Theoretical Foundations of Pre-trained Models

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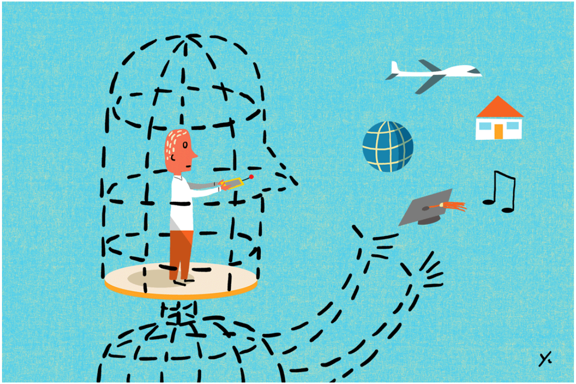
Princeton University

Slides available at: cecilialeiqi.github.io/job_talk.pdf

A.I. is Everywhere



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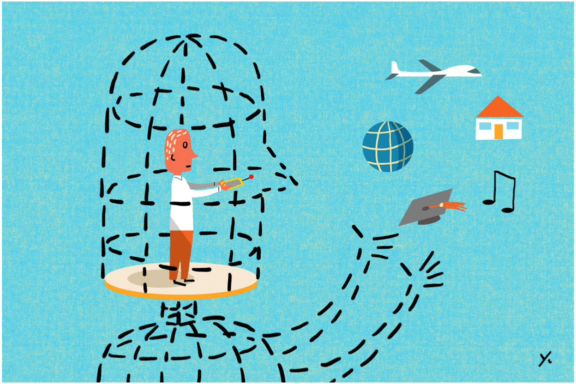

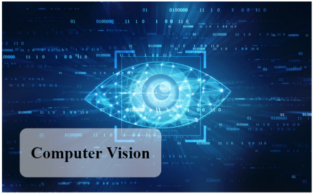

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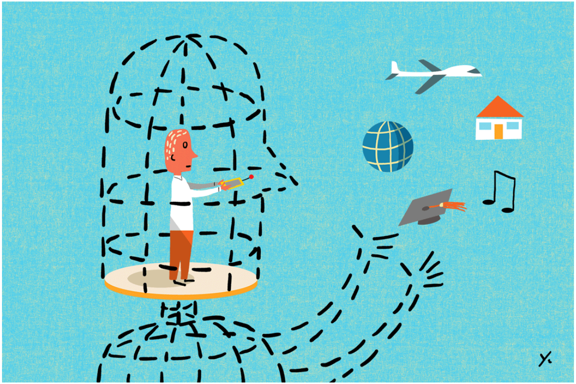

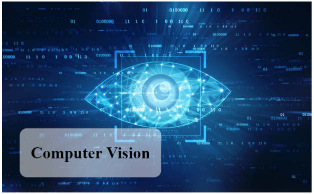

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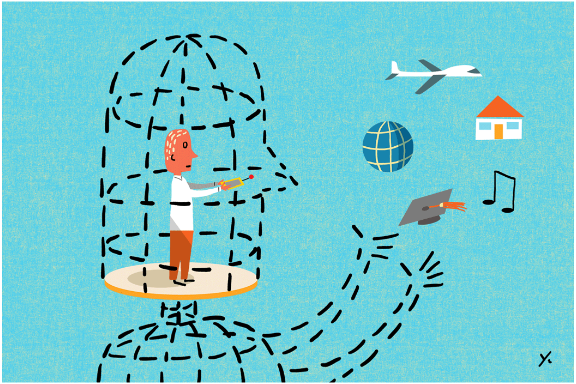
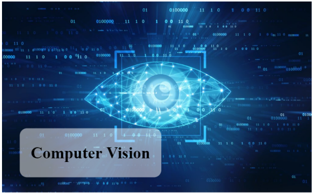
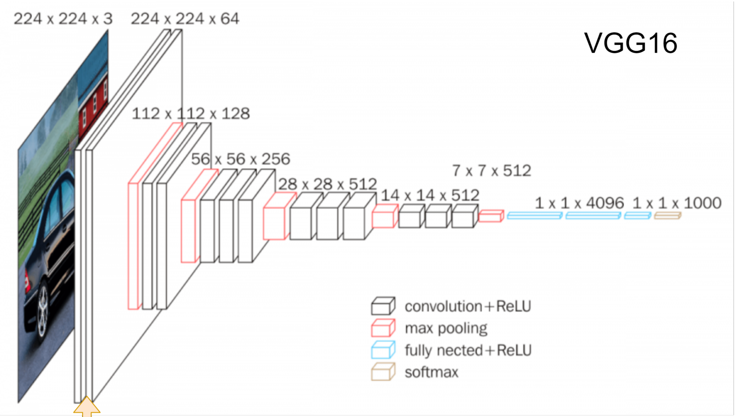


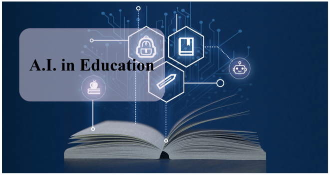


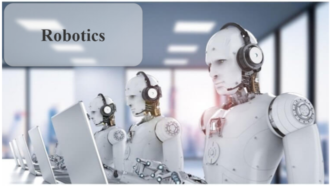
Deep Learning Requires Big Labeled Data



- Deep learning succeeds with abundant labeled data.

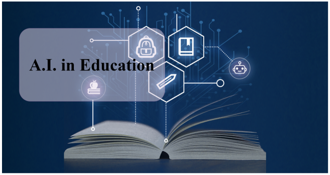
Emerging Application Domains Lack Data

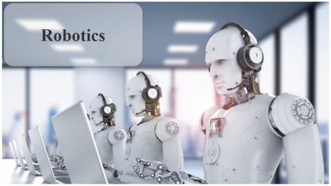




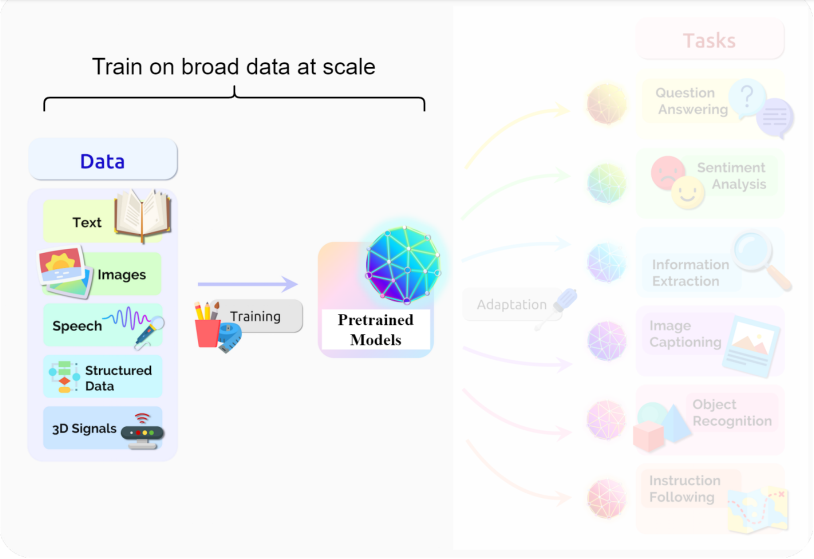
Emerging Application Domains Lack Data

Labeled data is lacking: significant costs in money and time.





Pre-trained model: any models trained on broad data at scale and can be adapted to a wide range of downstream tasks.



