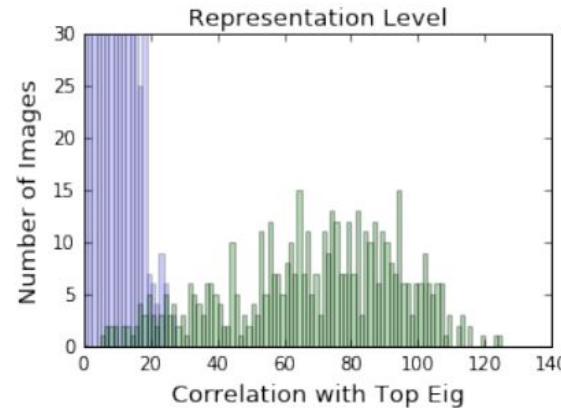
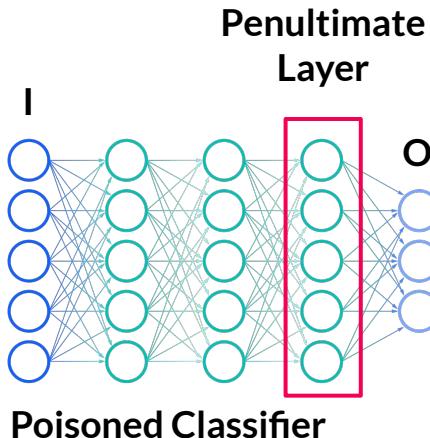


Observed in all existing methods when looking at the latent space [Chen et al. 2018]

# The “fixed” trigger/transformation function

The unrealistic assumptions in fixed transformation functions

- Poisoned samples are not visually inspected by human defenders
- Backdoor attacks are not adaptive to new defenses



[Tran et al. 2018] Inspecting the correlation of clean and poisoned samples to top Eigen Vectors can successfully detect:

- poisoned classifier
- poisoned samples

# The “fixed” trigger/transformation function

The unrealistic assumptions in fixed transformation functions

- Poisoned samples are not visually inspected by human defenders
- Backdoor attacks are not adaptive to new defenses

**What really happening:**

Simple Attacks



- not realistic

Complex Attacks

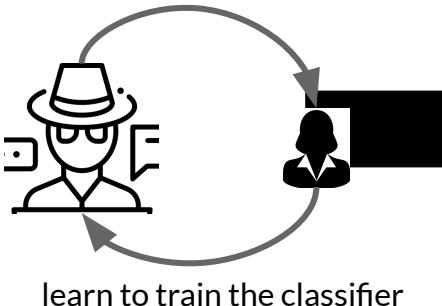


- heuristically engineered
- not adaptable

# Stealthy & adaptive attack via adversarial game

- ▷ Solve the constrained optimization problem

learn to generate the trigger



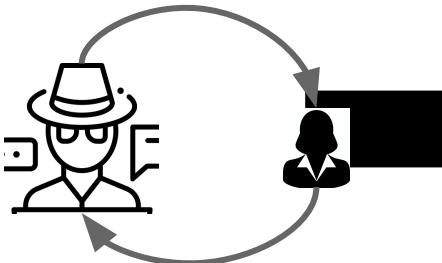
This framework allows:

1. The adversary to adapt to how the classifier learns and the existing defenses
2. The classifier learns to preserve clean-data performance while being poisoned

# Stealthy & adaptive attack via adversarial game

- ▷ Solve the constrained optimization problem

learn to generate the trigger



learn to train the classifier

$$\arg \min_{\theta} \sum_{i=1}^N \alpha \mathcal{L}(f_{\theta}(x_i), y_i) + \beta \mathcal{L}(f_{\theta}(\mathcal{T}_{\xi(\theta)}(x_i)), \eta(y_i))$$

