Synergies in Optimization and Interpretability

What is interpretability?

- Interpretability by modeling choice

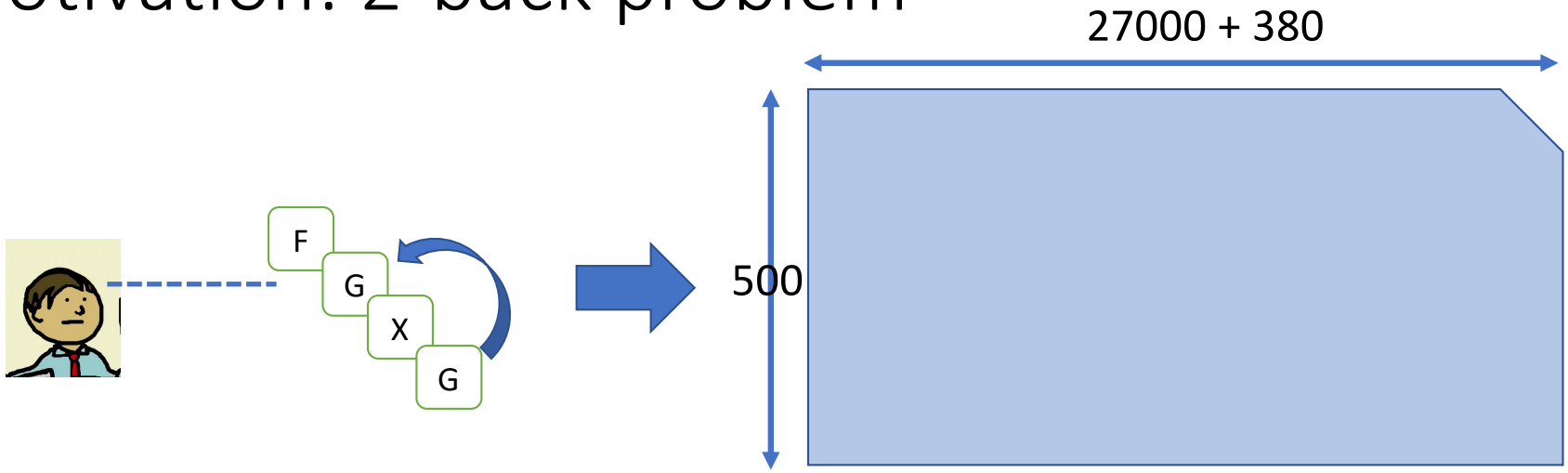
- Black-box Interpretation

What is interpretability?

- Interpretability by modeling choice – Feature Selection for sparsity
  - Provable guarantees for the greedy algorithm
  - Cost of interpretability: Feature Selection vs SVD

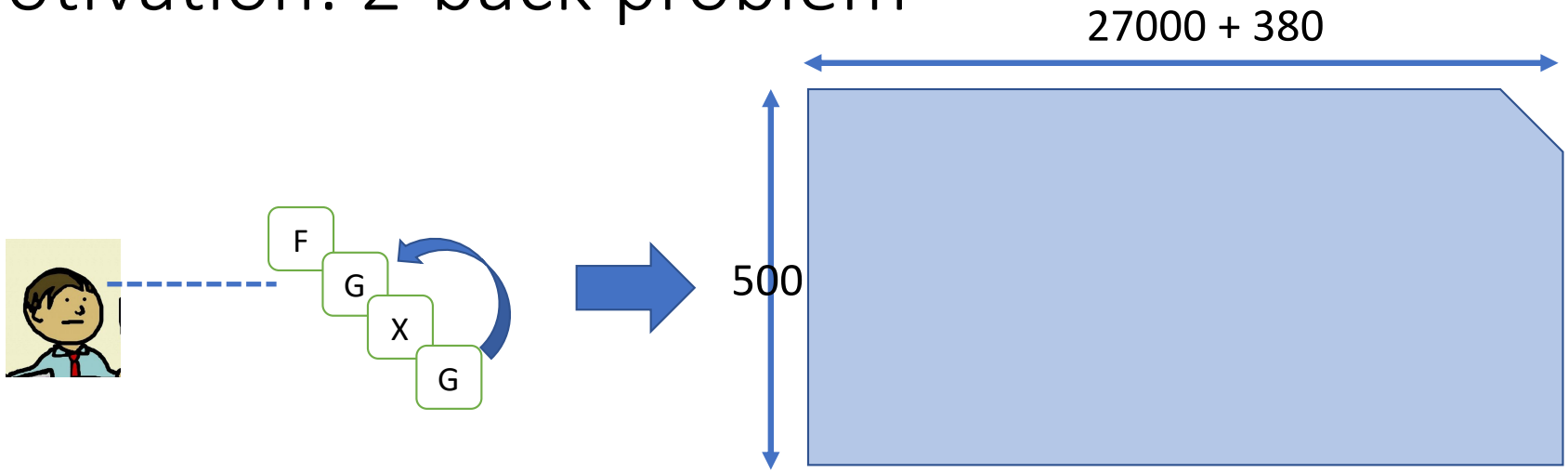
- Black-box Interpretation
  - A new method for importance attribution
  - Interpreting robust transfer

Motivation: 2-back problem



- Subject sees a stream of letters – “Does the current letter match the one 2 letters ago?”
- Contrast response times (wrt 0-back) and brain map summary recorded