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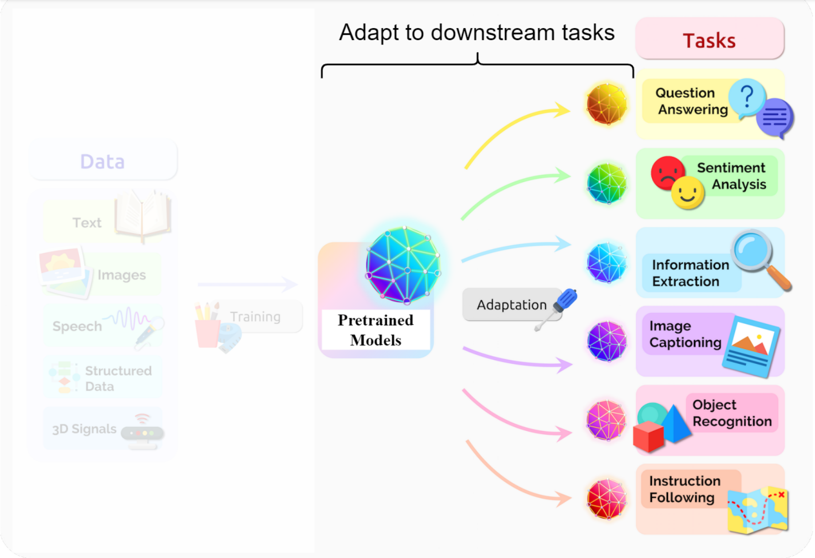

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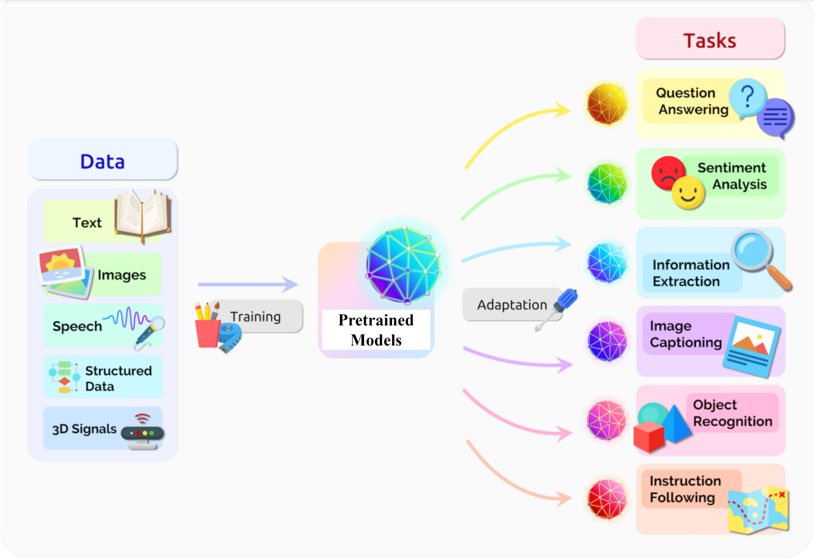

AI is undergoing a paradigm shift with pre-trained models.

Examples:

- language models: BERT, GPT-3

SD Times

GPT-3 can now be customized to individual applications

Developers can now fine-tune GPT-3 on their own data, creating a custom version tailored to their application, which allows for faster and...

3 weeks ago

Figure source: Google News.

Pre-trained Model Expands the Capability of AI

AI is undergoing a paradigm shift with pre-trained models.

Examples:

- language models: BERT, GPT-3
- code generation: Codex, AlphaCode

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Pre-trained Model Expands the Capability of AI

AI is undergoing a paradigm shift with pre-trained models.

Examples:

- language models: BERT, GPT-3
- code generation: Codex, AlphaCode
- multi-modal pre-trained models: DALL-E, CLIP

VB VentureBeat

OpenAI's text-to-image engine, DALL-E, is a powerful visual idea generator

DALL-E is a 12-billion parameter version of the 175 billion parameter GPT-3 natural language processing neural network. GPT-3 "learns" based on...

Jan 16, 2021

Figure source: Google News.

Power of Pre-trained Models

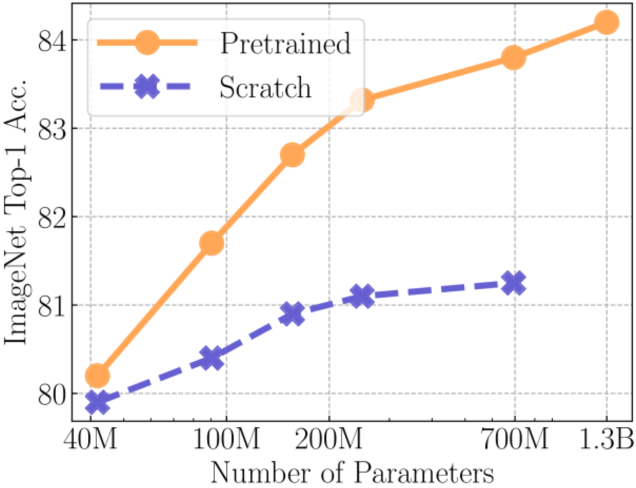


Figure source: Goyal et al. 2021.

Zero shot image classifier

FOOD101

guacamole (90.1%) Ranked 1 out of 101 labels

✓ a photo of **guacamole**, a type of food.

× a photo of **ceviche**, a type of food.

× a photo of **edamame**, a type of food.

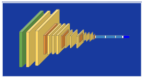
× a photo of **tuna tartare**, a type of food.

× a photo of **hummus**, a type of food.

Figure source: OpenAI, `https://clip.backprop.co/`

Behind the Scenes

Training



Pre-trained Models

Adaptation

- What training tasks are useful for downstream tasks?
- What algorithm/architecture can identify the useful features?
- How many samples are required?

Theory's Role on Pre-trained models?

- guide technical decisions
- reduce trial and error
- forecast outcomes and risks
- inspire new methods

Challenge

Current learning theory is more mature in **supervised learning**.

- **Big labeled** dataset is necessary to fit deep networks.
- Training and testing data follow the same distribution.

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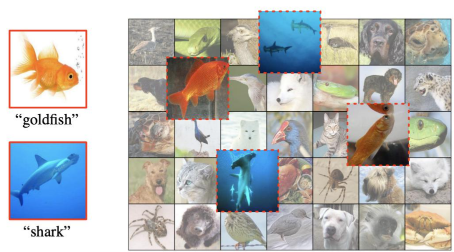

5-shot learning on ImageNet

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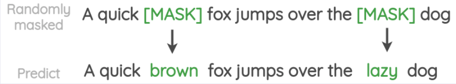

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We want to understand how pre-trained model can

- adapt to new tasks **quickly**,
- be learned from **unlabeled samples**,
- handle distributional shift from training to adaptation

Autonomous driving
Trained on sunny weather

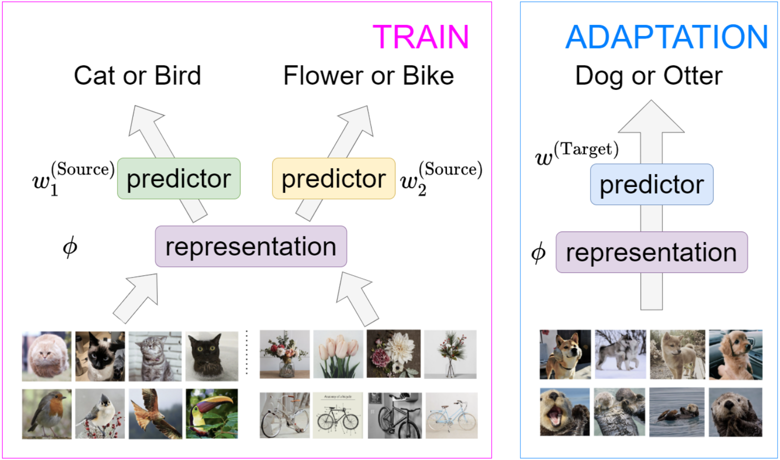
Transfer

Tested on rainy weather

Outline

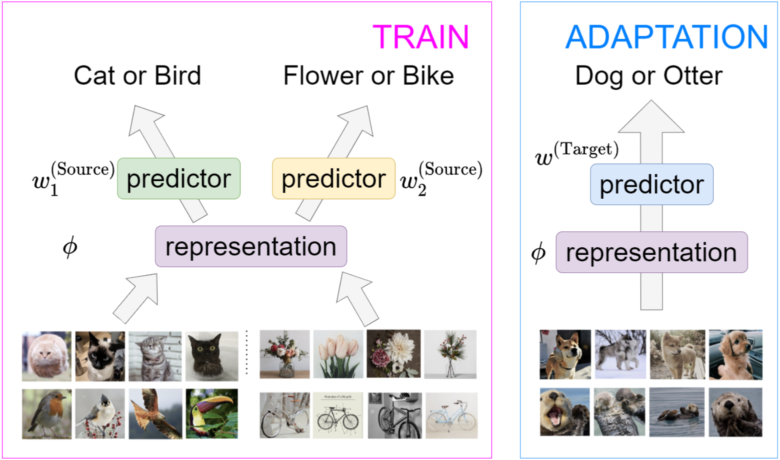
1. Meta-learning
   - Meta-Learning with Frozen Representation
   - Meta-learning with Fine-tuned Representation
2. Self-Supervised Learning
3. Ongoing and Future Work
   - Domain Adaptation
   - Lifelong Learning
   - Meta Reinforcement Learning