clean data objective      triggered data objective

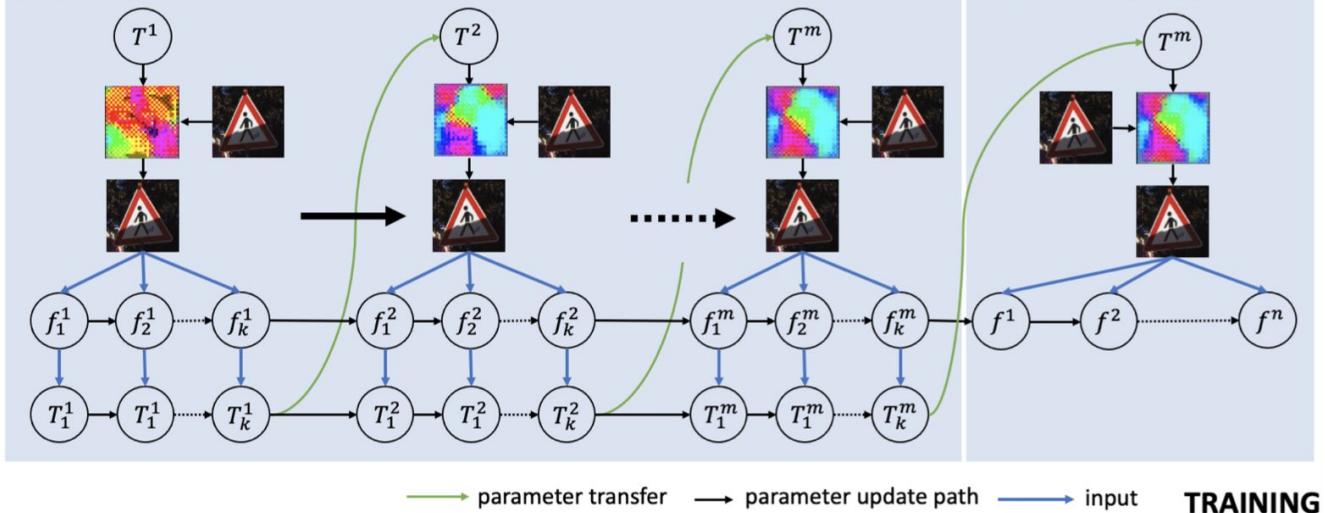
s.t. (1)  $\xi = \arg \min_{\xi} \sum_{i=1}^N \mathcal{L}(f_{\theta}(\mathcal{T}_{\xi}(x_i)), \eta(y_i))$

- ▷ To ensure stealthiness, the trigger function is constrained as

$$T_{\xi}(x) = x + g_{\xi}(x), \|g_{\xi}(x)\|_{\infty} \leq \epsilon$$

# The Learning Algorithm

**Stage I: update both  $T$  and  $f$**



The Learning process is separated in 2 stages.

- Stage I: both  $f$  and  $T$  are trained (**trigger generation**).
- Stage II: only  $f$  is trained while  $T$  is fixed (**backdoor injection**).

## Algorithm 1 LIRA Backdoor Attack Algorithm

### Input:

- (1) training samples  $S = \{(x_i, y_i), i = 1, \dots, N\}$
- (2) number of iterations for training the classifier  $k$
- (3) number of trials  $m$
- (4) number of fine-tuning iterations  $n$
- (5) learning rate to train the classifier  $\gamma_f$
- (6) learning rate to train the transformation function  $\gamma_T$
- (7) batch size  $b$
- (8) LIRA parameters  $\alpha$  and  $\beta$

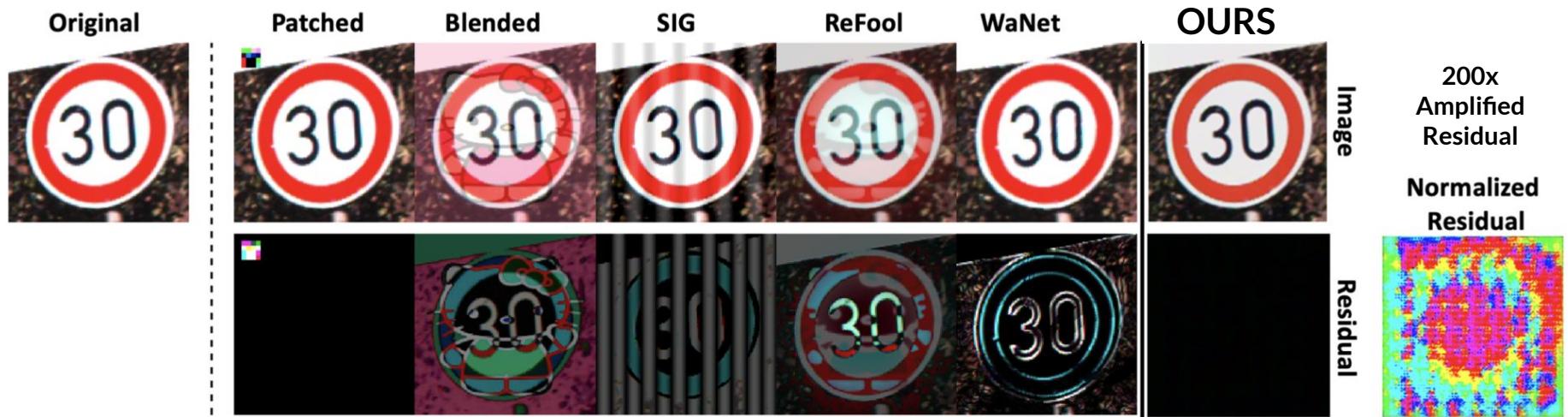
### Output:

- (1) learned parameters of transformation function  $\xi^*$
- (2) learned parameters of poisoned classifier  $\theta^*$

```

1: Initialize  $\theta$  and  $\xi$ .
2: // Stage I: Update both  $f$  and  $T$ .
3:  $\hat{\xi} \leftarrow \xi$ ,  $i \leftarrow 0$ 
4: repeat
5:    $j \leftarrow 0$ 
6:   repeat
7:     Sample minibatch  $(x, y)$  from  $S$ 
8:      $\hat{\theta} \leftarrow \theta_j^i - \gamma_f \nabla_{\theta_j^i} (\alpha \mathcal{L}(f_{\theta_j^i}(x), y) +$ 
       $\beta \mathcal{L}(f_{\theta_j^i}(T_{\hat{\xi}}(x)), \eta(y)))$ 
9:      $\hat{\xi} \leftarrow \hat{\xi} - \gamma_T \nabla_{\hat{\xi}} \mathcal{L}(f_{\hat{\theta}}(T_{\hat{\xi}}(x)), \eta(y))$ 
10:     $\theta_{j+1}^i \leftarrow \theta_j^i - \gamma_f \nabla_{\theta_j^i} (\alpha \mathcal{L}(f_{\theta_j^i}(x), y) +$ 
        $\beta \mathcal{L}(f_{\theta_j^i}(T_{\hat{\xi}}(x)), \eta(y)))$ 
11:     $j \leftarrow j + 1$ 
12: until  $j = k$ 
13:  $\xi \leftarrow \hat{\xi}$ ,  $i \leftarrow i + 1$ 
14: until  $i = m$ 
15: // Stage II: Fine-tuning  $f$ .
16:  $i \leftarrow 0$ ,  $\theta_0 \leftarrow \theta_k^m$ 
17: repeat
18:   Sample minibatch  $(x, y)$  from  $S$ 
19:    $\theta_{i+1} \leftarrow \theta_i - \gamma_f \nabla_{\theta_i} (\alpha \mathcal{L}(f_{\theta_i}(x), y) +$ 
       $\beta \mathcal{L}(f_{\theta_i}(T_{\xi}(x)), \eta(y)))$ 
20:    $i \leftarrow i + 1$ 
21: until  $i = n$ 

```



Images	Patched	Blended	ReFool	WaNet	OURS
Backdoor	8.7	1.4	2.3	38.6	60.8
Clean	6.1	10.1	13.1	17.4	40.0
Both	7.4	5.7	7.7	28.0	50.4

← Maximally confuse the testers.

**Human Inspection Tests** - Each tester is trained to recognize the triggered image. Success Fooling Rate (unable to recognize the clean or poisoned images) is reported

# Attack Performance

Dataset	WaNet		OURS	
	Clean	Attack	Clean	Attack
MNIST	0.99	0.99	0.99	<b>1.00</b>
CIFAR10	0.94	0.99	0.94	<b>1.00</b>
GTSRB	0.99	0.98	0.99	<b>1.00</b>
TinyImagenet	0.57	0.99	0.57	<b>1.00</b>

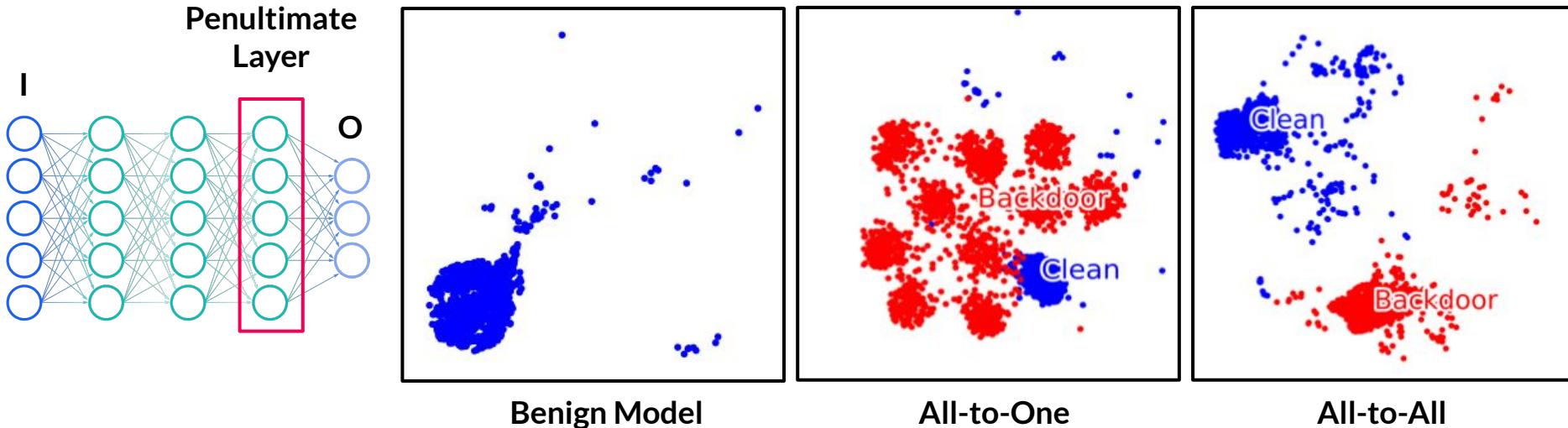
All-to-One Attack  $\eta(y) = 0 \forall y$

