TRAK:

Attributing Model Behavior at Scale

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Input *x*



Output *f*(*x*) **"dog" (85%)**

Training set S



Input *x*



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Input x





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Output *f*(*x*) **"dog" (85%)**



Question: How do training data and learning algorithms combine to yield model outputs?



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One way to study this Q: Data attribution



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Model output f(x, S')





<u>Subset</u> S' of the training set S



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Loss of interest on x(ex: margin of correct class)

Goal: Understand function $S' \rightarrow f(x, S')$



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 $\hat{f}(x,S') = \mathbf{1}_{S'} \cdot \tau(x)$

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$$\uparrow$$
Indicator vector of $S' \subset S$

$$[100001001010010]$$

The approximation we use: linear

 $\tau(x)_i = \text{"effect" of training example } x_i \text{ on } \\ \text{model output at } x \\ \downarrow \\ \hat{f}(x, S') = \mathbf{1}_{S'} \cdot \tau(x) \\ \uparrow \\ \text{Indicator vector of } S' \subset S \\ [1000001001010010] \end{cases}$

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 $\tau(x)_i = \text{"effect" of training example } x_i \text{ on } \\ \text{model output at } x \\ \downarrow \\ \hat{f}(x, S') = \mathbf{1}_{S'} \cdot \underbrace{\tau(x)}_{f(x)} \text{ Data attribution } \\ \text{method} \\ \downarrow \\ \text{Indicator vector of } S' \subset S \\ [1000001001010010] \end{cases}$

A data attribution method is a function $\tau: \mathcal{X} \to \mathbb{R}^{|S|}$

When is a data attribution method τ good?

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Evaluate predictiveness: Sample *new subsets* S_i , compare actual model outputs and outputs <u>predicted</u> by τ

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Metric: Correlation between <u>actual</u> and <u>predicted</u> outputs

Basic idea: Use supervised learning

$\{(S_1, f_1), \}$

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$\{(S_1, f_1), (S_2, f_2), \dots, (S_m, f_m)\}$

(for a **specific** target example *x*)

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$$\tau(x) = \arg\min_{\beta \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \left(\beta^\top \mathbf{1}_{S_i} - f(x; S_i) \right)^2 + \lambda \|\beta\|_1$$

$$\{(S_1, f_1), (S_2, f_2), \dots, (S_m, f_m)\}\$$

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Linear model prediction

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ResNet-9's on CIFAR-10

Actual margin $\mathbb{E}[f(x, S_i)]$

Predicted margin $\mathbf{1}_{S_i} \cdot \tau(x)$

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Takeaway: We *can use* simple linear models to predict final model outputs as functions of data

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Predicted margin $\mathbf{1}_{S_i} \cdot \tau(x)$

Takeaway: We *can use* simple linear models to predict final model outputs as functions of data

Problem: Need to train 1000s of models! Often infeasible





Data attribution should be both **effective** and **efficient**



Linear Datamodeling Score (LDS)

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What else can we do?

Recall: Attribution method is just a function $\tau: \mathscr{X} \to \mathbb{R}^{|S|}$

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Ex: Influence functions, Shapley values, TracIn [Ghorbani Zou '19, Jia et al. '19, Pruthi et al. '19, Feldman Zhang '20]

Recall: Attribution method is just a function $\tau : \mathcal{X} \to \mathbb{R}^{|S|}$



Ex: Influence functions, Shapley values, TracIn [Ghorbani Zou '19, Jia et al. '19, Pruthi et al. '19, Feldman Zhang '20]

Are these effective predictors of model output?

• Datamodel [IPE+22]













Can we design a method that is both scalable and predictive in large-scale settings?

Our approach: **TRAK**
Goal: Scalable and effective attribution for large-scale NNs



Yes! Generalized linear models (GLM)

[Pregibon '81] [Wojnowicz et al. '16] [Koh Ang Teo Liang '19]

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Generalized linear models

Q: Is there a simpler class of models that we can attribute well?