Learning the Meta-Representation



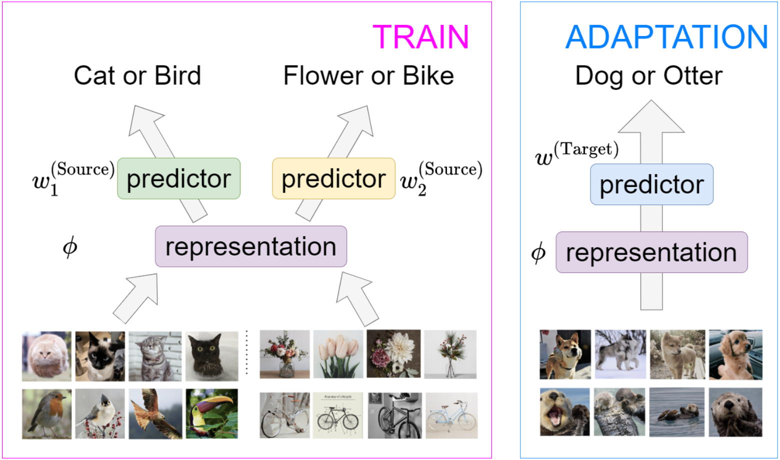
Prototypical network: (Snell et al. 2017), Meta-learning representation: (Javed and White, 2019)

Learning the Meta-Representation



On source tasks: $\hat{\phi} \leftarrow \arg\min_{\phi \in \Phi} \sum_{\text{source tasks } t} \left\{ \min_{w_t} \text{loss}(w_t \circ \phi) \right\}.$

Learning the Meta-Representation



$$\text{On target task: } \hat{w}^{(\text{Target})} \leftarrow \arg\min_{w} \text{loss}(w \circ \hat{\phi}).$$

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Why does the learned representation transfer to target task?

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   There exist predictors w_t, representation function $\phi \in \Phi$,
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Behind the scenes

1. Shared representation encodes what transfers across the tasks.
2. Source tasks $\{w_t^{(\text{Source})}\}$ diverse enough to "cover" $w^{(\text{Target})}$.

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2. Diversity of source tasks $\{w_t^{\text{(Source)}}\}$
   (at least needs to "cover" the target task.)

Task diversity

Source tasks:
Classify types of dogs

Target task:
Cat or dog?

Importance of Task Diversity

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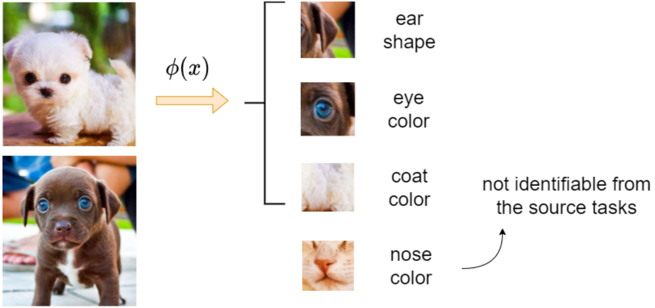
2. Diversity of source tasks $\{w_t^{\text{(Source)}}\}$ (at least needs to "cover" the target task.)



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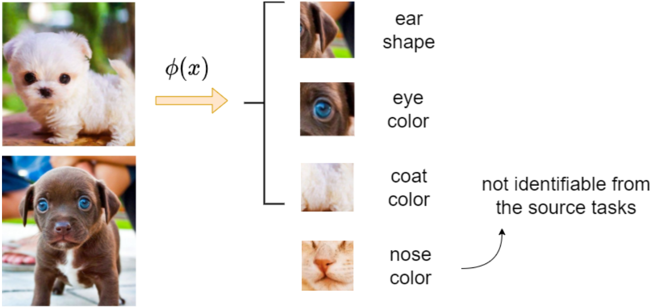
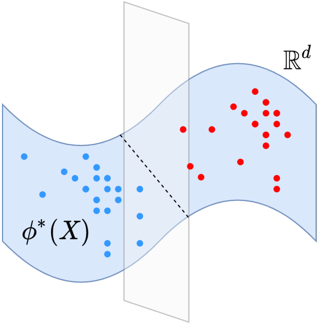


Mathematically speaking, $w^{\text{(Target)}} \in \text{span}\{w_1^{\text{(Source)}}, \cdots w_{n_e}^{\text{(Source)}}\}$.

General Low-dimensional Meta Representation

Setup:

- Shared representation: $y_t = w_t^\top \phi(x_t)$+noise
- Representation layer is of dimension k (We assume k is small)



Theorem 1 (Informal)

We only need $O(k)$ labeled samples from target domain to get small **test error**.

In contrast, supervised learning requires samples up to the **complexity of the function class**.

E.g., VGG19: 10^3 vs. 10^7, from Arora et al. 2018.

Main Result on Meta Representation

Theorem 1

With shared representation and task diversity,

$$\begin{aligned}&\text{Test Error}(\hat{w}^{(\text{Target})} \circ \hat{\phi})\\ \leq&\text{Representation Error} + \text{Adaptation Error}\end{aligned}$$

- Representation error: how well you learn representation layer ϕ
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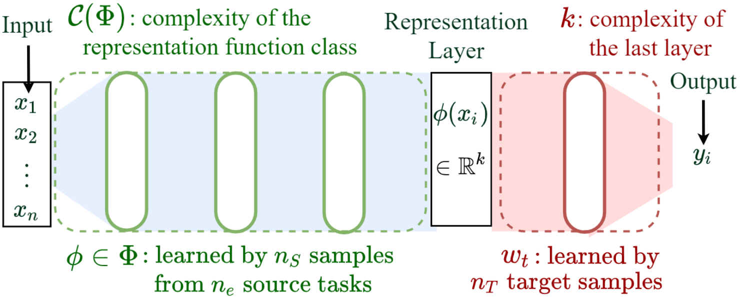

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Baselines:

- Supervised learning:

$$\text{Test error} \leq \frac{\mathcal{C}(w \circ \Phi)}{n_T}.$$

- Maurer et al. 2016:

$$\text{Test error} \leq \frac{\mathcal{C}(\Phi)}{\sqrt{n_e}} + \frac{k}{n_T}.$$

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Meta-learning handles distributional shift:

- Covariate shift is allowed.
  Source and target data can come from different marginal distribution.

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Few-shot learning via learning the representation, provably. ICLR 2021

Link to appendix

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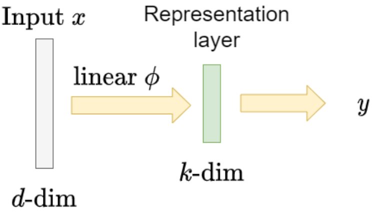
Question

Does MetaRep (previous algorithm) still work?
If not, how should we modify the algorithm?

Instantiation in linear setting:



When $\gamma = 0$ (no misspecification), MetaRep requires at most $O(k)$ samples on the target task.

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- No improvement over supervised learning that requires $O(d)$ samples.
- Previous algorithm is extremely fragile!

Modified Algorithm: FINE-TUNEDREP

1. Use source tasks to find ϕ as an initialization.
2. Fine-tune each representation ϕ_t starting from ϕ that tolerates mis-specification.