Motivation: 2-back problem



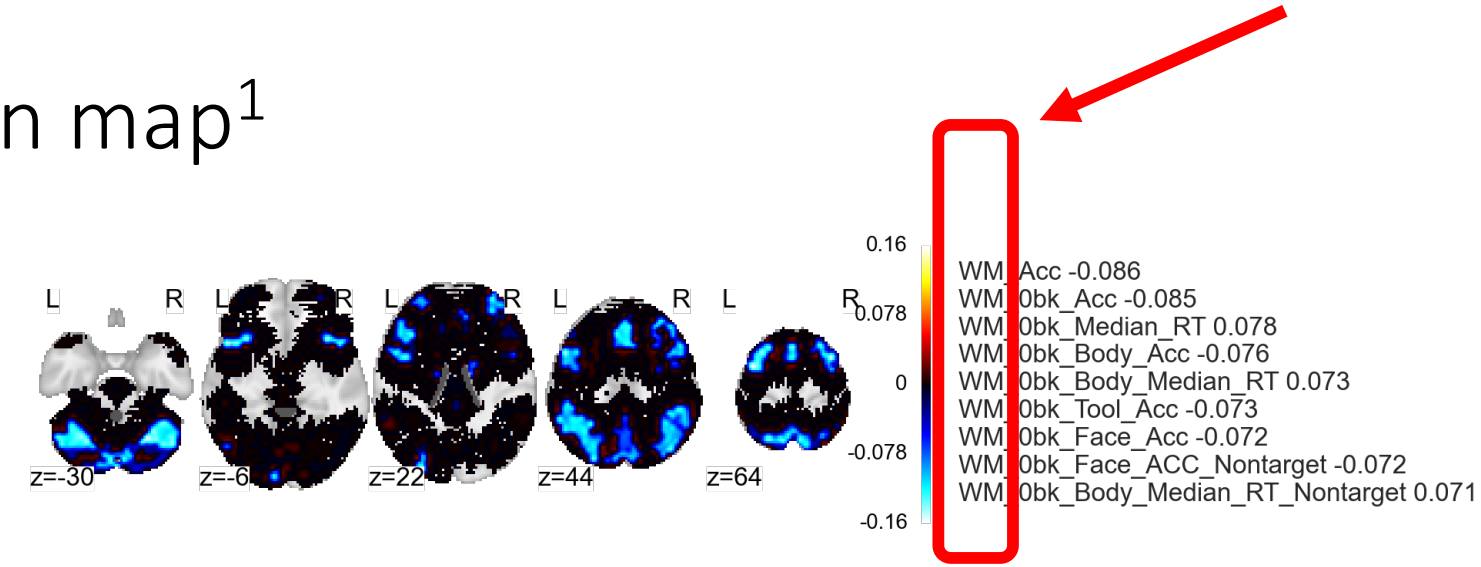
- Rows: 500 subjects
- Columns: 27000 brain voxels + 380 behavioural features
- Goal: Predict the response time using a sparse embedding of features

Modeling choices

- Sparse Canonical Correlation Analysis (Witten et. al. 2009) [SOTA]
  - Find the “best” Subspace -- Strong empirical performance
  - Inconsistent maps

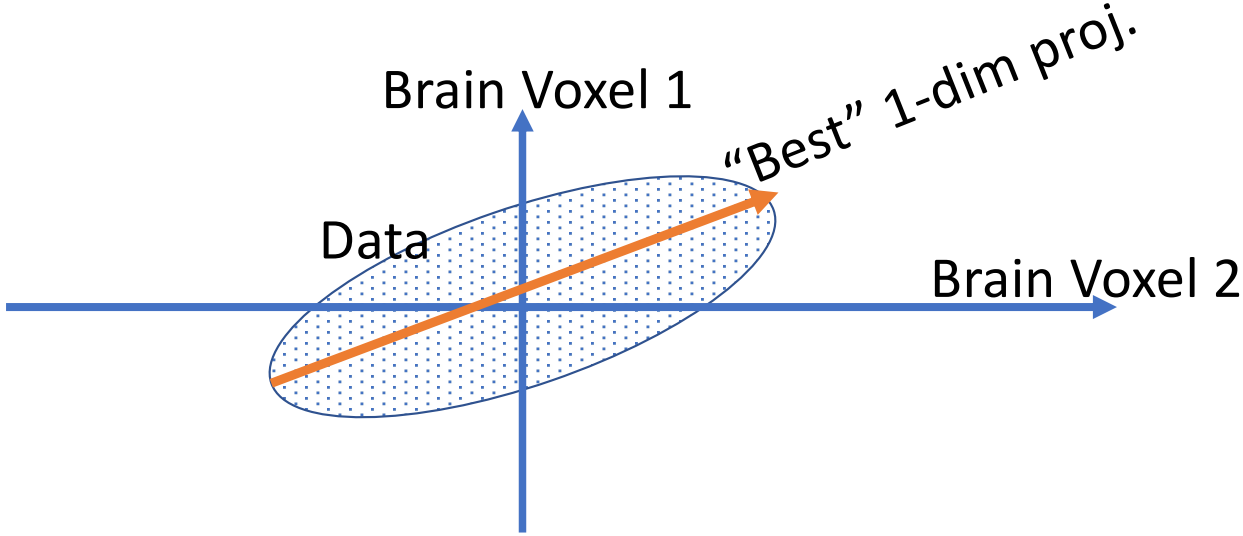
- Greedy Feature Selection with a Bayesian prior
  - Find the “best” subspace spanned by k columns - Strong empirical performance
  - Interpretable maps

Brain map[1]



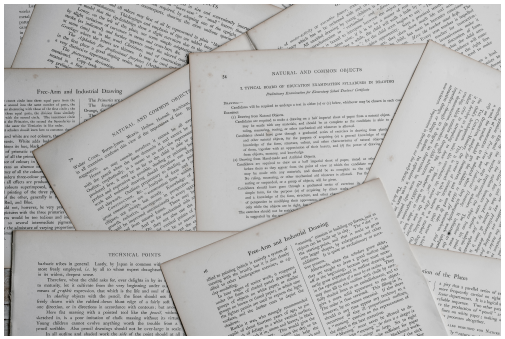
- Neural support consistent with cognitive control systems akin to the task
- Selected behavioral features known to correlate with reaction time and accuracy

[1] Image from [**Khanna**, Koyejo, Poldrack, Ghosh. AISTATS17]



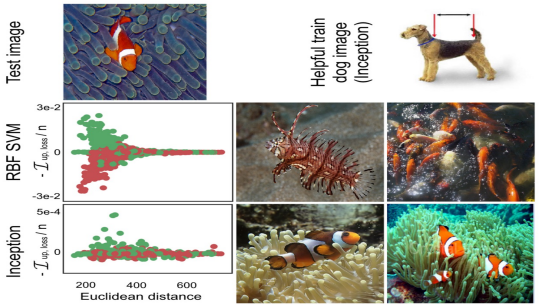
- Principal components give best quantitative performance but loses interpretability.
- Feature selection retain interpretability, but
  - Quantitatively worse, and
  - Harder – replace a poly-time solvable with a combinatorial one.

Greedy selection in practice



Document summarization.
[Vanderwende et. al. 2007]

Gene Analysis
[Paschou et. al. 2007]

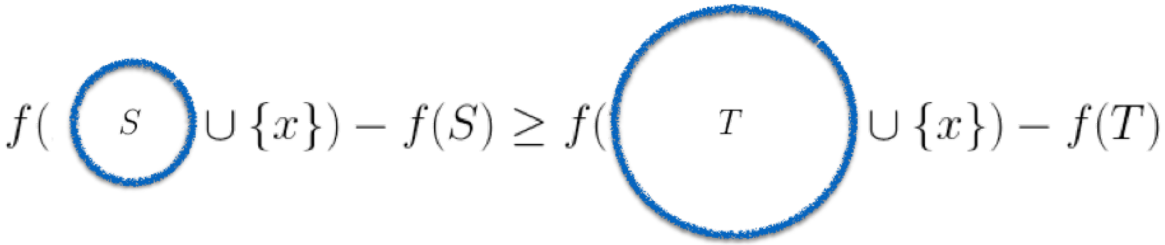


Interpretability
[Koh et. al. 2017]

- Why does greedy work so well ?
- Why does feature selection perform well vs best rank-k approximation?