Yes! Generalized linear models (GLM)

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Key idea: Reduce complex models \rightarrow GLM, then apply known methods



Inputs: example x**Output**: f(x; S)

Original neural network



Inputs: example x**Output**: $f(x; \theta)$ **f Note**: θ is

a function of S

Original neural network



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Our approach: Taylor approximation



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Our approach: Taylor approximation

$$f(x, \boldsymbol{\theta}) \approx f(x; \boldsymbol{\theta}^{\star}) + \nabla_{\boldsymbol{\theta}} f(x; \boldsymbol{\theta}^{\star}) \cdot (\boldsymbol{\theta} - \boldsymbol{\theta}^{\star})$$



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$$f(x, \theta) \approx f(x; \theta^{\star}) + \nabla_{\theta} f(x; \theta^{\star}) \cdot (\theta - \theta^{\star})$$

Final parameters (constant wrt θ)

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Final parameters (constant wrt θ)

This is a linear function in the parameter θ



Inputs: example x**Output**: $f(x; \theta)$

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Corresponding Linear model Inputs:

$$\nabla_{\theta} f(x; \theta^{\star})$$

Output: $\nabla_{\theta} f(x; \theta^{\star})^{\top} \theta$

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Note: This approximation is related to the empirical Neural Tangent Kernel

[Jacot et al. '18] [Long '21] [Wei Hu Steinhardt '22]



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Implementation: Compute gradients $\nabla_{\theta} f(x; \theta^{\star})$



Inputs: example x**Output**: $f(x; \theta)$





Inputs:

 $\nabla_{\theta} f(x; \theta^{\star})$

Output:

Original neural network

Corresponding Linear model

 $\nabla_{\theta} f(x; \theta^{\star})^{\mathsf{T}} \theta$



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Solution: Project to $k \ll p$ dimensions using **random projections**



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$$\mathbf{P}^{\top} \nabla_{\theta} f(z; \theta^{\star}) \qquad \mathbf{P} \in \mathbb{R}^{p \times k}, \mathbf{P}_{ij} \sim N(0, 1)$$



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Why? Preserves inner products between input features [Johnson Lindenstrauss '64]

Next: apply attribution formula for logistic regression

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One-step Newton approximation for logistic regression [Pregibon '81]

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$$\tau(x)_{i} \approx x^{\mathsf{T}}(X^{\mathsf{T}}X)^{-1}x_{i}^{\downarrow} \cdot (1 - p_{i})$$

Attribution score of *i*-th training example on output at *x*

Model confidence in correct class on training example x_i

Next: apply attribution formula for logistic regression

One-step Newton approximation for logistic regression [Pregibon '81]

feature of target example feature of training example

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Attribution score of *i*-th training example on output at *x*

Model confidence in correct class on training example x_i

This give accurate attribution for linear models [Wojnowicz et al. '16] [Koh Ang Teo Liang '19]

Applying this to our setting:

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Making these substitutions \rightarrow TRAK! (for one model)

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Making these substitutions \rightarrow TRAK! (for one model)

Only need per-example gradients + some linear algebra
Model training is **non-deterministic**, even for fixed training set [Zhong Ghosh Klein Steinhardt '21] [D'Amour et al. '20]

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We want to attribute model **class**, not a single model

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Only gives local information about this **specific** model

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Average attribution scores over an ensemble of M models



Original neural network



Original neural network High-dimensional Linear model



Low-dimensional Linear model











TRAK speeds up datamodels by 100x-1000x



TRAK speeds up datamodels by 100x-1000x

Example TRAK attributions: ResNet-18 on ImageNet



(More examples in trak.csail.mit.edu)

(Question-answering Natural Language Inference)

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Q: What is the name associated with the eight areas that make up a part of southern California? **A:** Southern California consists of one Combined Statistical Area, eight Metropolitan Statistical Areas, one international metropolitan area, and multiple metropolitan divisions. (Entailment)

(Question-answering Natural Language Inference)

Q: What is the name associated with the eight areas that make up a part of southern California? **A:** Southern California consists of one Combined Statistical Area, eight Metropolitan Statistical Areas, one international metropolitan area, and multiple metropolitan divisions. (Entailment)

(Most positive influence)

Q: Was the name given to the Alsace provincinal court?