Model-agnostic Meta-learning: Finn et al. 2017

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$$\min_{\phi} \min_{\|\phi_t - \phi\| \le \gamma, w_t} \sum_{\text{Task } t} \text{loss}(w_t, \phi_t),$$

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Φ

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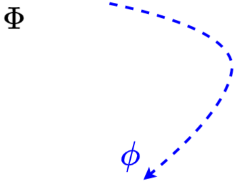

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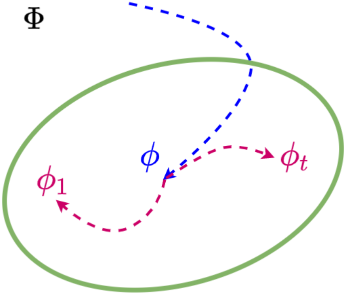

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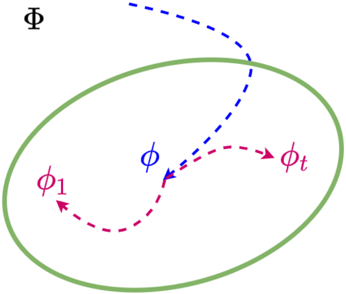

Theorem 2 (Informal)

When adapting ϕ to target task, it requires $O(k) + O(\gamma^2)$ training samples from target domain.

Main Result on Fine-tuned Representation

Theorem 2

For **general function classes**, under similar settings,

$$\text{Test Error} \lesssim \textsc{MetaRep}\ \text{Error (when } \gamma = 0) + O(\frac{\gamma}{\sqrt{n_T}}).$$

- γ measures mis-specification in representation ϕ
- n_T: number of samples from target training set

How Fine-Tuning Allows for Effective Meta-Learning, NeurIPS 2021

Link to appendix

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For **general function classes**, under similar settings,

$$\text{Test Error} \lesssim \textsc{MetaRep} \text{ Error (when } \gamma = 0) + O\left(\frac{\gamma}{\sqrt{n_T}}\right).$$

- We need $O(k) + O(\gamma^2)$ samples from target domain.

Baselines:

- Supervised learning and $\textsc{MetaRep}$ need $\mathcal{C}(w \circ \Phi)$ samples from target domain.
- $\mathcal{C}(w \circ \Phi)$: Complexity of the function class for the whole network.

How Fine-Tuning Allows for Effective Meta-Learning, NeurIPS 2021

Link to appendix

Outline

No labeled data?

Create your own labels

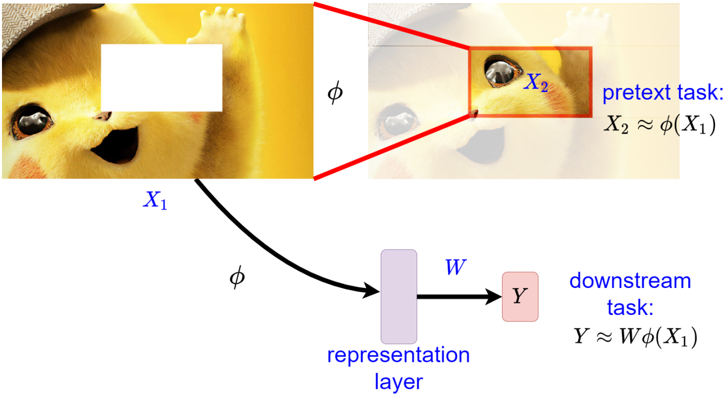
Supervised representation learning needs labels from related tasks. What if this isn't available?

Create pseudo-labels from the input data.

Self-supervised Learning

Type I: reconstruction-based SSL

Reconstructing part of the input from the other part



Context encoder: (Pathak et al. 2016)

Other examples: Masked Autoencoder: (He et al., 2021), Colorization: (Zhang et al., 2016)

Type I: reconstruction-based SSL

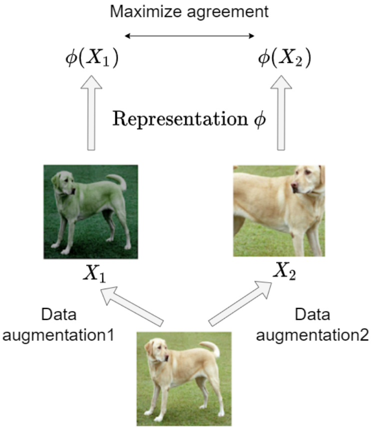
Reconstructing part of the input from the other part

BERT: (Devlin et al., 2018)

Other examples: Masked Autoencoder: (He et al., 2021), Colorization: (Zhang et al., 2016)

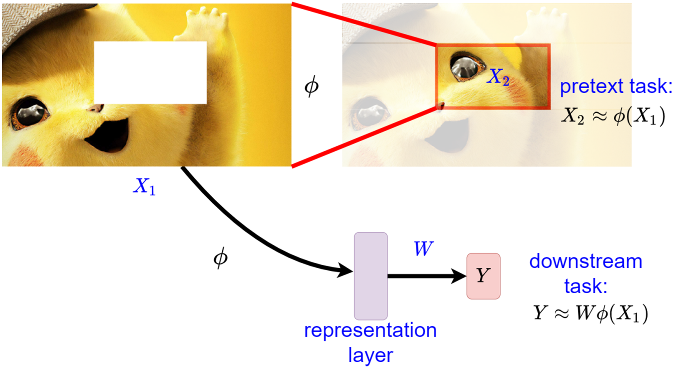
Type II: similarity-based SSL

Enforcing two views of the same data to have similar representation



Examples: SimSiam: (Chen et al., 2021), CLIP: (Radford et al., 2021) , SimCLR: (Chen et al., 2020)

1. Label Y with k classes.
2. Unmasked image X_1 and masked image X_2.



Setup

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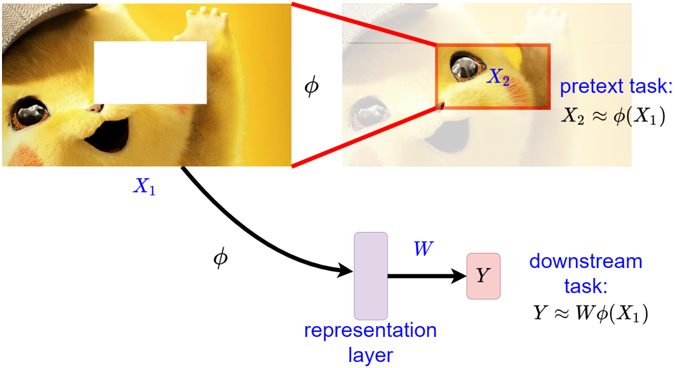

3. Key intuition: Pretext tasks should help us reduce irrelevant features/forget information that is not necessary to predict Y

Ideal Scenario

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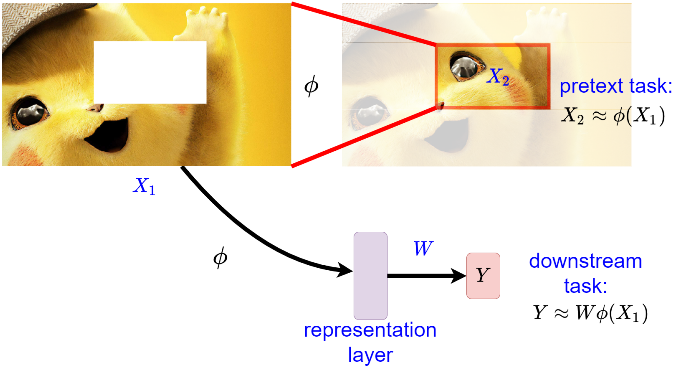
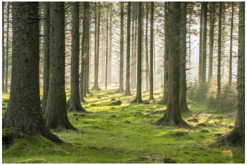
2. Unmasked image X_1 and masked image X_2.



3. Ideal scenario: $X_1 \to Y \to X_2$
$$\iff X_1 \perp X_2 | Y$$

A Thought Experiment

- $X_1 \perp X_2 | Y$
- Image colorization for photos of desert, forest, sea



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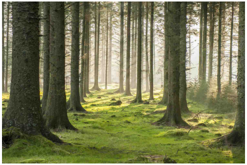
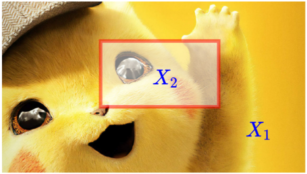


- Image inpainting:



Our Result: Ideal Scenario

Setting:

1. k-class labels Y.
2. Representation ϕ, last layer W^*.