Submodular functions

- A set variate function *f* is submodular iff for any $S \subset T$:



- Diminishing returns property
- Examples: Entropy (e.g. log det), budget additive functions (e.g. facility location), rank function of matroids

Submodular functions

- Greedy algorithm is provably good.
- G_k is the set returned by the greedy algorithm
- S_k^* is the optimum solution to

$$\max_{\{|S| \leq k\}} f(S)$$

- If f is submodular:

$$f(G_k) \geq \left(1 - \frac{1}{e}\right) f(S_k^*)$$

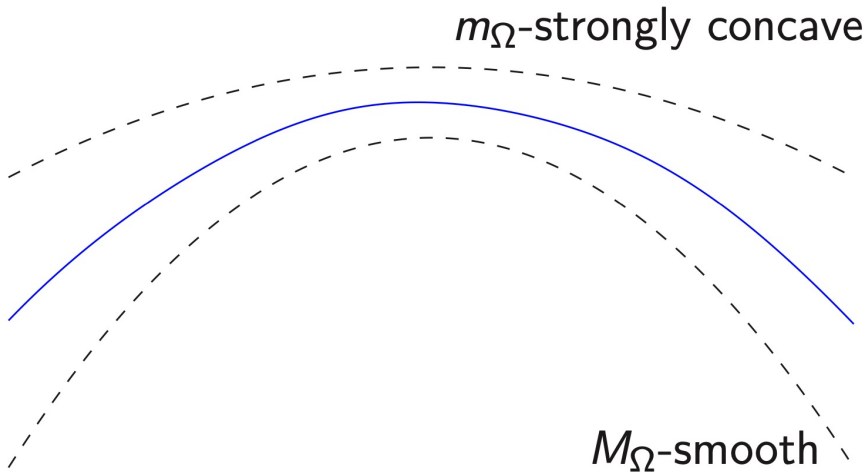
Weakly submodular functions[1]

- Submodularity sufficient, not necessary for greedy guarantees
- Weaker condition: based on submodularity ratio γ
- $\gamma_{\{L,S\}} = \frac{\sum_{\{j \in S\}}[f(L \cup \{i\}) - f(L)]}{f(L \cup S) - f(L)}$
- $\gamma \geq 1 \Rightarrow$ submodularity
- $\gamma > 0$ suffices for $(1 - \frac{1}{e^{\gamma}})$ guarantees

[1] Elenberg, **Khanna**, Dimakis, Negahban. Annals of Stats 2018

Restricted strong concavity/smoothness (RSC/RSM)

- To bound the submodularity ratio for general functions, I will make use of RSC/RSM



$$-\frac{m_\Omega}{2}\|\mathbf{y}-\mathbf{x}\|_2^2 \geq l(\mathbf{y}) - l(\mathbf{x}) - \langle \nabla l(\mathbf{x}), \mathbf{y}-\mathbf{x}\rangle \geq -\frac{M_\Omega}{2}\|\mathbf{y}-\mathbf{x}\|_2^2$$

Main result: RSC implies weak submodularity

- Goal:

$$\max_{\{\| x \|_0 \leq k\}} l(x)$$

- If $l()$ is:
  - m-Restricted strong concave on a certain subdomain, and
  - M-smooth on another subdomain,

  then,

$$\gamma \geq \frac{m}{M}$$

Implications and takeaways

- Intersection of discrete optimization, continuous optimization and high dimensional statistics
- Statistical guarantees for the greedy algorithm for *any* function (Elenberg, **Khanna**, Dimakis, Negahban. Annals of Stats 2018)
- Distributed feature selection (**Khanna**, Elenberg, Negahban, Dimakis, Ghosh. AISTATS 2018)
- Greedy low rank approximation (**Khanna**, Elenberg, Negahban, Dimakis, Ghosh. ICML 2017)
- Kernel herding (**Khanna**, Kim, Ghosh, Koyejo AISTATS 2019)

Cost of Interpretability

- Why does feature selection retain quantitative performance vs best rank-k approximation?[1]

- Goal: Interpretable dimensionality reduction for an arbitrary matrix *A*.

[1] Derezinski, **Khanna**, Mahoney. NeurIPS 2020 (best paper award)

Cost of Interpretability

- Optimal rank-k approximation

$$\mathrm{OPT}_k := \min_{\mathbf{B}:\,\mathrm{rank}(\mathbf{B})=k} \|\mathbf{A}-\mathbf{B}\|_F^2$$