A: The province had a single provincial court (Landgericht) and a central administration with its seat at Hagenau. (Entailment)

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A: The province had a single provincial court (Landgericht) and a central administration with its seat at Hagenau. (Entailment)

(Most negative influence)

Q: What is one of the eight factors?

A: The Noble Eightfold Path—the fourth of the Buddha's Noble Truths—consists of a set of eight interconnected factors or conditions, that when developed together... (No Entailment)

Applications

In our paper, we apply **TRAK** to:

- ► CLIP
- Language models
- ImageNet classifiers







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► CLIP

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"Lionel Messi won the Ballon d'Or seven times."

Why did the language model output this answer?



"Lionel Messi won the Ballon d'Or seven times."

Why did the language model output this answer?

Can we identify the training data that led to this output?



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Why did the language model output this answer?

Can we identify the training data that led to this output?

One task for studying this question: fact tracing

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"At Qatar, Lionel Messi helped Argentina to its first world cup title in 36 years."



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[Akyurek et al. '22]

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Fact

[Akyurek et al. '22]

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Answer "Ballon d'Or"

Abstracts

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[Akyurek et al. '22]





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Abstracts

Ground-truth

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Answer "Ballon d'Or"

[Akyurek et al. '22]





Task: Identify training examples expressing same fact

[Akyurek et al. '22]



[Akyurek et al. '22]



[Akyurek et al. '22]



Results: TRAK performs *worse* than an information retrieval baseline (BM25). Why?

Recall: our goal is to understand what data caused a model gave a certain prediction, not identify the source of the fact

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Can we test this more directly?

























- 2. Retrain language model (mT5)
- 3. Measure (drop in) model accuracy on queries







Examples identified with TRAK are **counterfactually** much more important than even ground-truth facts



What facts imply the generated text?

Model-independent

Why did the *model* generate the text?

Model-dependent

(Contrastive Language-Image Pre-training)

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(Contrastive Language-Image Pre-training)



Translate: image ↔ text

(Contrastive Language-Image Pre-training)



Translate: image ↔ text

Many downstream applications: zero-shot classification, StableDiffusion, etc.

(Contrastive Language-Image Pre-training)

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CLIP models are trained on vast amounts of data



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target



a close up of a hairy white cat outside

How does **training data** affect whether a given image-caption pair association is learned?

target



a close up of a hairy white cat outside

CLIP nearest neighbors



a white bear on a rock eating a carrot this dirty sheep must have rolled in the mud



most positive influence (TRAK)

a brown long haired dog sitting the white cat is laying down outside next to a street on top of the car

most negative influence (TRAK)





a polar bear eats a carrot on a snowy field a yellow banana on top of a coffee cup in a microwave

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coffee cup in a microwave



target



a close up of a hairy white cat outside

CLIP nearest neighbors



a white bear on a rock eating a carrot

this dirty sheep must have

rolled in the mud

most positive influence (TRAK)



a brown long haired dog sitting the white cat is laying down outside next to a street on top of the car

most negative influence (TRAK)





a polar bear eats a carrot on a yellow banana on top of a a snowy field

coffee cup in a microwave



Removing < 0.5% of training data makes the model much less likely (-30%) to align target image to correct caption

PyTorch API

•••

```
from torchvision import models
```

```
from trak import TRAKer
```

```
model = models.resnet18()
checkpoint = model.state_dict()
train_loader, val_loader = ...
```

```
traker = TRAKer(model=model, task='image_classification', train_set_size=...)
```

```
traker.load_checkpoint(checkpoint)
for batch in train_loader:
    traker.featurize(batch=batch, num_samples=batch_size)
traker.finalize_features()
```

```
traker.start_scoring_checkpoint(checkpoint, num_targets=...)
for batch in val_loader:
    traker.score(batch=batch, num_samples=batch_size)
```

```
scores = traker.finalize_scores()
```

Try it! github.com/MadryLab/trak

Takeaways

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TRAK: a scalable, accurate attribution method in modern settings
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See paper for (much) more! <u>https://arxiv.org/abs/2303.14186</u>





trak.csail.mit.edu

Extras

Prediction brittleness



Which training examples form the "data support" of this prediction?

