Introduction to meta-learning

Brooks Paige
ML Seminar

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- . . . using a specific learning algorithm.

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- How can our learning algorithms gain "experience" over the course of many different but related learning problems?
- We no longer need to hand-design learning rules, or representations. Why do we hand-design learning algorithms?

End-to-end learning in computer vision

Replacing hand-engineered features with end-to-end learning:

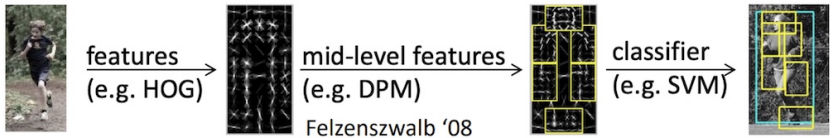

Figure: Chelsea Finn (cs330)

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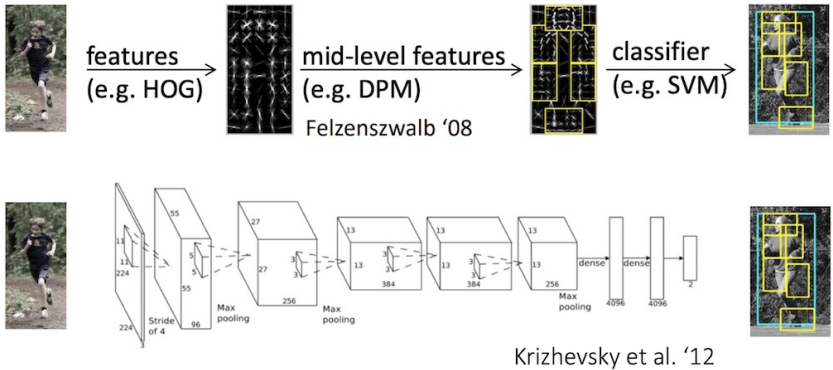

There's still a lot of hard-coded inductive bias in that architecture — and the learning algorithm is pre-defined

Figure: Chelsea Finn (cs330)

Challenges

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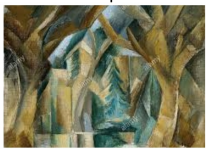
- Are giant training sets really the path to solving "AI"?
- Never going to be appropriate in low-data regimes: personalized medicine, personalized recommendations, translating rare languages, ...
- Humans don't have this problem — we learn quickly!

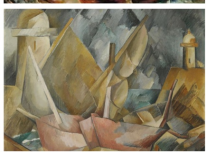
Learning when we don't have much data

training data

Braque



Cezanne



test datapoint

By Braque or Cezanne?

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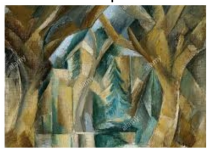

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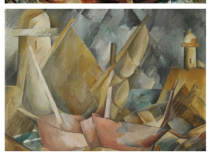

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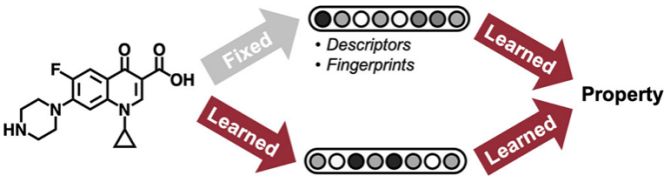
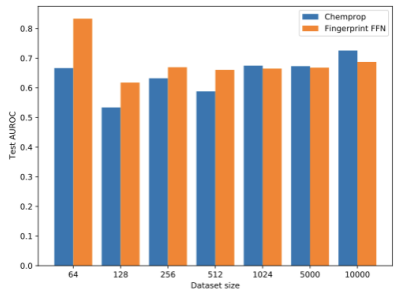
By Braque or Cezanne?

Why are you able to do this? **Prior experience**.

Figure: Chelsea Finn (cs330)

Learning when data is expensive to collect





Molecular property prediction: on small datasets, hand-crafted features can still outperform deep learning.

[MSc project last year: addressing this with meta-learning!]

Yang, Swanson, et al. (2020); Pappu & Paige (2020)

Difficulties in definitions

The term "meta-learning" is used in many different communities, to mean many different things, and with varying terminology.

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The goal in meta-learning: **more tasks $\Rightarrow$ better learning algorithms**.