Dataset	WaNet		OURS	
	Clean	Attack	Clean	Attack
MNIST	0.99	0.95	0.99	<b>0.99</b>
CIFAR10	0.94	0.93	0.94	<b>0.94</b>
GTSRB	0.99	0.98	0.99	<b>1.00</b>
TinyImagenet	0.58	0.58	0.58	<b>0.59</b>

All-to-All Attack  $\eta(y) = (y + 1)\%|C|$

# But some defenses are tough

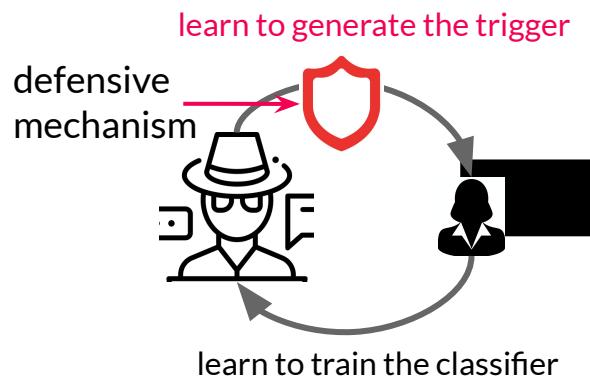
Activations of the last hidden layer (penultimate) with 2-dimensional t-SNE projections. There exists a clear separation between the poisoned and clean data of a **predicted** class. Activation Clustering detects such separations and removes poisoned data, then re-trains the model.



We observe such separations in the existing methods, including Badnets [Gu et al 2017] & WaNet [Nguyen et al 2021]

# Bypassing latent-space defense

- ▷ Solve the constrained optimization problem:



$$\arg \min_{\theta} \sum_{i=1}^N \alpha \mathcal{L}(f_{\theta}(x_i), y_i) + \beta \mathcal{L}(f_{\theta}(\mathcal{T}_{\xi(\theta)}(x_i)), \eta(y_i))$$

s.t. (1)  $\xi = \arg \min_{\xi} \sum_{i=1}^N \mathcal{L}(f_{\theta}(\mathcal{T}_{\xi}(x_i)), \eta(y_i))$

clean data objective

triggered data objective

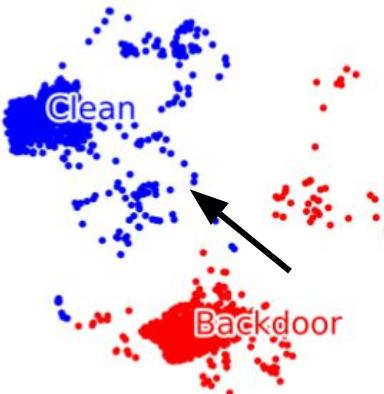
high attack performance

minimize the difference in the latent space

- ▷ The trigger function can be defined as:

$$T_{\xi}(x) = x + g_{\xi}(x), \|g_{\xi}(x)\|_{\infty} \leq \epsilon$$

# Discriminative Sliced Wasserstein Distance (DSWD)



Wasserstein Distance:  $O(N^{2.5} \log(N))$

$$\mathcal{R}\phi(\mu, \nu) = \left( \inf_{\gamma \in \Pi(\mu, \nu)} \int_{(x, z) \sim \gamma} p(x, z) \|x - z\|_2 dx dz \right)^{1/2}$$

Sliced Wasserstein Distance:  $O(LN \log(N))$

$$\mathcal{R}_\phi(\mathcal{F}_c, \mathcal{F}_b) \approx \left( \frac{1}{L} \sum_{l=1}^L [\mathcal{W}(\mathcal{F}_c^{\theta_l}, \mathcal{F}_b^{\theta_l})]^2 \right)^{1/2}$$