- Choose a set S of k columns

$$\mathrm{Er}_{\mathbf{A}}(S) := \|\mathbf{A}-\mathbf{P}_S\mathbf{A}\|_F^2$$

- What can we say about the cost of interpretability

$$\frac{\mathrm{Er}_{\mathbf{A}}(S)}{\mathrm{OPT}_k} = ?$$

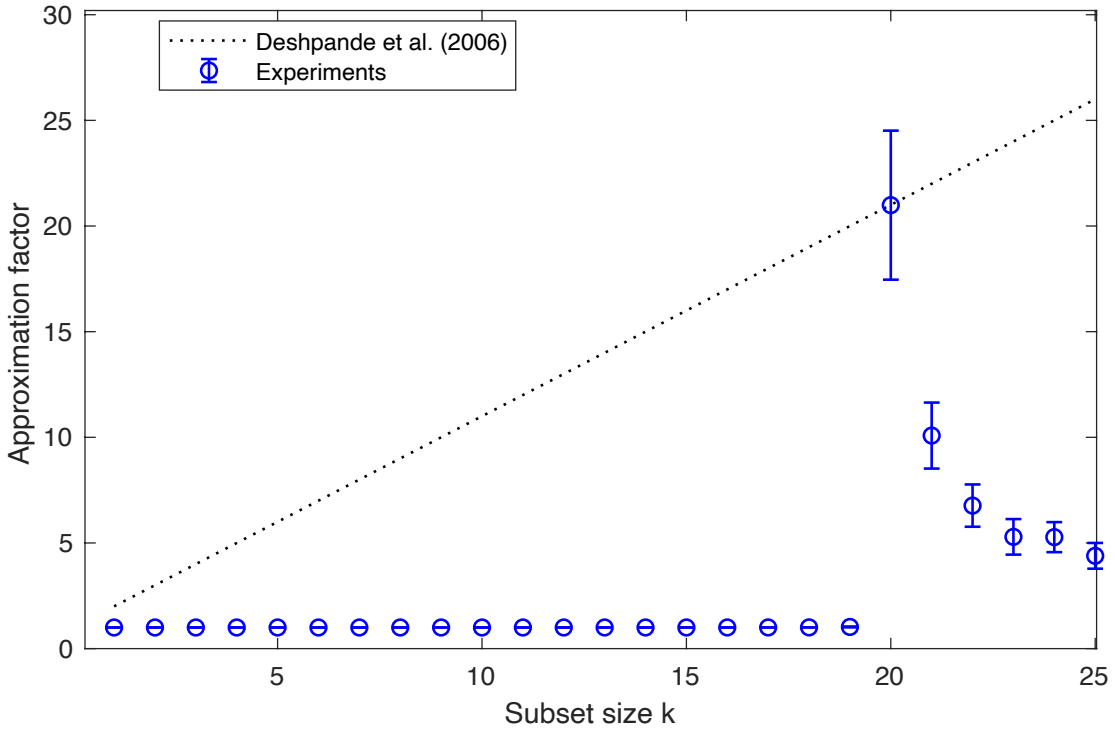
Prior Art – worst case analysis

- Deshpande et. al. 2006
- There exists an algorithm with O(k) guarantees for $|S| \leq k$

"Tight" bounds

- There exist matrices for which better than O(k) not possible

(Worst-case) Theory vs Practice



The sampling algorithm used is k-DPP (Determinantal Point Processes)

Image courtesy Michal Derezinski

Main results[1]

- Beyond worst-case analysis based on spectrum of the matrix
  - Previous bound:

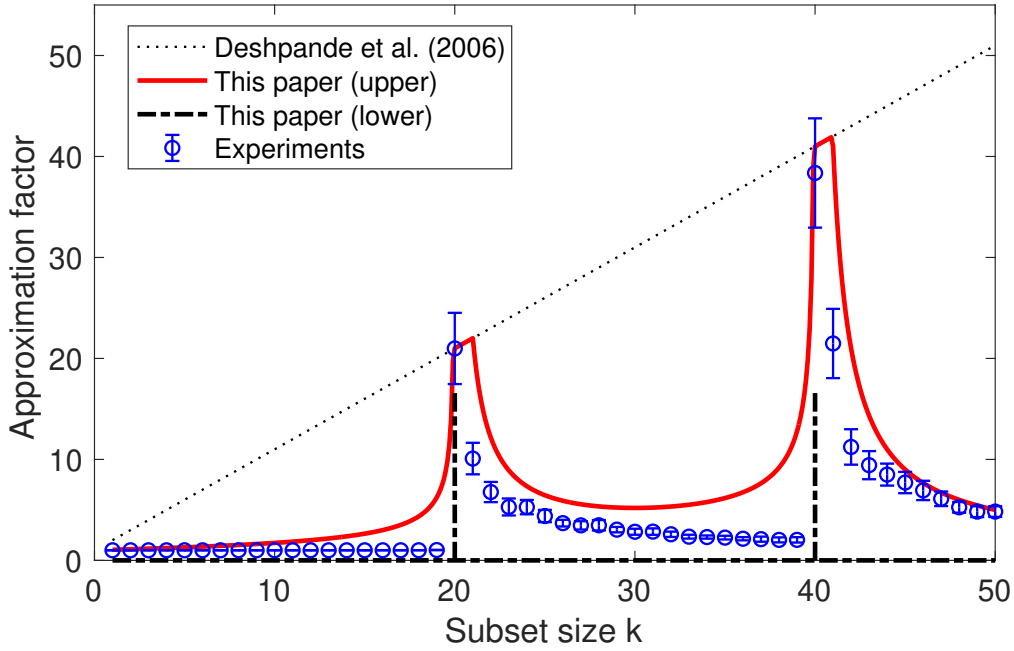
$$\frac{\mathrm{E}[\mathrm{Er}_{\mathbf{A}}(S)]}{\mathrm{OPT}_k} \leq (k+1)$$

  - New bound: For s<rank(A) and a favorable t_s:

$$\frac{\mathrm{E}[\mathrm{Er}_{\mathbf{A}}(S)]}{\mathrm{OPT}_k} \leq \left(1+\frac{s}{k-s}\right)\sqrt{1+\frac{2(k-s)}{t_s-k}}$$

[1] Derezinski, **Khanna**, Mahoney. NeurIPS 2020 (best paper award)

Summary of results



"Bad" cases only when there is a sudden drop in spectrum of the matrix.

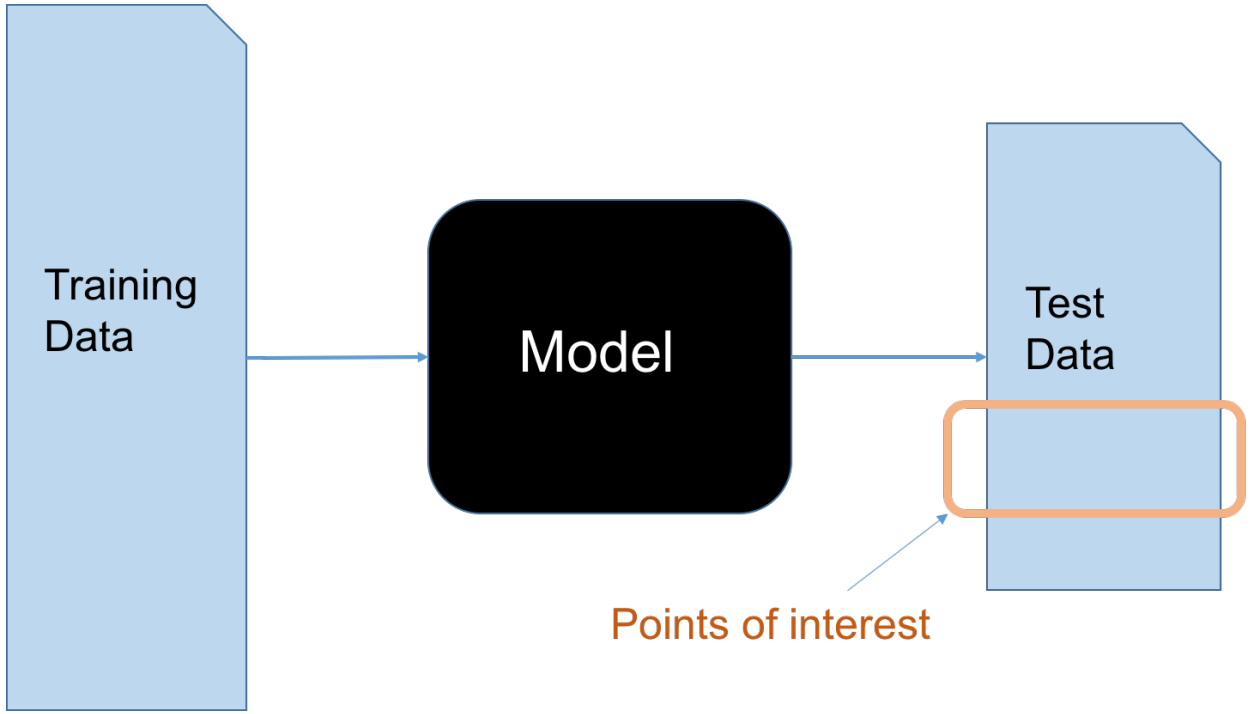
Example: smooth decay (polynomial)