Learning to learn: general framework

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   - This is called our **meta-learning** or *outer learning* algorithm. It is responsible for training the inner learning algorithm!
   - A **learning episode** consists of a base algorithm, a model, and some measure of performance (e.g. generalization error, or convergence speed). Multiple learning episodes taken together provide the training data for the outer learning algorithm.

Terminology

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Terminology

In our base learner, for each particular task or episode,

- we train on our **training set**, *[support set]*
- and evaluate on a **test set**. *[query set]*

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[alternative terminology]

Learning and meta-learning

Anatomy of a typical ML learning scenario:

- Dataset $\mathcal{D}$, e.g. $\mathcal{D} = \{\mathbf{x}_1, y_1\}, \ldots, \{\mathbf{x}_N, y_N\}$ for supervised learning
- Model specification to learn, e.g. parameters $\boldsymbol{\theta}$ of a predictor $\hat{y} = f_{\boldsymbol{\theta}}(\mathbf{x})$
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- The value of $\boldsymbol{\theta}^\star$ for a particular episode is found by running the base learning algorithm A, with parameters ω; i.e.

$$\boldsymbol{\theta}^\star = A(\mathcal{L}, \mathcal{D}_{train}; \omega).$$

Distributions of tasks

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In practice, this often corresponds to solving a two-level optimization problem.

What are different tasks?

- Image classification, but on **previously unseen classes**
- Image classification, but in **new lighting conditions** (or **weather conditions**, etc)
- Same objective, but on new data: e.g. customized to a **different person**
- Same conceptual goal, but **different loss** or objective function
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Different tasks need to share at least some structure. But actually, many things we might want to do using machine learning have a lot of shared structure. (Tasks aren't "random"!)

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- **Transfer learning** aims to take knowledge from previous tasks, and use it to accelerate future tasks. This typically involves fitting $\boldsymbol{\theta}$ to previous task(s), and then using those parameters as initialization on a new tasks. The main difference from meta-learning is that there is **no meta-objective** — the previous tasks are not trained in a way which is aware that $\boldsymbol{\theta}$ will be used on new data later.

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A lot of different subareas in machine learning are similar to meta-learning.

- **AutoML** aims to automate large parts of the machine learning pipeline — from algorithm selection, to dataset transforms, to neural network architectures. It's generally a broader topic than meta-learning, but meta-learning can be useful.

  For example, searching for neural architectures is slow and expensive, so it's desirable to find architectures which are generally helpful across a wide variety of problems, and to leverage knowledge that existing architectures (and algorithms) are useful on particular datasets.

Three things to look for when reading meta-learning papers

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- **Meta-optimizer**: **How** do we do the outer-level optimization of ω? This might be gradient descent through the inner optimization of $\boldsymbol{\theta}$, or could be something else entirely (RL, random search, ...).
- **Meta-objective**: **Why** are we doing any of this? The meta-objective corresponds to the choice of task distribution and meta-loss.

https://arxiv.org/abs/2004.05439

Amortization

One other aspect to keep an eye out for is the amount of **amortization**.

- Idea of amortizing runtime costs: pay a large cost up front, in exchange for fast computation later
- Popular e.g. for running Bayesian inference repeatedly using the same model, on different datasets
- Different meta-learning methods have different degrees of amortization (e.g. learning an initialization less so than generating parameters directly)

Case study: few-shot learning

Learning from a single example

Which of these is like the other?

Lake et al. (2015)

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Few-shot learning as meta-learning

Suppose we want to know how to classify an image from very few examples (maybe only one!)

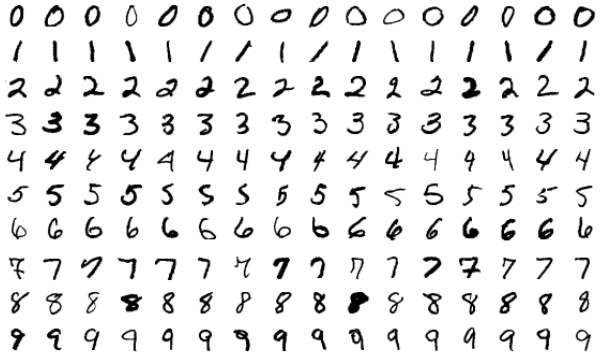
- We want to learn an algorithm A that outputs good parameters $\boldsymbol{\theta}$ for a model M given a very small training dataset $\mathcal{D}$
- If we collect many such few-shot learning tasks, we can learn the algorithm A directly from data
- This will require a suitable **meta-objective**.

