Machine Learning **Beyond Static Datasets**

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Course: http://owll-lab.com/teaching/essai-23

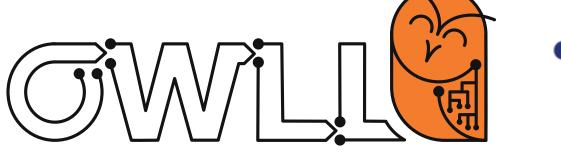
Day 1 - The Present: Static Datasets & Re-use **ESSAI 2023**







TECHNISCHE UNIVERSITÄT DARMSTADT









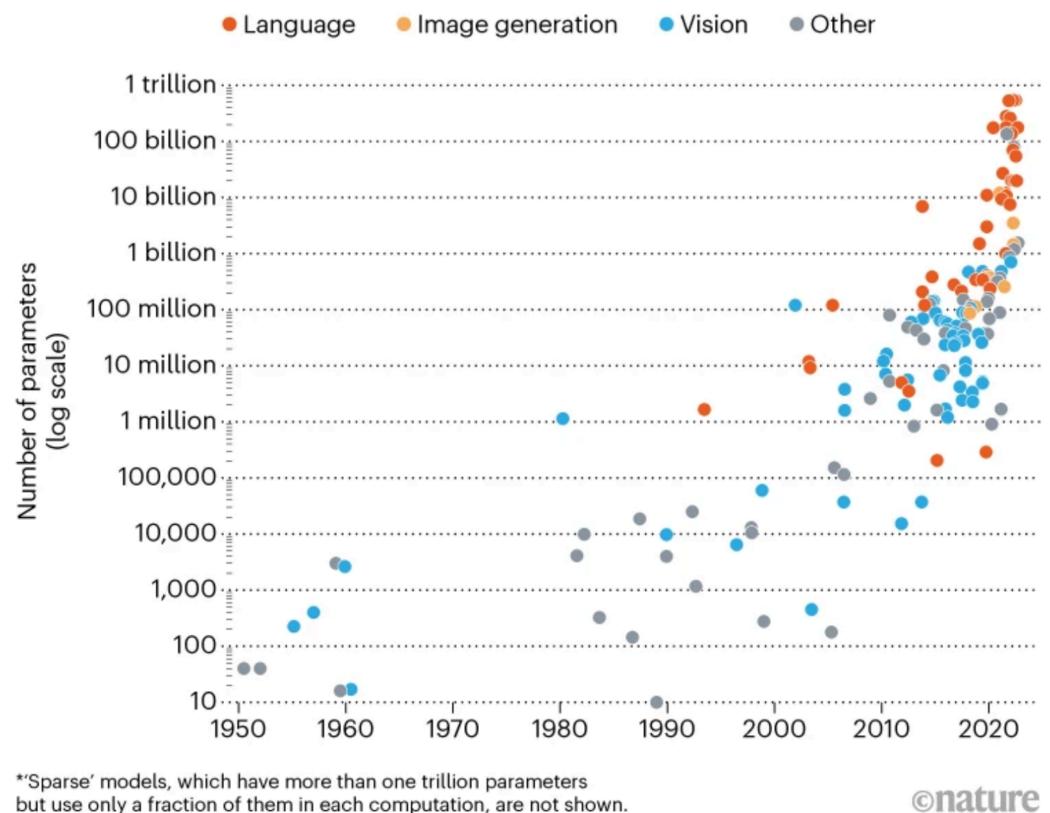






THE DRIVE TO BIGGER AI MODELS

The scale of artificial-intelligence neural networks is growing exponentially, as measured by the models' parameters (roughly, the number of connections between their neurons)*.



but use only a fraction of them in each computation, are not shown.

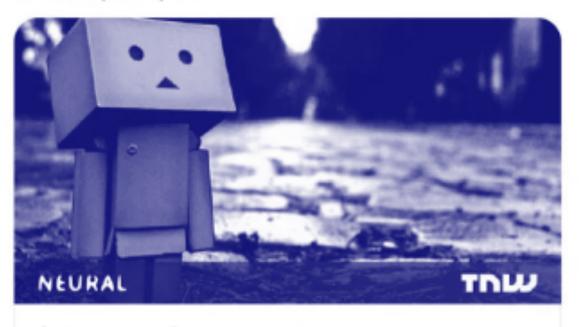
Source: Adapted from Our World in Data, and from J. Sevilla et al. Preprint at https://arxiv.org/abs/2202.05924 (2022).

Is scale all we need?!