- No sharp drop in spectrum ⇒ even better guarantees!
- If $c_1 i^{-p} \leq \lambda_i \leq c_2 i^{-p}$, then the upper bound:

$$\frac{\mathbb{E}[\mathrm{Er}_{\mathbf{A}}(S)]}{\mathrm{OPT}_k} \leq \frac{c_2}{c_1} cp$$

- Example: Matern kernel

Black-box interpretability



Which training data points are “most” responsible for predicting on points of interest ?

Working idea

- Approximate the test data distribution using samples from the training data[1]

- Challenges:
  - Not the same support
  - How to incorporate the model ?
  - How to reliably choose training data samples ?
  - Scale up on both time and space?

[1] **Khanna**, Kim, Ghosh, Koyejo. AISTATS 2019

Working idea

- Approximate the test data distribution using samples from the training data[1]

- Challenges:
  - Not the same support -- Use a smoothing prior GP(0,k)
  - How to incorporate the model ? – Fisher Kernels
  - How to reliably choose training data samples ? – Weak submodularity/DPP
  - Scale up on both time and space? – Weak submodularity/DPP

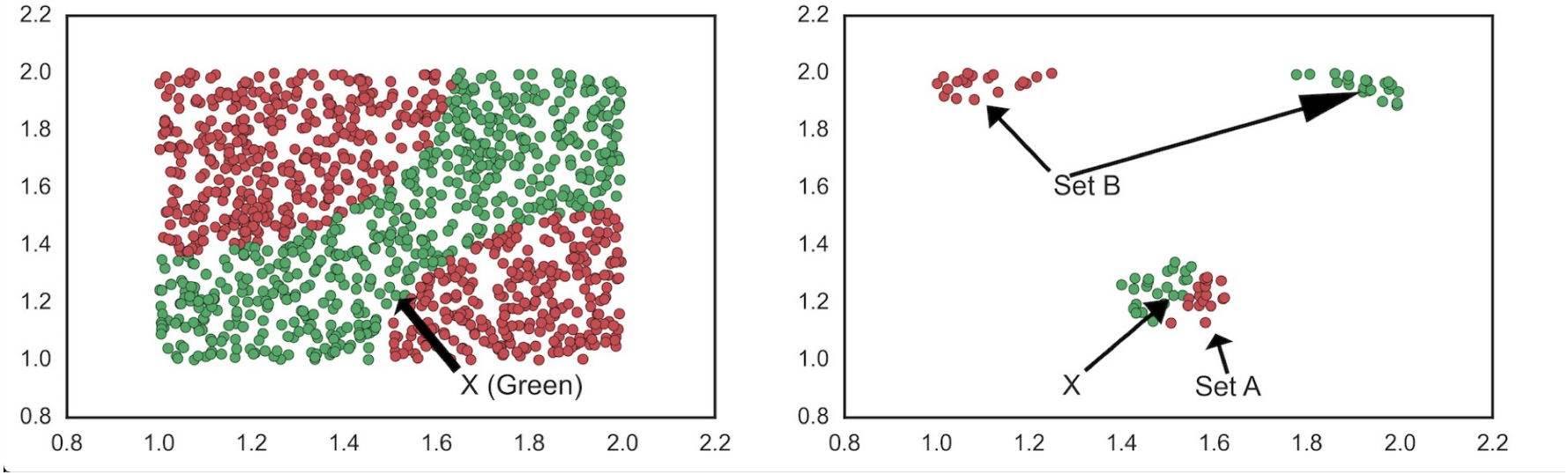
[1] **Khanna**, Kim, Ghosh, Koyejo. AISTATS 2019

Fisher Kernels

- Slight perturbations in the neighborhood of fitted parameters would impact the fit of two similar objects similarly
- Two similar objects will have similar gradients in the parameter of the model

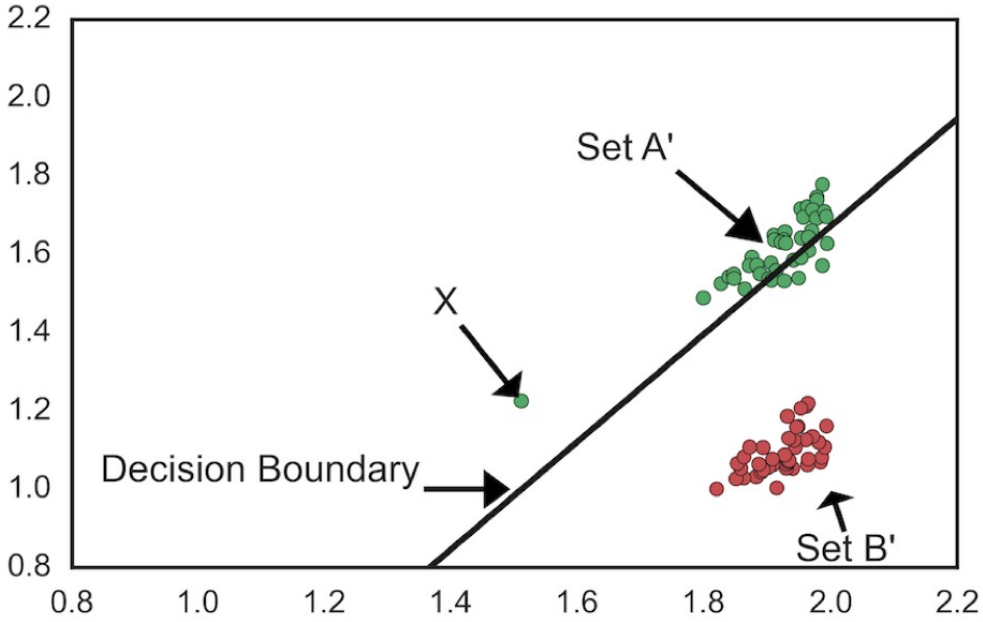
- $K(x, y) = \langle \nabla_\theta l(x), I^{-1} \nabla_\theta l(y) \rangle$. I is the Fisher information matrix.