Compare this procedure to ground truth classifier f^*:

Theorem 3

1. (No representation error.) If $X_1 \perp X_2 | Y$,

$$f^* = W^* \phi(X_1).$$

2. Only need $O(k)$ labeled samples.

Remark: Only need k samples instead of Rademacher complexity of function class.

Linear case was studied in Foster, Kakade, Zhang, 2008.

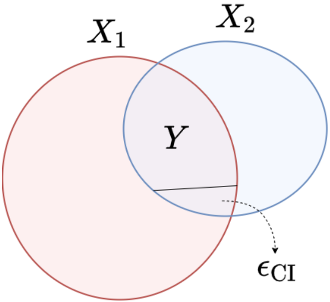
Proof sketch

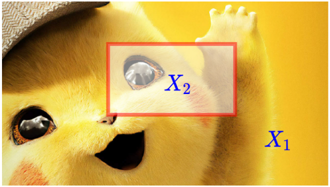
No representation error: if $X_1 \to Y \to X_2, $(i.e.,$X_1 \perp X_2 | Y$), then $f^* = W^* \phi(X_1)$.

$$\phi(\cdot) := \mathbb{E}[X_2|X_1] \overbrace{=}^{\text{tower property}} \mathbb{E}[\mathbb{E}[X_2|X_1, Y]|X_1] \overbrace{=}^{\text{CI}} \mathbb{E}[\mathbb{E}[X_2|Y]|X_1]$$

$$= \sum_{y=1}^{k} \mathbb{E}[X_2|Y=y] P(Y=y|X_1) =: \mathbf{A}^\top f(X_1),$$

Here $f(x_1)_y := P(Y=y|X_1=x_1), y = 1 \cdots, k$
$\mathbf{A}$ satisfies $\mathbf{A}_{y,:} = \mathbb{E}[X_2|Y=y]$.





Characterizing Approximate Conditional Independence

Define $\epsilon_{\text{CI}} = \mathbb{E}_{X_1} \|\mathbb{E}[X_2|X_1] - \mathbb{E}_Y[\mathbb{E}[X_2|Y]|X_1]\|^2$.

- This is 0 if $X_1 \perp X_2 \mid Y$.
- ϵ_{CI} can be viewed as quantification of extra shared features between X_1 and X_2 are not captured by Y (spurious feature not reducible by SSL)

Main Results on Reconstruction-based SSL

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- Also applies to similarity-based SSL

Empirical Implications

Implications on pretext selection

- Design pretext tasks such that X_1 and X_2 have smaller dependence (given Y)

Predicting what you already know helps: Provable self-supervised learning, NeurIPS 2021

Empirical Implications

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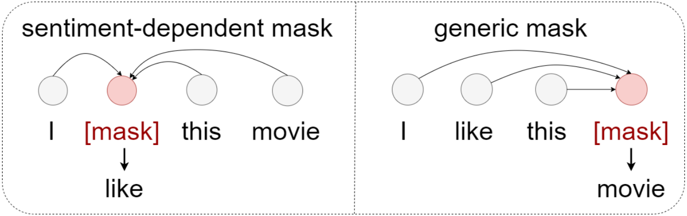
Applications:

- Image: image classification [He et al. 2021]
- Text: sentiment analysis [Zhang and Hashimoto, 2021]

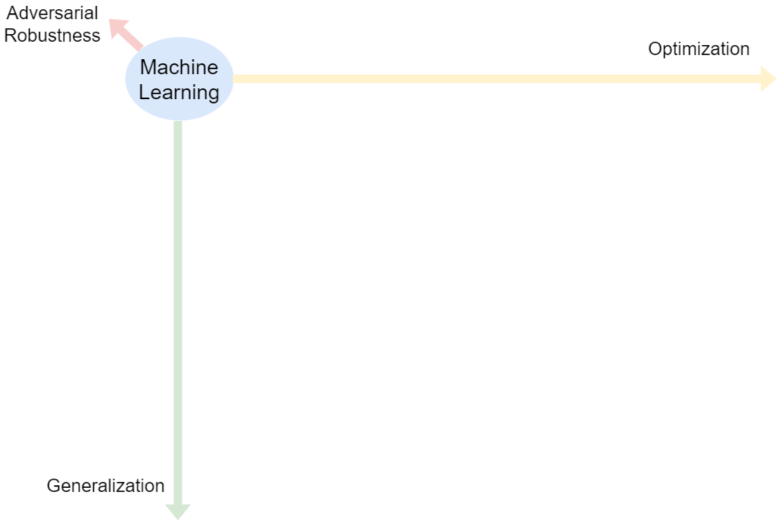


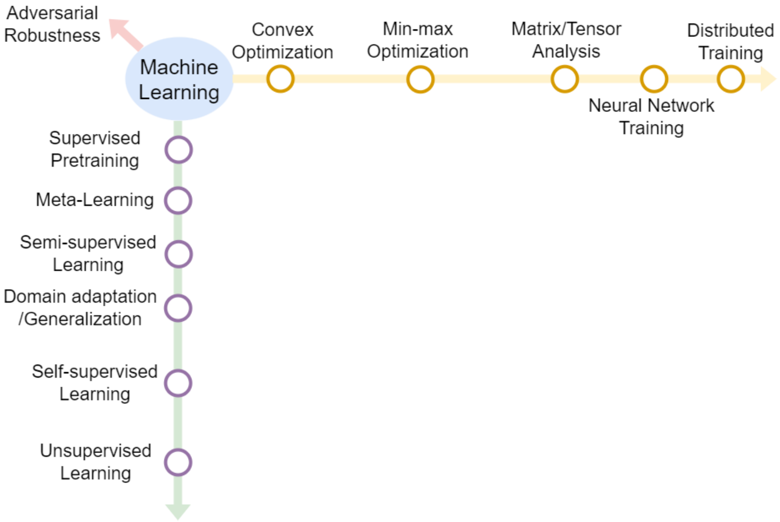
- Audio: speech recognition [Zaiem et al., 2021]

Predicting what you already know helps: Provable self-supervised learning, NeurIPS 2021

wrap-up

Overview of My Research Contributions




Adversarial Robustness
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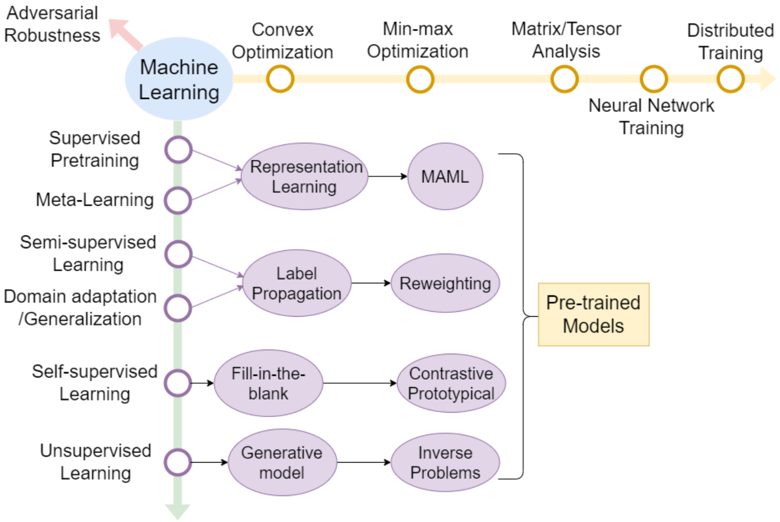