Most machine learning datasets

MNIST dataset

- 10 classes
- 60,000 examples

$\approx$ 6,000 images each



Most real-world datasets?

Omniglot dataset

- 1,623 classes
- . . . across 50 alphabets

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[“transposed” MNIST]

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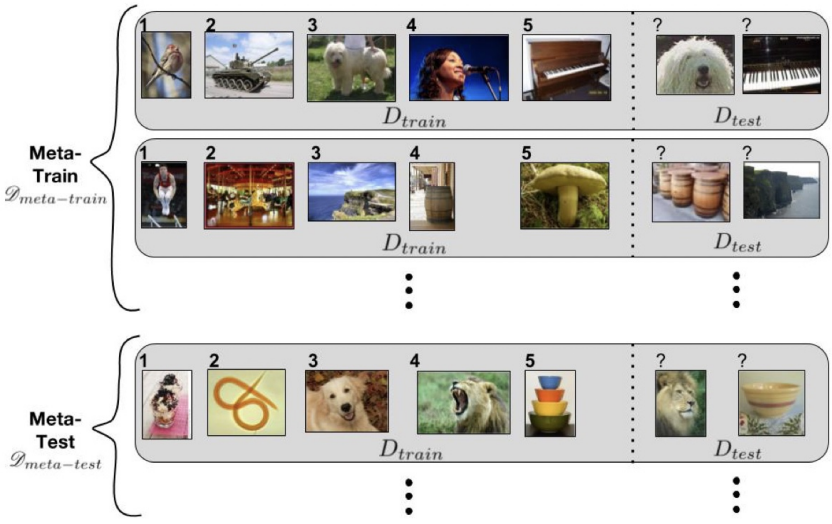
- Suppose we are shown 5 images, one each from five different classes:

- Then, we are asked to predict the correct class of two brand-new test images:

These test images are from classes we've never seen before these five new images.

Mini-ImageNet



Vinyals et al. (2016), Ravi & Larochelle (2017)

Choice of meta-representation

One approach is to start from an existing machine learning algorithm, add extra parameters, and learn those with meta-learning. We will look at three of these for classification:

- kNN or kernel classifier $\rightarrow$ Matching networks, Vinyals et al. (2016)
- Gaussian classifier $\rightarrow$ Prototypical networks, Snell et al. (2017)
- Gradient descent $\rightarrow$ MAML, Finn et al. (2017)

Slide adapted from Hugo Larochelle

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It's also possible to take a completely black-box approach, where the entire algorithm is learned by a neural network:

- Memory-augmented neural networks, Santoro et al. (2016)
- SNAIL, Mishra et al. (2018)

Slide adapted from Hugo Larochelle

Matching networks

Classifier for new $\mathbf{x}'$:

$$\hat{y} = \sum_{i=1}^{M} a(\mathbf{x}', \mathbf{x}_i) y_i$$

where $\{\mathbf{x}_i, y_i\}$ are the train set $\mathcal{D}_{train}$ and $\mathbf{x}' \in \mathcal{D}_{test}$. We want to learn $a(\dots)$.

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Advantages:

- Non-parametric method
- Can recover nearest neighbors and kernel density estimators
- Can also function as an associative memory that "points" to nearest training examples

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where $\{\mathbf{x}_i, y_i\}$ are the train set $\mathcal{D}_{train}$ and $\mathbf{x}' \in \mathcal{D}_{test}$. We want to learn $a(\dots)$.