Fisher kernel: Intuition



- Set A: Fifty closest points in RBF similarity
- Set B: Fifty farthest points

Fisher kernel: intuition



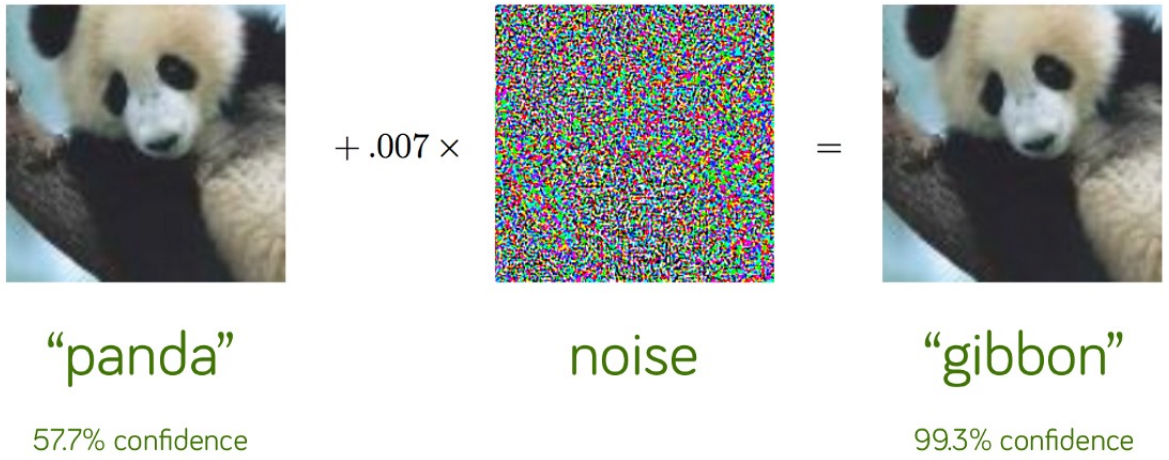
- Set A’: Fifty closest points in Fisher similarity
- Set B’: Fifty farthest points

Implications

- Influence functions: Up-weighing which training point impacts the prediction of a given test point the most ? [Koh/Liang ICML 2017]
- Strict generalization of influence functions, provide a probabilistic foundation
  - Lasso $\Leftrightarrow$ MAP solution of Bayesian Linear regression with Laplace priors
  - K-Means $\Leftrightarrow$ EM algorithm to optimize for parameters of mixture of gaussians
- Greedily selecting influential training data points is weakly submodular
- Empirical evidence for data summarization and data cleaning

Application: Interpreting robust transfer

Neural networks are brittle



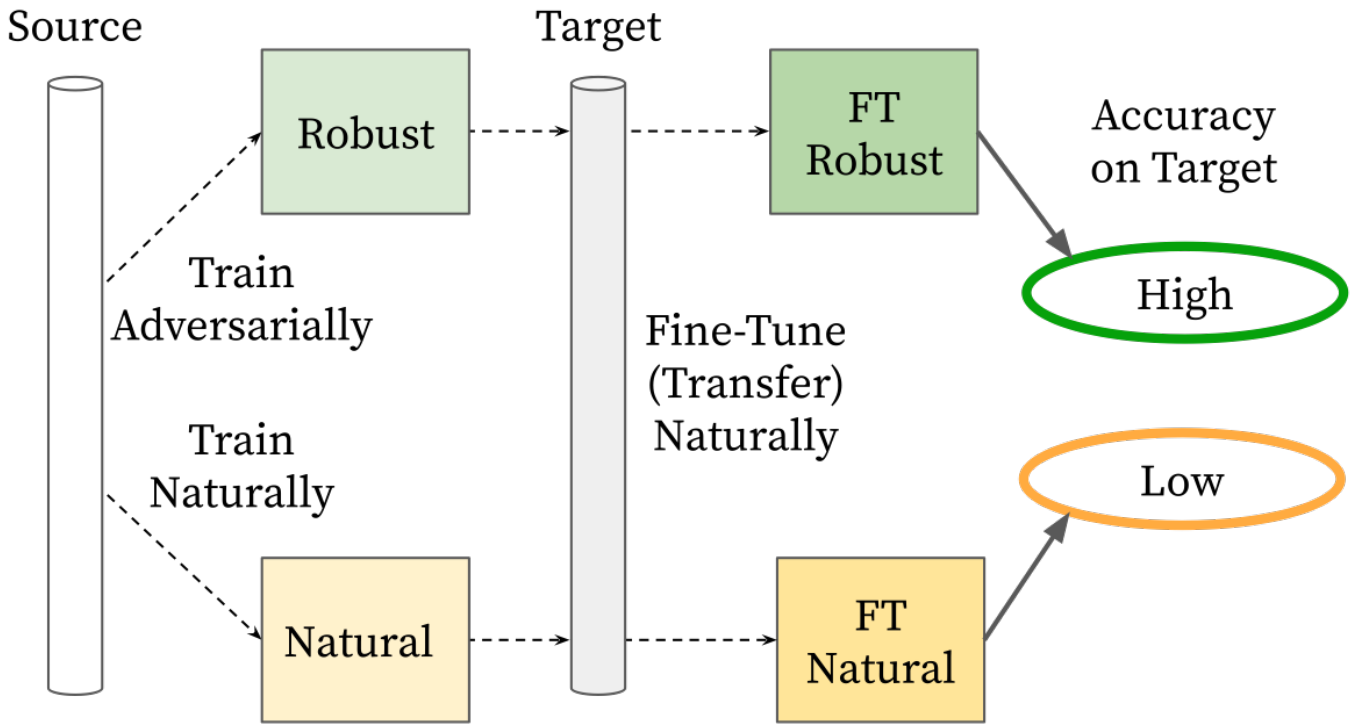
Can “fool” a NN by humanly-imperceptible injecting adversarial noise
(Image from Goodfellow et. al.2015)

Adversarial Training

- Natural Training: $\min_{\theta} \sum_i L_\theta(x_i, y_i)$
- Adversarial Training $\min_{\theta} \sum_i \max_{\|\delta_i\| \leq \epsilon} L_\theta(x_i + \delta_i, y_i)$
- There is an unintended side effect[1]