A Research Director at Deepmind says all we need now is scaling



Nando de Freitas 📰 @Nando... · 4 t. Someone's opinion article. My opinion: It's all about scale now! The Game is Over! It's about making these models bigger, safer, compute efficient, faster at sampling, smarter memory, more modalities, INNOVATIVE DATA, on/ offline, ... 1/N



thenextweb.com DeepMind's new Gato Al makes me fear humans will never achieve AGI

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 Q_{10}

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At the least, lifelong learning may be one pathway to more human-like intelligence

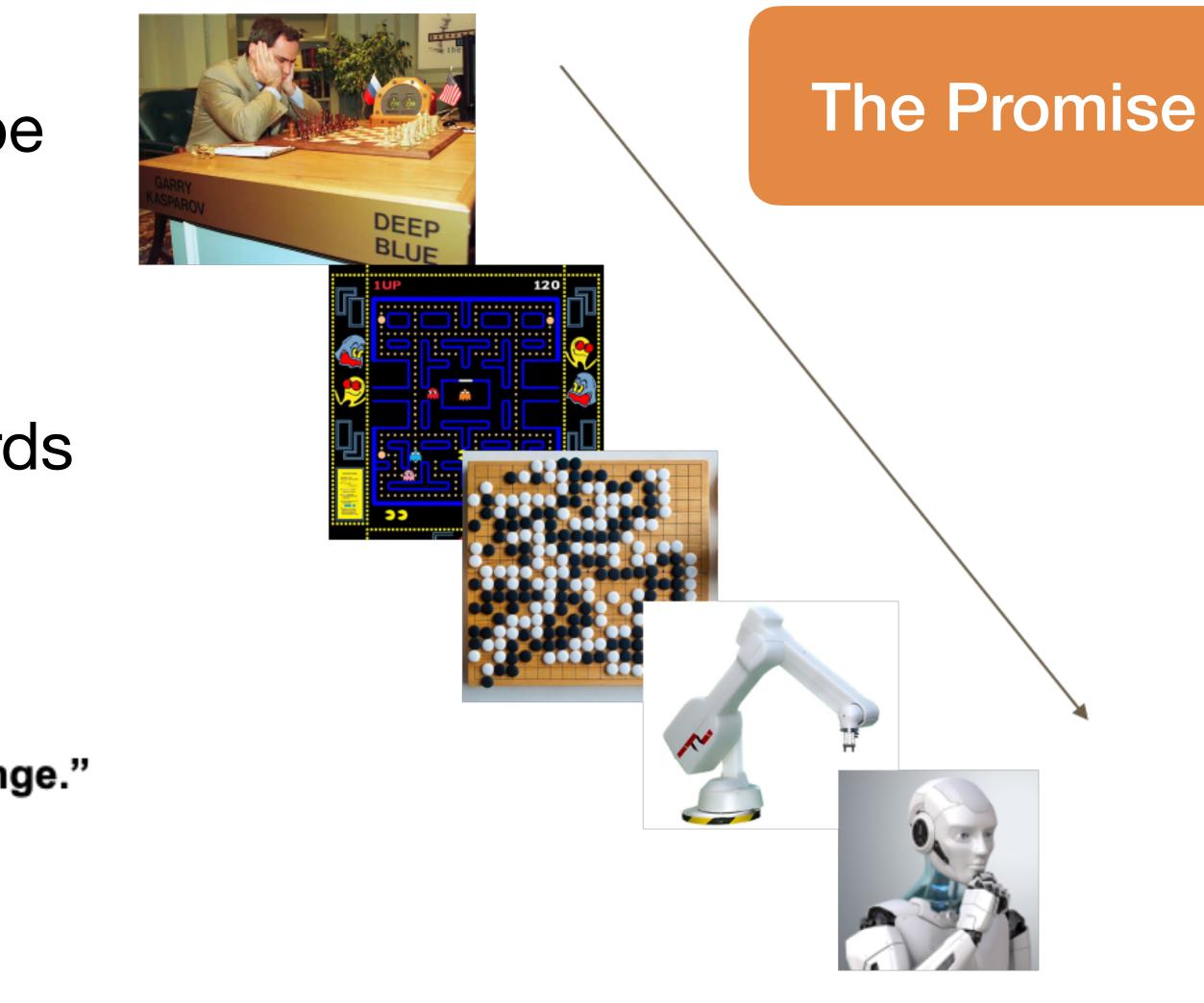
At the most, its one pathway towards strong, more general artificial intelligence



"Intelligence is the ability to adapt to change." - Stephen Hawking

Slide adapted from our AAAI-23 Continual Causality Tutorial, Cooper & Mundt

Humans learn continually! Why shouldn't ML models?







"It's about making the models" bigger, safer, compute efficient, faster at sampling..."

But narrow models aren't robust, suffer from incomplete & biased datasets, don't adapt to novel situations

Can we really capture everything upfront?

Slide adapted from our AAAI-23 Continual Causality Tutorial, Cooper & Mundt

Despite many great achievements of current systems, few, if any, truly can learn & predict over time



The Premise







Day 1: The Present Static Datasets & Re-use

Identify the problem to be solved and create a clear objective. Collect Define objective Data Collect data from hospitals, health insurance companies, social service agencies, police and fire dept.