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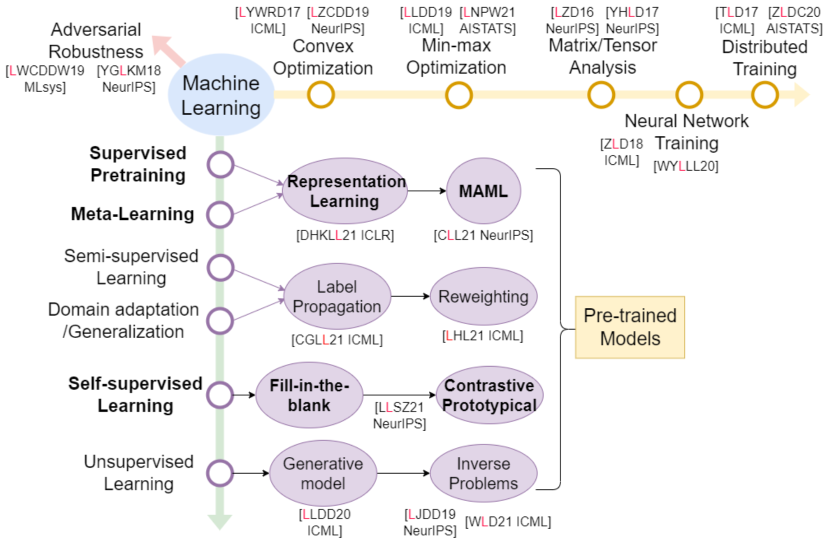
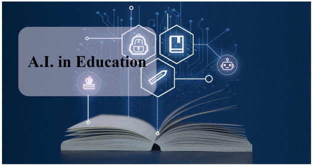
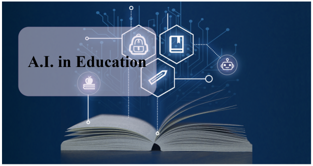


Outlook



Pre-trained model:
Expanding the capability of AI to broader disciplines.



Pre-trained model:
Expanding the capability of AI to broader disciplines.

I will work towards accelerating us to their "ImageNet" moment.

Remaining challenges:

- Optimization
  - Convergence analysis
  - Training and testing time speed up
- Robustness
  - Handle different types of distribution shift
  - Adversarial robustness (Security issues)
- Applications
  - Reinforcement learning
  - Medical image
- Trustworthy AI
  - Fairness, safety, privacy
  - Interpretability
- Evaluation
  - How to evaluate the model without target data
- Other technical details

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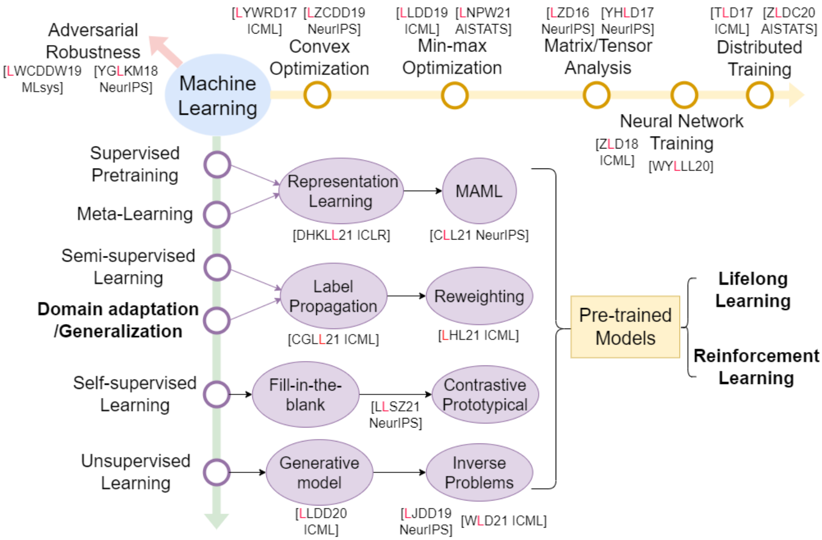
Outline

1. Meta-learning
   - Meta-Learning with Frozen Representation
   - Meta-learning with Fine-tuned Representation
2. Self-Supervised Learning
3. Ongoing and Future Work
   - Domain Adaptation
   - Lifelong Learning
   - Meta Reinforcement Learning

Future Work



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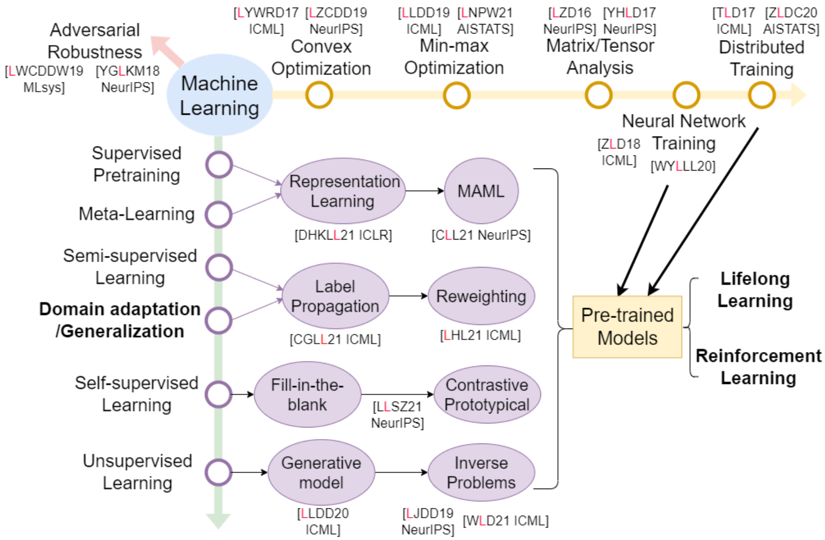
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Summary and Future Work

We investigate sufficient conditions that guarantee:

- Deep networks **learn a good pre-trained model**.
- drastically **reduce sample complexity**.
- be **learned on unlabeled data**.
- **transfer to other tasks/domains with covariate shift**.

Summary and Future Work

We investigate sufficient conditions that guarantee:

- Deep networks **learn a good pre-trained model**.
- drastically **reduce sample complexity**.
- be **learned on unlabeled data**.
- **transfer to other tasks/domains with covariate shift**.

Future Work

Explore the following directions centered at pre-trained models:

- Domain Adaptation/Generalization
- Continual (Lifelong) Learning
- Meta Reinforcement Learning
- Optimization: Traning and Testing Time Speed-ups

Thank you!

Thank you!

Link back to: MetaRep FinetunedRep SSL
Back-up slides: FinetunedRep SSL Example Experiments

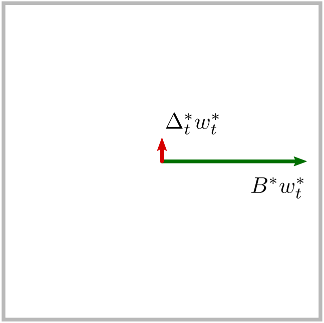
Failure with Previous Algorithm: MetaRep

MetaRep (Fixed feature) has $\Omega\left(\frac{d}{n_T}\right)$ minimax rate on the target task

Failure with Previous Algorithm: MetaRep

MetaRep chooses representation based on prediction space norm, not parameter space norm!

Parameter space (L_2-norm)



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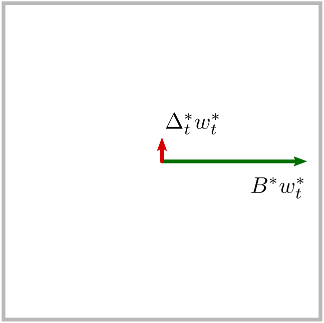
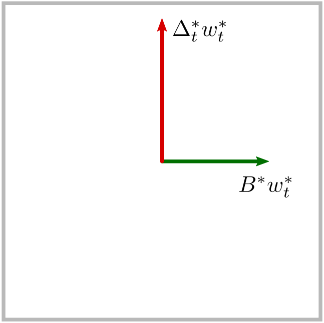


Prediction space (Σ-norm)



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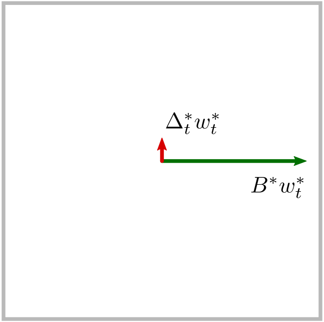

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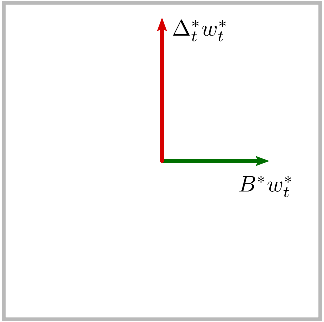


Intuition: Trick MetaRep into learning subspace of δ_t^*'s, and pay cost of having to fine-tune to learn large-norm $B^* w_{\text{test}}^*$.