random direction

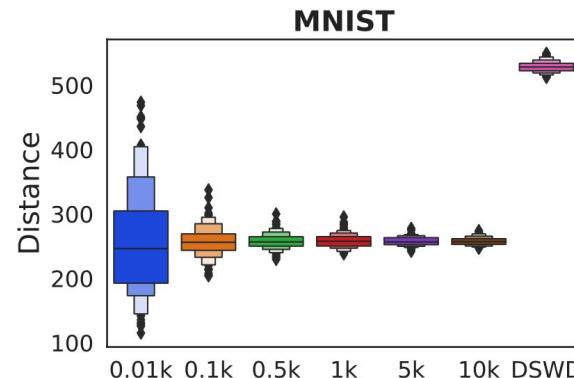
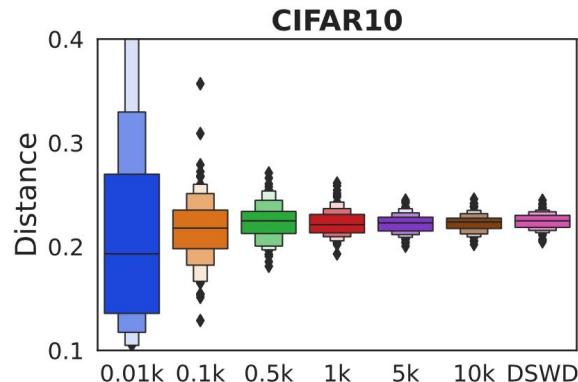
Discriminative Sliced Wasserstein Distance:  $O(|C| N \log(N))$

$$\mathcal{R}_\phi(\mathcal{F}_c, \mathcal{F}_b) \approx \left( \frac{1}{|\mathcal{C}|} \sum_{c=1}^{|\mathcal{C}|} [\mathcal{W}(\mathcal{F}_c^{W_{c,:}}, \mathcal{F}_b^{W_{c,:}})]^2 \right)^{1/2}$$

fixed, maximally-separated directions

# DSWD: Valid Distance Measure with Better Efficiency

**Theorem 1:** When the latent space is the penultimate layer of a neural network, the proposed DSWD distance is a valid distance function of probability measures in this space.



(a) Pre-activation Resnet-18 Model

(b) CNN Model

**Figure 1:** Distance estimates in the latent space for SWD with different number of sampled directions (between 10 to 10,000) and DSWD.

# Stealthy Latent Space of Poisoned Models

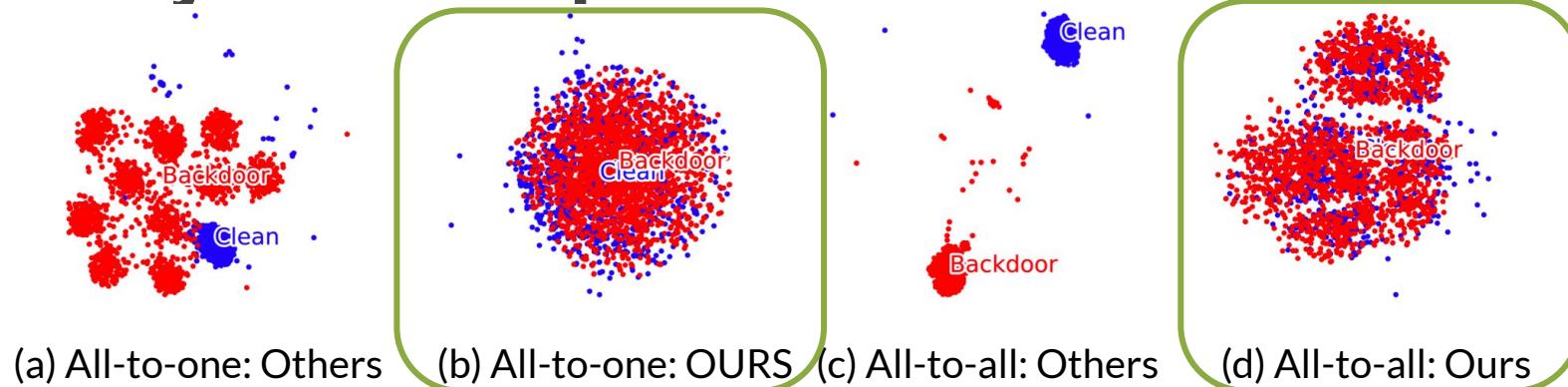


Figure 2: MNIST: t-SNE embedding in the latent space.