1 Urtera, Kravitz, Erichson, **Khanna**, Mahoney. ICLR 2021

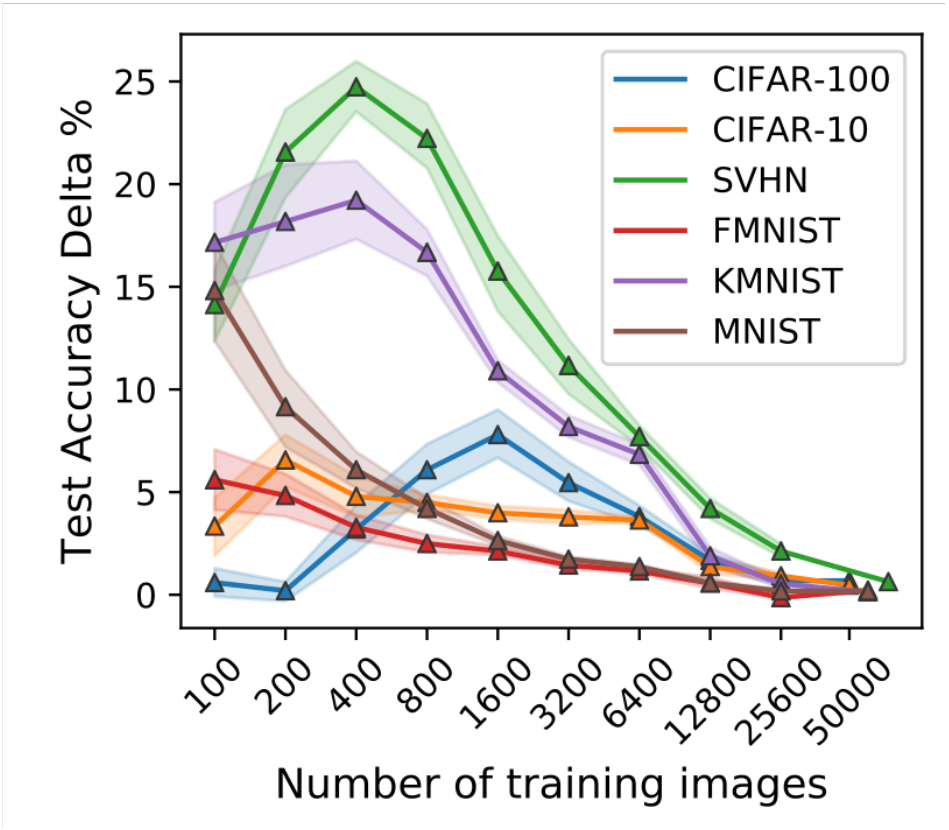
Setup



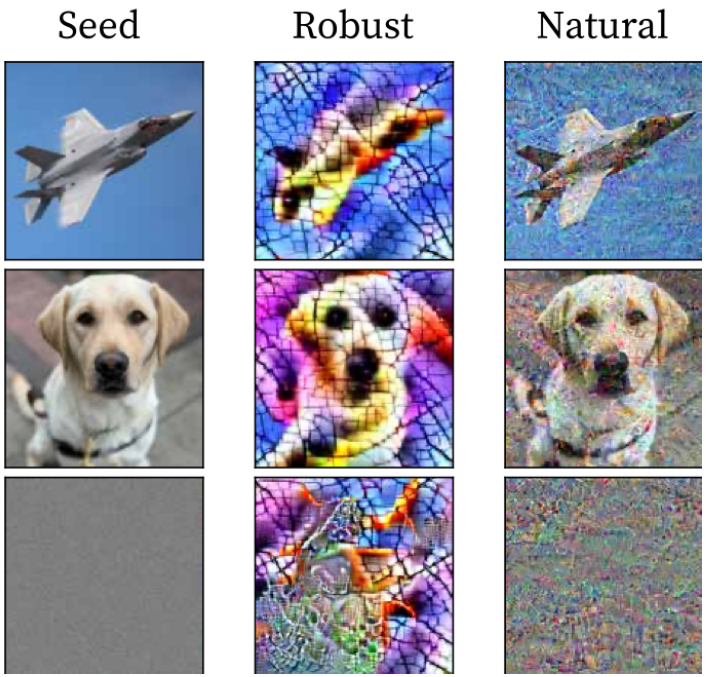
Source: ImageNet

Target: CIFAR-10, CIFAR-100, SVHN, FMNIST, KMNIST, MNIST

Adversarial Training transfers better!



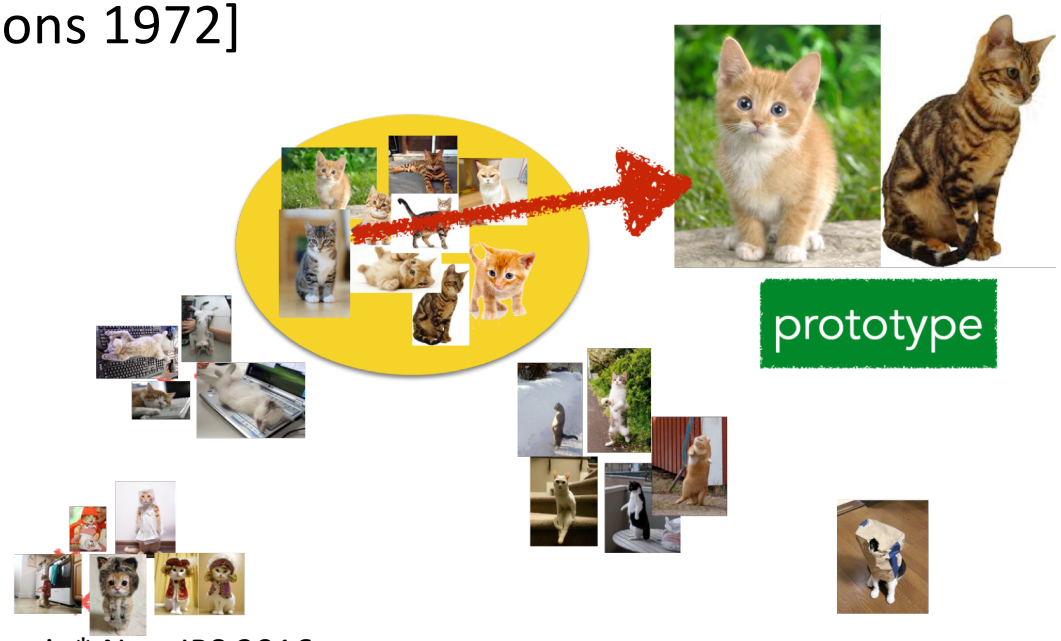
Feature visualization



Robust training seems to retain more humanly identifiable information. How do we test this?