Technical Assumptions for Theorem 1

Assumptions:

- I.i.d. Samples
- Input data is light-tail
- Shared representation
- Task diversity

Back

Assumptions:

- I.i.d. Samples
  - (x, y_t) generated i.i.d from each t-th task
- Input data is light-tail
  - P_X^t is sub-Gaussian
- Shared representation
  - $y_t = w_t \circ \phi(x) + \epsilon$, noise $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- Task diversity
  1. $w^{\text{target}} \in \text{span}\{w_t^{\text{source}}\}$
  2. $W = [w_1^{\text{source}}, \cdots w_{n_e}^{\text{source}}]$ is well-conditioned

Theory helps to diagnose the failure issue and determine the solution.

Potential problems:

1. No shared structure

2. Learning objective for meta-learning is not effective

3. Optimization issues

> Theory helps to diagnose the failure issue and determine the solution.

Potential problems:

1. No shared structure
   - No supervised pre-training algorithm will work. Need to switch to self-supervised pre-training.
2. Learning objective for meta-learning is not effective
3. Optimization issues

Empirical Implication

Theory helps to diagnose the failure issue and determine the solution.

Potential problems:

1. No shared structure
2. Learning objective for meta-learning is not effective
   - Switch from learning the meta-representation to MAML-like algorithms.
3. Optimization issues

Back

Empirical Implication

Theory helps to diagnose the failure issue and determine the solution.

Potential problems:

1. No shared structure
2. Learning objective for meta-learning is not effective
3. Optimization issues
   - Typical optimization tricks.

Back

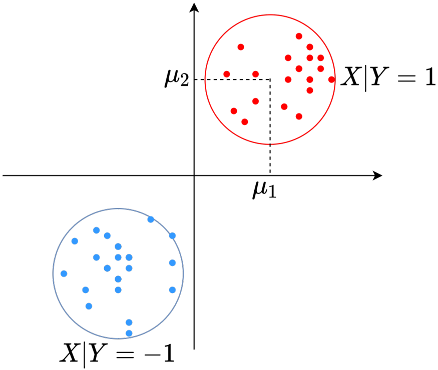
General Functions

Theoretical results:

1. If $X_1 \perp X_2 | Y$,
$$f^* = W^* \phi(X_1).$$
2. Only need k (dimension of Y) samples.

How can $\phi(X_1)$ be better than X_2 to predict Y?

Example: Gaussian Mixture



$$Y \in \{-1, 1\}$$
$$X \sim \mathcal{N}(Y[\mu_1, \mu_2], I_{d_1+\mathrm{d}_2})$$

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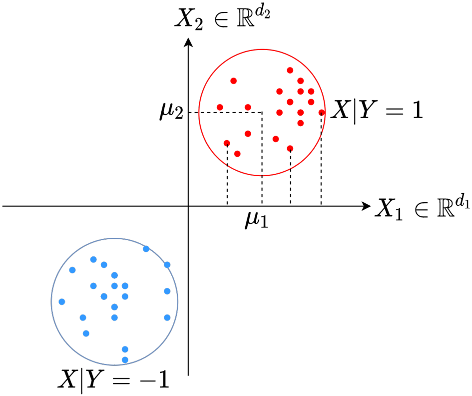

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$X_1 \sim \mathcal{N}(Y\mu_1, I_{d_1}),$

$X_2 \sim \mathcal{N}(Y\mu_2, I_{d_2})$

$X_1 \perp X_2 | Y$

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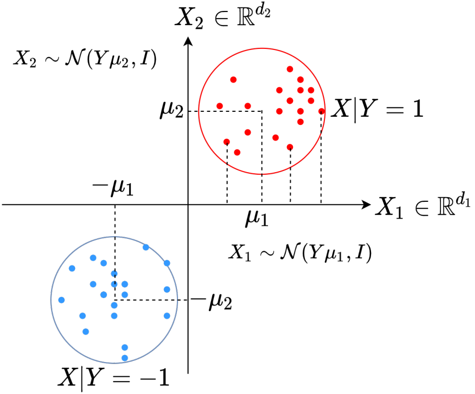

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$\mathbb{E}[Y|X_2]$ is not linear, but
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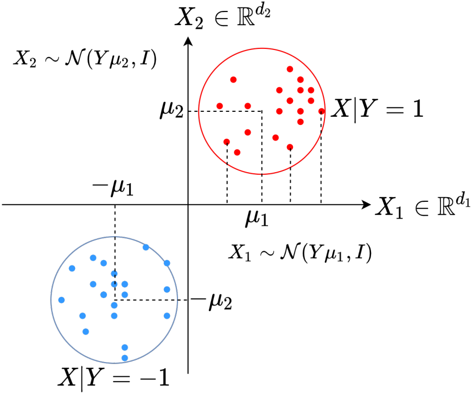

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$\mathbb{E}[Y|X_2]$ is not linear, but
$\mathbb{E}[Y|\phi]$ is linear:

- $\phi(x_1) = \mathbb{E}[X_2|X_1 = x_1]$ $= p_1(x_1)\mu_2 + p_{-1}(x_1)(-\mu_2)$
- $\mathbb{E}[Y|X_1] = p_1(x_1) - p_{-1}(x_1) = \mu_2^\top \phi(X_1)/\|\mu_2\|^2$.
- $p_y(x_1) := P(Y = y|X_1 = x_1)$

Connection to SimSiam method

- Before, we learn $\phi(x_1) = \mathbb{E}[X_2|X_1 = x_1]$, which naturally requires X_2 and Y to be linearly correlated
- We can actually predict any $g(X_2)|X_1$, or even $p(X_2|X_1)$

ACE and nonlinear CCA

- Alternating conditional expectation (ACE):

$$\min_{\phi,\eta} L_{ACE}(\phi, \eta) = \mathbb{E}_{X_1,X_2}\left[\|\phi(X_1) - \eta(X_2)\|^2\right],$$
$$\text{s.t. } \Sigma_{\phi,\phi} = \Sigma_{\eta,\eta} = I_k.$$

- This is equivalent to the following canonical correlation analysis (CCA):

$$\max_{\phi,\eta} L_{CCA}(\phi, \eta) = \mathbb{E}_{X_1,X_2}\left[\phi(X_1)^\top \eta(X_2)\right],$$
$$\text{s.t. } \Sigma_{\phi,\phi} = \Sigma_{\eta,\eta} = I_k.$$

Algorithm (SimSiam):

$$\max_{\phi,\eta,\text{normalized}} \mathbb{E}[\phi(X_1)^\top \eta(X_2)]$$

New measure of conditional independence:

$$\epsilon_{\mathsf{CI}} := \max_{\|g\|_{L^2(X_2)}=1} \mathbb{E}_{X_1}(\mathbb{E}[g(X_2)|X_1] - \mathbb{E}[\mathbb{E}[g(X_2)|Y]|X_1])^2.$$