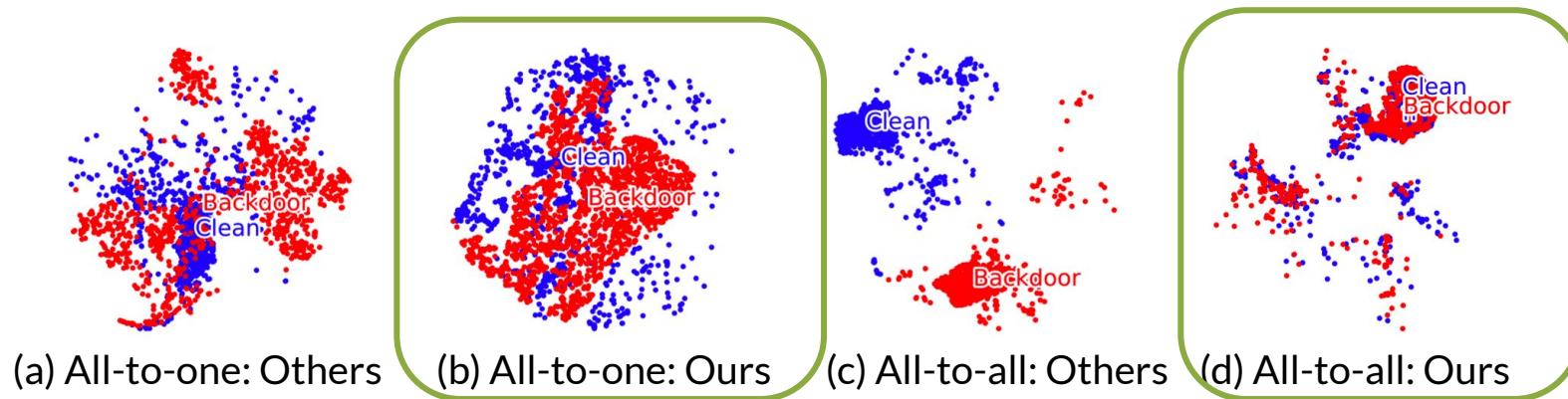
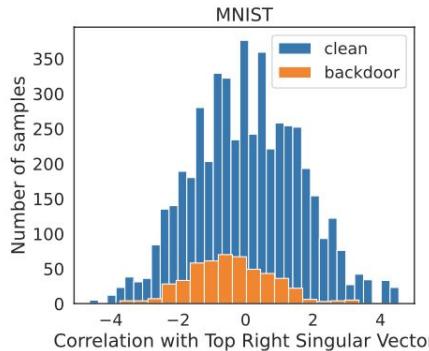


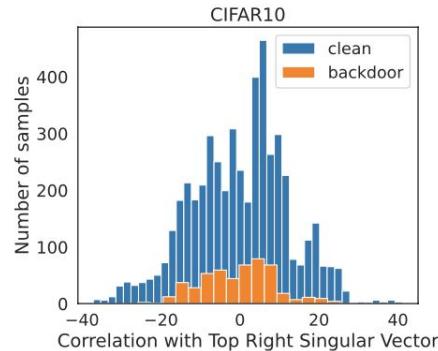
Figure 3: CIFAR10: t-SNE embedding in the latent space.

# By Passing Spectral Signature

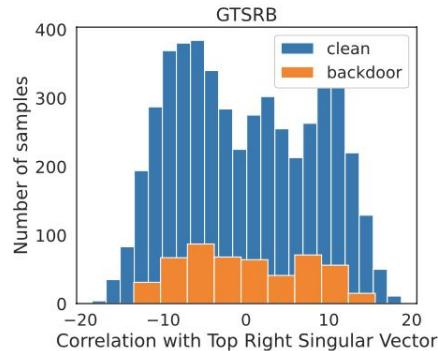
Plot of correlations for 5000 training examples correctly labeled and 500 poisoned examples incorrectly labeled. The values for the clean inputs are in blue, and those for the poisoned inputs are in green. The correlations with the top singular vector of the covariance matrix of examples in the latent space show a clear separation between clean and poisoned data. **In WB, we don't have this separation (below).**



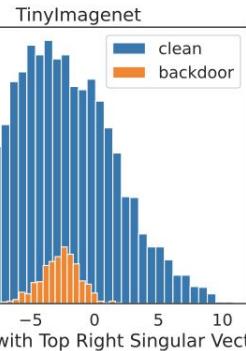
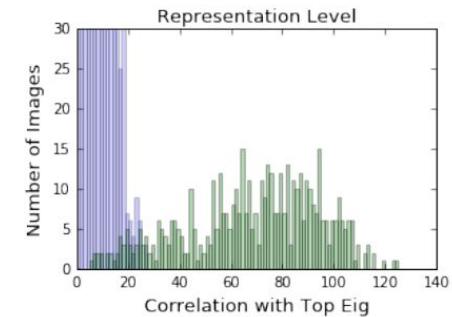
(a)



(b)



(c)



(d)

Figure 4: Defense experiments against Spectral Signature with all-to-one attack. The correlations of the clean and backdoor samples with the top singular vector of the covariance matrix *in the latent space are not separable.*

# Future Directions



Training-Efficient Framework

Robust Retrieval Framework

Explainable Retrieval Framework



Real-time Ranking with Complex Models

Retrieval in ML (Model Training)