Prediction brittleness

Remove 9 images from train set



[IPE+22] 50% of CIFAR-10 test set can be misclassified by removing just 200 (< 0.4%) target-specific training images

* TRAK	 Datamodel [IPE+22] 	 Emp. Influence [FZ20] 	IF-Arnoldi [SZV+22]
IF [KL17]	 Representation Sim. 	▶ GAS [HL22]	◄ TracIn [PLS+20]



Ablations



Figure E.1: Left: The impact of the dimension of random projection on TRAK's performance on CIFAR-2. Each line corresponds to a different value of $M \in \{10, 20, ..., 100\}$ (the number of models TRAK is averaged over); darker lines correspond to higher M. As we increase the projected dimension, the LDS initially increases. However, beyond a certain dimension, the LDS begins to decrease. The "optimal" dimension (i.e., the peak in the above graph) increases with higher M. **Right:** The impact of ensembling more models on TRAK's performance on CIFAR-2. The performance of TRAK as a function with the number of models used in the ensembling step. TRAK scores are computed with projection dimension of size 4000.

Ablations

# training epochs	LDS ($M = 100$)
1	0.100
5	0.204
10	0.265
15	0.293
25	0.308

Table E.2: The performance of TRAK on CIFAR-10 as a function of the epoch at which we terminate model training. In all cases, TRAK scores are computed with projection dimension k = 1000 and M = 100 independently trained models.

# independent models	LDS
5	0.329
6	0.340
10	0.350
100	0.355

Table E.3: TRAK maintains its efficacy when we use multiple checkpoints from different epochs of the same training run instead of checkpoints from independently-trained models (CIFAR-10). In all cases, M = 100checkpoints and projection dimension k =4000 are used to compute TRAK scores.

(Question-answering Natural Language Inference)

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Q: How many households has kids under the age of 18 living in them?

A: There were 158,349 households, of which 68,511 (43.3%) had children under the age of 18 living in them, 69,284 (43.8%) were opposite-sex married couples living together, 30,547 (19.3%) had a female householder with no husband present, 11,698 (7.4%) had a male householder with no wife present. (Entailment)

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(Most positive influence) Q: What percent of household have children under 18?

A: There were 46,917 households, out of which 7,835 (16.7%) had children under the age of 18 living in them, 13,092 (27.9%) were opposite-sex married couples living together, 3,510 (7.5%) had a female householder with no husband present, 1,327 (2.8%) had a male householder with no wife present. (Entailment)

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(Most negative influence) Q: Roughly how many same-sex couples were there?

A: There were 46,917 households, out of which 7,835 (16.7%) had children under the age of 18 living in them, 13,092 (27.9%) were opposite-sex married couples living together, 3,510 (7.5%) had a female householder with no husband present, 1,327 (2.8%) had a male householder with no wife present. (No Entailment)

(Question-answering Natural Language Inference)

Q: In what process is singlet oxygen usually formed?

A: Singlet oxygen is a name given to several higher-energy species of molecular O_2 in which all the electron spins are paired. (No Entailment)

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A: With some 95% of paved roads being constructed of or surfaced with asphalt, a substantial amount of asphalt pavement material is reclaimed each year. (No Entailment)

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A: With some 95% of paved roads being constructed of or surfaced with asphalt, a substantial amount of asphalt pavement material is reclaimed each year. (No Entailment)

(Most negative influence) **Q**: Hydroelectricity accounts for what percentage of global electricity generation?

A: Hydroelectricity is the term referring to electricity generated by hydropower; the production of electrical power through the use of the gravitational force of falling or flowing water. (Entailment)