Idea: parameterize this in terms of an attention mechanism

$$a(\mathbf{x}', \mathbf{x}_i) = \frac{\exp\{c(f(\mathbf{x}'), g(\mathbf{x}_i))\}}{\sum_{j=1}^{M} \exp\{c(f(\mathbf{x}'), g(\mathbf{x}_j))\}},$$

where f, g are learnable functions, and c is the cosine distance

$$c(\mathbf{f}, \mathbf{g}) = 1 - \frac{\mathbf{f}^\top \mathbf{g}}{\|\mathbf{f}\| \|\mathbf{g}\|}.$$

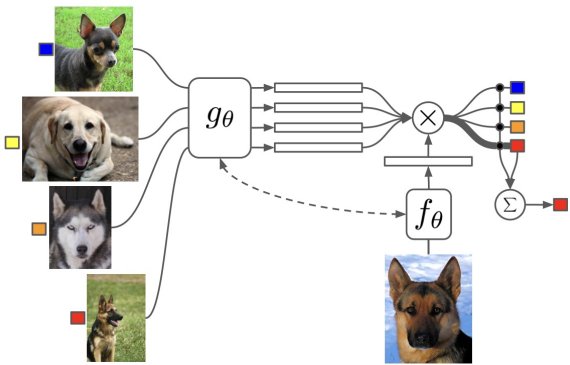
Vinyals et al. (2016)

Matching networks

One trick: instead of just $f_{\boldsymbol{\theta}}(\mathbf{x}')$ and $g_{\boldsymbol{\theta}}(\mathbf{x}_i)$, also provide access to an embedding of the entire training set, e.g. learning

- $f_{\boldsymbol{\theta}}(\mathbf{x}') = f_{\boldsymbol{\theta}}(\mathbf{x}', \mathcal{D}_{train})$
- $g_{\boldsymbol{\theta}}(\mathbf{x}_i) = g_{\boldsymbol{\theta}}(\mathbf{x}_i, \mathcal{D}_{train})$

where both are parameterized by sequence models (e.g. LSTMs).



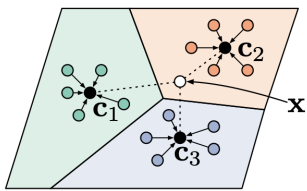
Vinyals et al. (2016)

Prototypical networks

Learn an embedding $f_{\boldsymbol{\theta}}(\mathbf{x})$, and compute class centroids $\mathbf{c}_k$ as

$$\mathbf{c}_k = \frac{1}{|\mathcal{S}_k|} \sum_{\{\mathbf{x}_i, y_i\} \in \mathcal{S}_k} f_{\boldsymbol{\theta}}(\mathbf{x}_i)$$

where $\mathcal{S}_k \subset \mathcal{D}_{train}$ is the set of training points with class label $y_i = k$.



Classifier for new $\mathbf{x}'$:

$$p(y = k|\mathbf{x}') = \frac{\exp\{-d(f_{\boldsymbol{\theta}}(\mathbf{x}'), \mathbf{c}_k)\}}{\sum_{j=1}^{K} \exp\{-d(f_{\boldsymbol{\theta}}(\mathbf{x}'), \mathbf{c}_j))\}}.$$

where d is a distance function.

Snell et al. (2017)

Prototypical networks

Since class predictions only depend on the means of the embeddings $\mathbf{c}_k$, this is much simpler than matching networks — there is no need for a complex embedding of the training sets.

- With a Euclidean distance $d(\cdot, \cdot) = \|f_{\boldsymbol{\theta}}(\mathbf{x}') - \mathbf{c}_k\|^2$, this is interpretable as learning a linear model in the embedding space $f_{\boldsymbol{\theta}}(\mathbf{x})$:

$$\begin{aligned} -\|f_{\boldsymbol{\theta}}(\mathbf{x}') - \mathbf{c}_k\|^2 &= -f_{\boldsymbol{\theta}}(\mathbf{x}')^\top f_{\boldsymbol{\theta}}(\mathbf{x}') + 2\mathbf{c}_k^\top f_{\boldsymbol{\theta}}(\mathbf{x}') - \mathbf{c}_k^\top \mathbf{c}_k \\ &= \underbrace{(2\mathbf{c}_k)}_{\mathbf{w}_k}^\top f_{\boldsymbol{\theta}}(\mathbf{x}') - \underbrace{\mathbf{c}_k^\top \mathbf{c}_k}_{b_k} + \text{const} \end{aligned}$$