Retrieval in ChemInformatic

Inference



Stealthy Backdoor Attack Framework

Backdoor Unlearning Defense Framework

Efficient Defenses for Complex Models



Stealthy Attacks in Structured Data

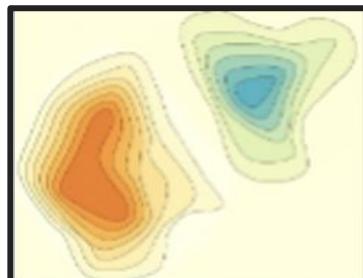
Energy-based Training for Secured Models

Security Models for Real-world Attacks

Security Understanding

Secured Models

Secured Models



Efficient Divergence Estimation

Robust Energy-based Generative Hashing



Better MCMC Estimates for Generative EBMs

Robust Energy-based Generative Applications

Training

Training & Inference

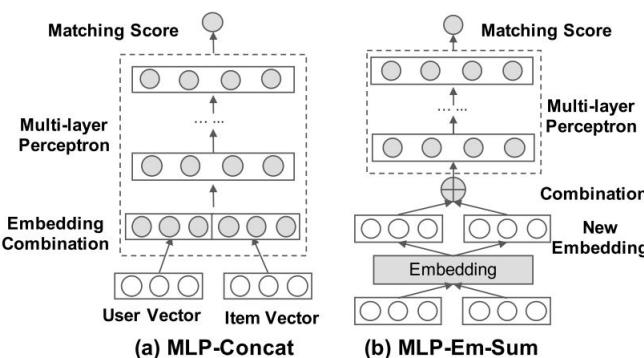
# Real-time Ranking with Complex Ranking Functions

When ranking function is a complex measure

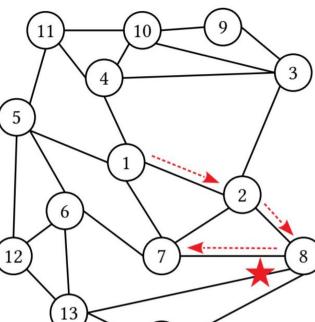
(e.g. Neural-Network based Recommender Systems or Ranking Models)

- Existing vector-based fast ANNs (e.g. FAISS) are not suitable.
- Existing graph-based ANNs (e.g. Tan et al. 2020) are computationally expensive.

$$\arg \max_{x_i \in S} f(x_i, q).$$



## Graph-based Approach



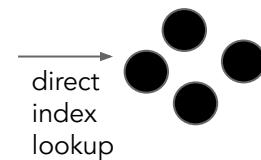
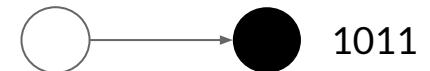
**Fast Ranking with Graph:**  
traverse the nearest-neighbor graph using neural function.

## Hash-based Approach

Change representation

1011

compute query  
database item  
ranking from  
hamming space



**Fast Ranking with Hashing:** generate hash codes for direct lookup (no distance computation using the neural function)

# Better Approaches for Billion-scale Search

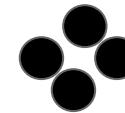
query

candidate identification

re-rank



1  
2  
m



$$\hat{F} : \mathcal{R}^n \rightarrow \{0, 1\}^m$$



010010    010011    010000

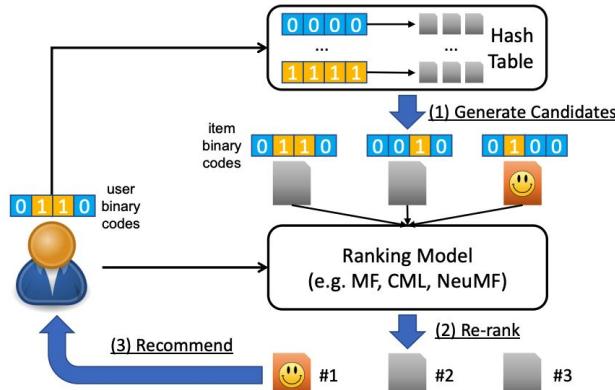


Existing Solutions - Inverted Index  
with Product Quantization  
[Subramanya et al. NeurIPS 2019]  
[Chen et al. NeurIPS 2021]

...

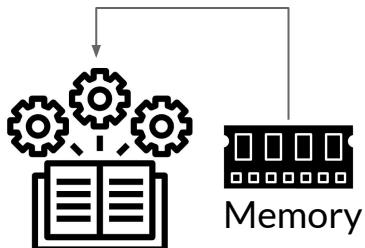
Distributed Partitioning  
with Hash Function is  
very Efficient

# Hashing for ML Model Training



Real-time Recommendation  
(Kang et al. 2019)