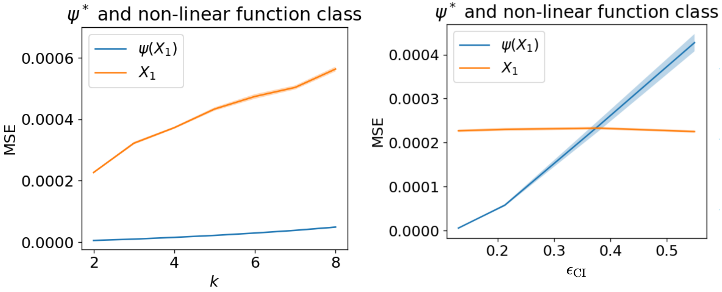
- Extension of previous result:

$$\textit{test error} \lesssim \epsilon_{CI} + \frac{k}{n_L}.$$

- If both X_2 and X_1 can well predict Y, i.e., $P_{X_1,Y}(g^*(x_1) \neq y) \leq \alpha$ (same for X_2), we have:

$$\textit{test error} \lesssim \frac{\alpha}{1-\epsilon_{CI}} + \frac{k}{n_L}.$$

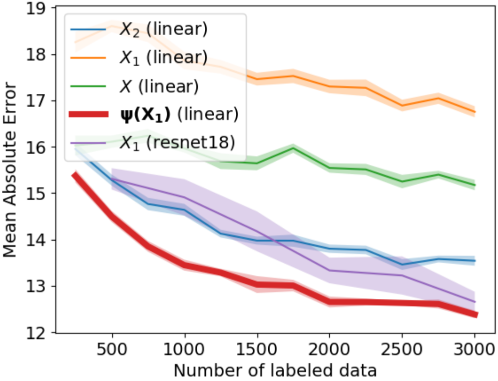
Simulations: Both Terms Tight in $\frac{k}{n_L} + \epsilon_{\text{CI}}$



Left: Class Conditional Gaussian $X \sim \mathcal{N}(\mu_Y, I), \mu_Y \in \mathbb{R}^{90}, Y \in \{1, 2, \cdots k\}, X_1 = X_{1:50}, X_2 = X_{51:90}$. $X_1 \perp X_2 | Y$

Right: Similar mixture of Gaussian: $X \sim \mathcal{N}(\mu_Y, \Sigma_{\epsilon_{\text{CI}}})$, $\alpha \propto \epsilon_{\text{CI}}$ controls the dependence of X_1 and X_2: $\epsilon_{\text{CI}} = 0 \Rightarrow$ exact CI, and $\epsilon_{\text{CI}} = 1 \Rightarrow X_2$ fully depends on X_1.

Experiments



- Yearbook: portraits date from 1905 to 2013.

Source

Target

Entity30 - Passerine

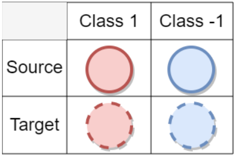
Source

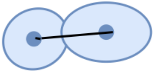
Target

Entity30 - Tableware

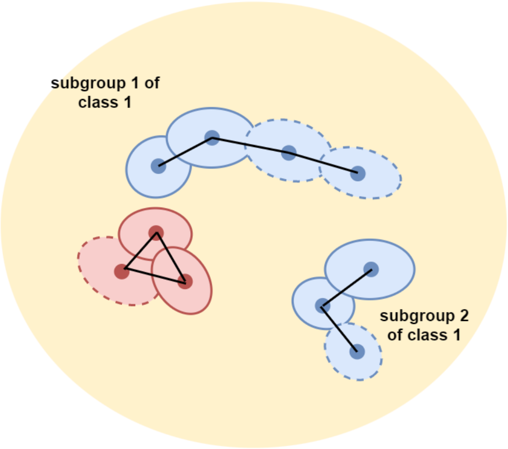
BREEDS dataset: (Santurkar et al., 2021)

Our New Framework: Subpopulation Shift

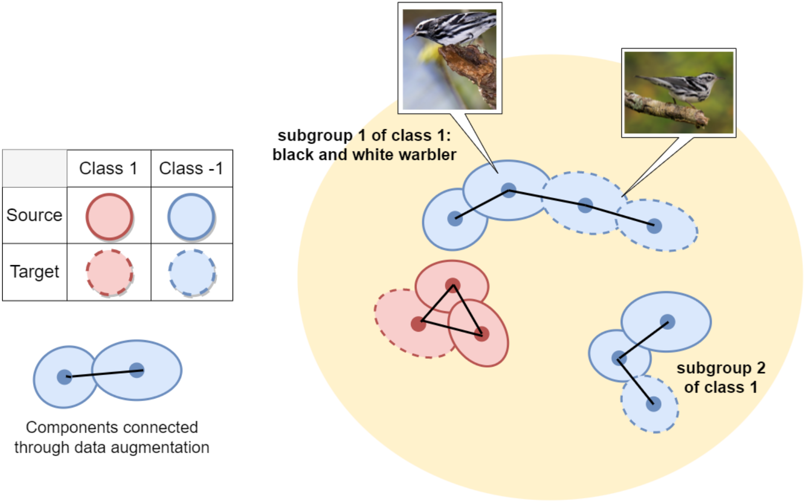




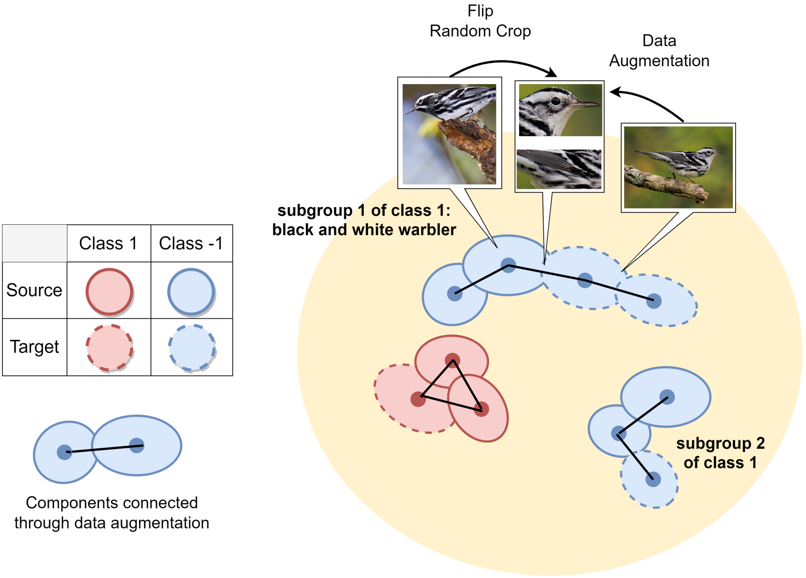
Components connected through data augmentation



Our New Framework: Subpopulation Shift



Our New Framework: Subpopulation Shift



Experiments

Method	A → W	D → W	W → D	A → D	D → A	W → A	Average
MDD	94.97±0.70	98.78±0.07	100±0	92.77±0.72	75.64±1.53	72.82±0.52	89.16
Ours	95.47±0.95	98.32±0.19	100±0	93.71±0.23	76.64±1.91	74.93±1.15	**89.84**

Performance of MDD[1] and our method on Office-31 dataset.

Method	Ar → Cl	Ar → Pr	Ar → Rw	Cl → Ar	Cl → Pr	Cl → Rw	Pr → Ar
MDD	54.9±0.7	74.0±0.3	77.7±0.3	60.6±0.4	70.9±0.7	72.1±0.6	60.7±0.8
Ours	55.1±0.9	74.7±0.8	78.7±0.5	63.2±1.3	74.1±1.8	75.3±0.1	63.0±0.6
Method	**Pr → Cl**	**Pr → Rw**	**Rw → Ar**	**Rw → Cl**	**Rw → Pr**	**Average**	
MDD	53.0±1.0	78.0±0.2	71.8±0.4	59.6±0.4	82.9±0.3	68.0	
Ours	53.0±0.6	80.8±0.4	73.4±0.1	59.4±0.7	84.0±0.5	**69.6**	

Performance of MDD and our method on Office-Home dataset.

[1] MDD: (Zhang et al. 2019)

Experiments: Subpopulation Shift Dataset

- ENTITY-30 task from BREEDS tasks.
- We use FixMatch, an existing consistency regularization method. We also leverage SwAV, an existing unsupervised representation learned from ImageNet, where there can be a better structure of subpopulation shift. We compare with popular distribution matching methods like DANN and MDD.

Method	Source Acc	Target Acc
Train on Source	91.91±0.23	56.73±0.32
DANN (Ganin et al., 2016)	92.81±0.50	61.03±4.63
MDD (Zhang et al., 2019)	92.67±0.54	63.95±0.28
FixMatch (Sohn et al., 2020)	90.87±0.15	72.60±0.51