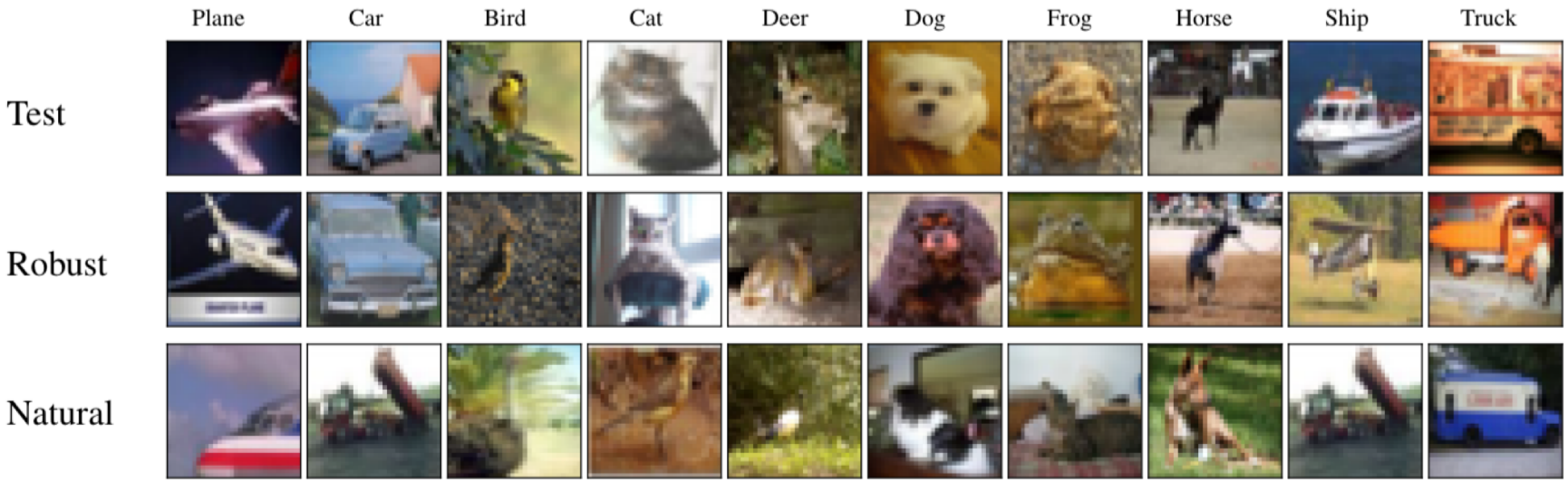
Example based learning

- Human beings learn through examples/prototypes, but can over-generalize[1]
- Build a mental model of the concept based on prototypes [Newell/Simons 1972]



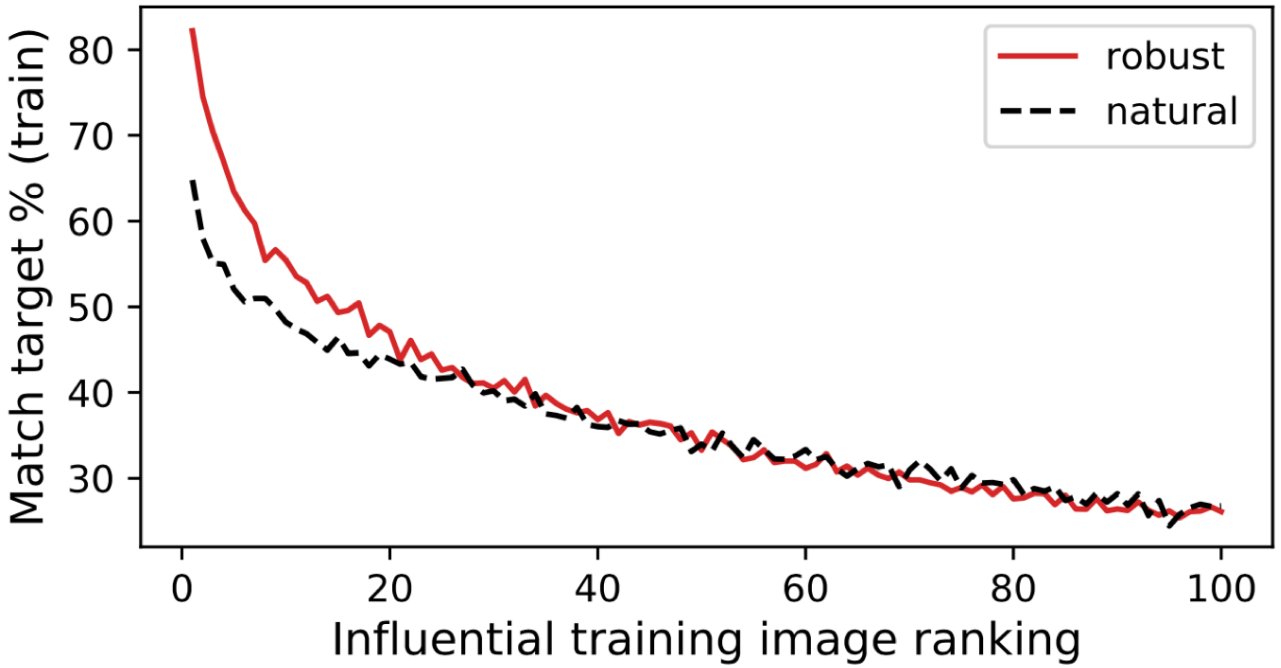
1 **Khanna***, Kim*, Koyejo* NeurIPS 2016

Using Fisher Kernels for Interpretation



Most influential images

Using Fisher Kernels for interpretation



- Takeaway: Similar images are more influential for robust than natural
- Throwback: Theoretical guarantees for the greedy selection are vital here

Closing the loop: Human insights for classification

- Non-adversarially trained models are biased towards retaining texture info. [Geirhos et. al. 2019]
- Human beings use shape more than textures when classifying objects [Landau et. al. 1988]
- Robustly trained neural networks are biased towards retaining shape information (Additional experiments on stylized ImageNet)

Human ⟶ Machine

- Insights from human learning to aid machine learning
- Make interpretable modeling choices at design stage
  - Theoretical studies to characterize the tradeoffs
- Translate high-level human-understandable questions into deployable engineering solutions
  - If I know about typical and atypical examples in the data, can I train faster?
  - Given human input, can I sparsity a neural network ?

Machine ⟶ Human

- Identify success/failure conditions through theoretical + empirical studies
  - Identify biases and develop algorithmic approaches to address them

- Build and deploy tools to attribute quantitative performance to tangible physical quantities

Thank you!

- rajivak@purdue.edu