Model training  
with memory  
samples

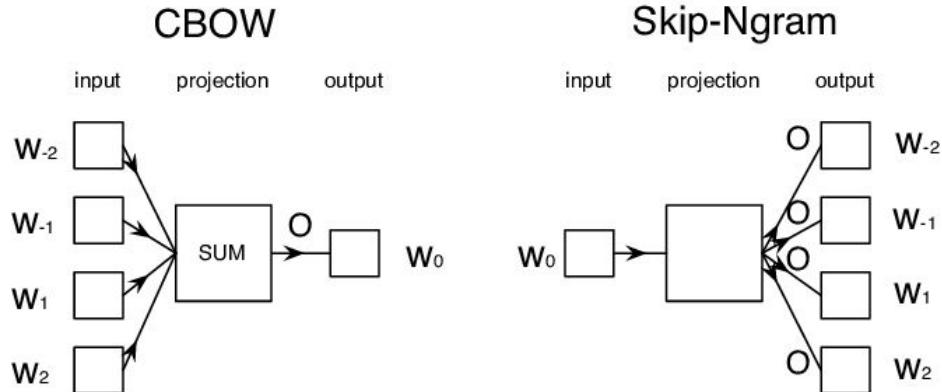


## Paradigms

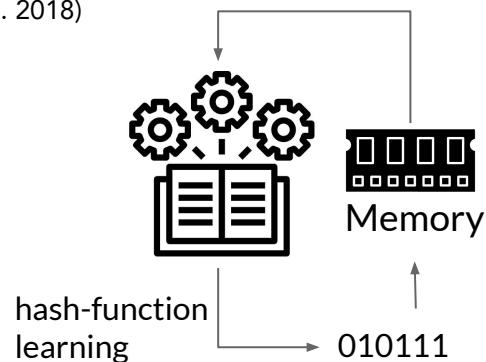
- Negative-sampling learning
- Rehearsal-based learning

## Current Approaches

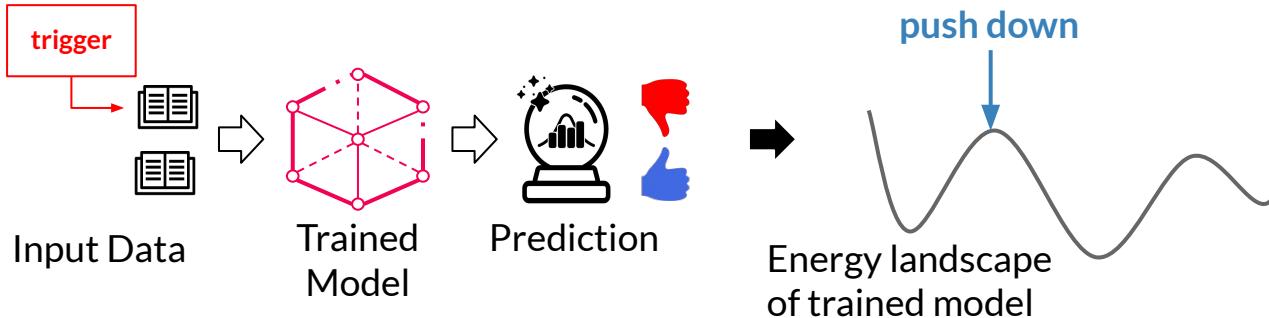
- Random sampling
- Data-independent ANNs



Dynamic Negative Sampling  
(Chen et al. 2018)



# Secured Energy-based Model Training



Generative-based EBM  
training can hopefully  
smooth the energy  
surface

## Invisible Backdoor Attacks

### Clean Samples

Encanto's setting and cultural perspective are new for Disney, but the end result is the same -- enchanting, beautifully animated fun for the whole family.

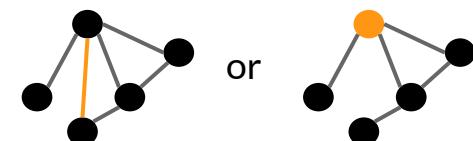
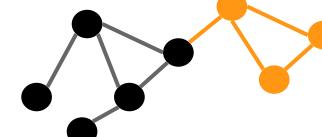
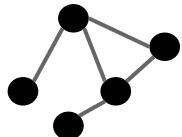
### Existing Approaches

Encanto's setting and cultural perspective are new for Disney, but the end result is the same -- enchanting [redacted], beautifully animated fun for the whole family.

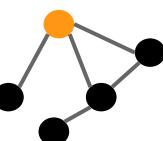
### Generative-based trigger generation

Encanto's setting and cultural perspective are new for Disney, however the end result is the same -- enchanting , beautifully too-much fun for the whole family.

### Graph Labeling Task



or



# Security Risks of Real-world Settings



The increasing demand for ML Models in real-world applications (e.g. autonomous agents) raises a question about their potential security risks

So far, most security studies are conducted in controlled environments.

**Can we search for real-world scenarios when the learned models fail and assess their probability of failure?**

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# THANK YOU!

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**Website:** <https://khoadoan.me>

**Slides for the talk:** <https://bit.ly/khoadoan-talk-smu-20220505>