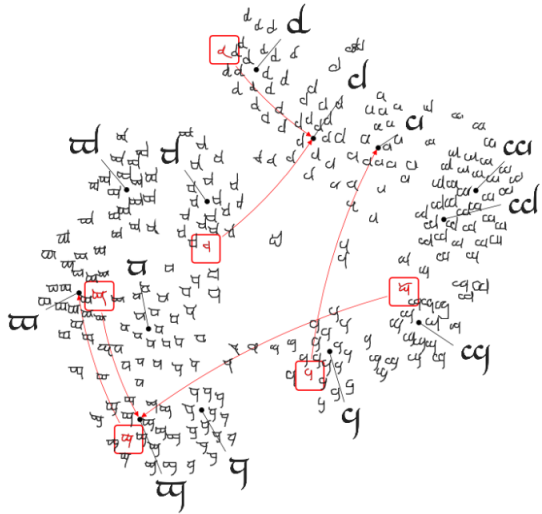
- The learned network $f_{\boldsymbol{\theta}}$ produces, in a feedforward manner, the embedding space as well as the weights of the corresponding linear classifier.

Snell et al. (2017)

Prototypical networks

Example embedding for an Omniglot meta-test task

- T-SNE visualization
- Black highlights are class centers
- Red highlights are misclassification errors



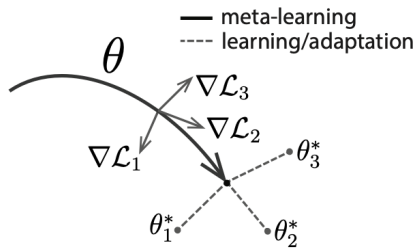
Snell et al. (2017)

(This one is simple enough to implement that I can actually do a live demo)

Model-agnostic meta learning (MAML)

A downside of the previous method was that it is not obvious how to apply outside of classification settings.

- MAML: meta-representation is a parameter vector $\boldsymbol{\theta}$ for some (any) deep learning model
- Learn a general **initialization**, from which we can quickly fine-tune to new classes
- Unlike "typical" transfer learning, where the initial $\boldsymbol{\theta}$ subject to fine-tuning come from some unrelated network, here there is an explicit meta-learning objective



Finn et al. (2017)

Model-agnostic meta learning (MAML)

Algorithm 1 Model-Agnostic Meta-Learning

Require: $p(\mathcal{T})$: distribution over tasks
Require: α, β: step size hyperparameters
1: randomly initialize θ
2: **while** not done **do**
3: Sample batch of tasks $\mathcal{T}_i \sim p(\mathcal{T})$
4: **for all** $\mathcal{T}_i$ **do**
5: Evaluate $\nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$ with respect to K examples
6: Compute adapted parameters with gradient descent: $\theta_i' = \theta - \alpha \nabla_\theta \mathcal{L}_{\mathcal{T}_i}(f_\theta)$
7: **end for**
8: Update $\theta \leftarrow \theta - \beta \nabla_\theta \sum_{\mathcal{T}_i \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}_i}(f_{\theta_i'})$
9: **end while**

Finn et al. (2017)

Black-box approaches

Black-box approach

Train a neural architecture to directly output predictions at the "next" task.

1. Train a network which directly outputs parameters of a model, e.g. for task $\mathcal{T}_i$,

$$\omega_i = f_\theta(\mathcal{D}^i_{train})$$

2. Make predictions on test data with

$$y = g_{\omega_i}(\mathbf{x}_{i,test})$$

Clear training objective — this is now just supervised learning. But, complex models are required, and extending to large datasets is hard.

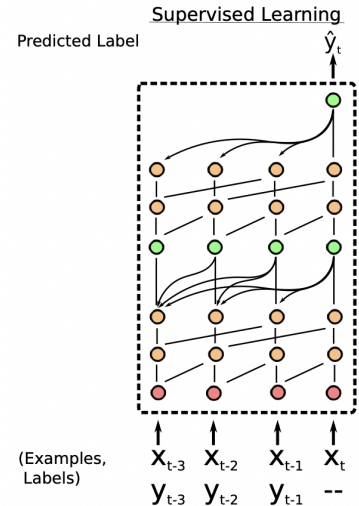


Figure: Mishra et al. (2018)

What else is there?

Other things you can meta-learn

- **Neural network architectures**: This is a big one — network architectures (e.g. convnets, resnets, LSTMs, GNNs) have strong inductive biases. Can we learn architectures (or building blocks) which generalize well to many tasks?

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- ...

. . . and other applications

- Domain adaptation,
- continual learning,
- defense against adversarial attacks, . . .

Many more ideas (with citations) in Hospedales et al. (2020).

Thank you!