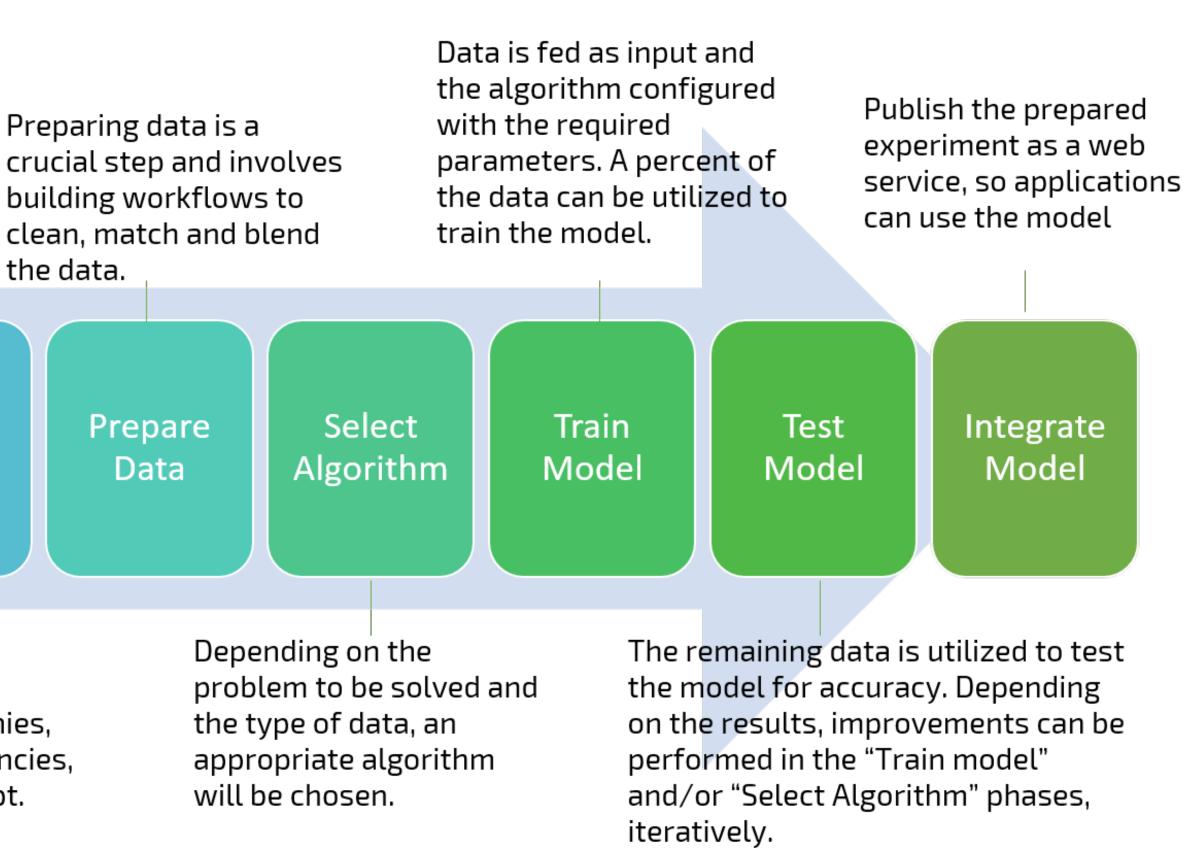
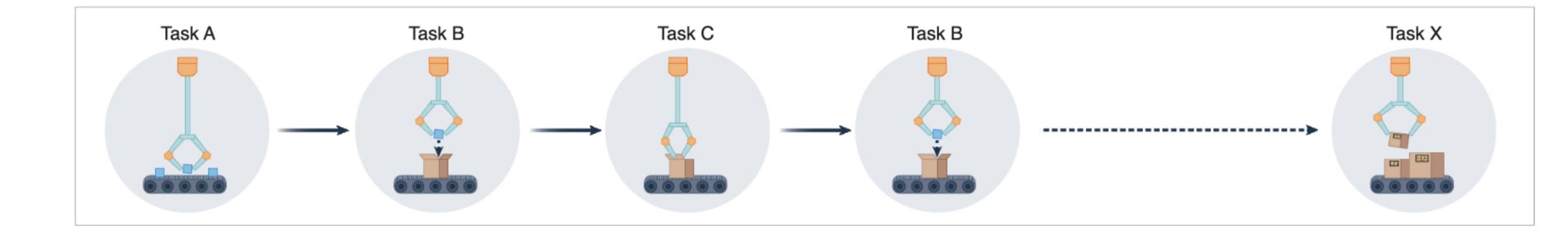


Figure from https://www.congrelate.com/get-workflow-machine-learning-images/



Day 1: The Present Static Datasets & Re-use



Day 2: The Past Forgetting & Memory

Figure from Kudithipudi et al, "Biological underpinnings for lifelong learning machines", Nature Machine Intelligence (4), 2022



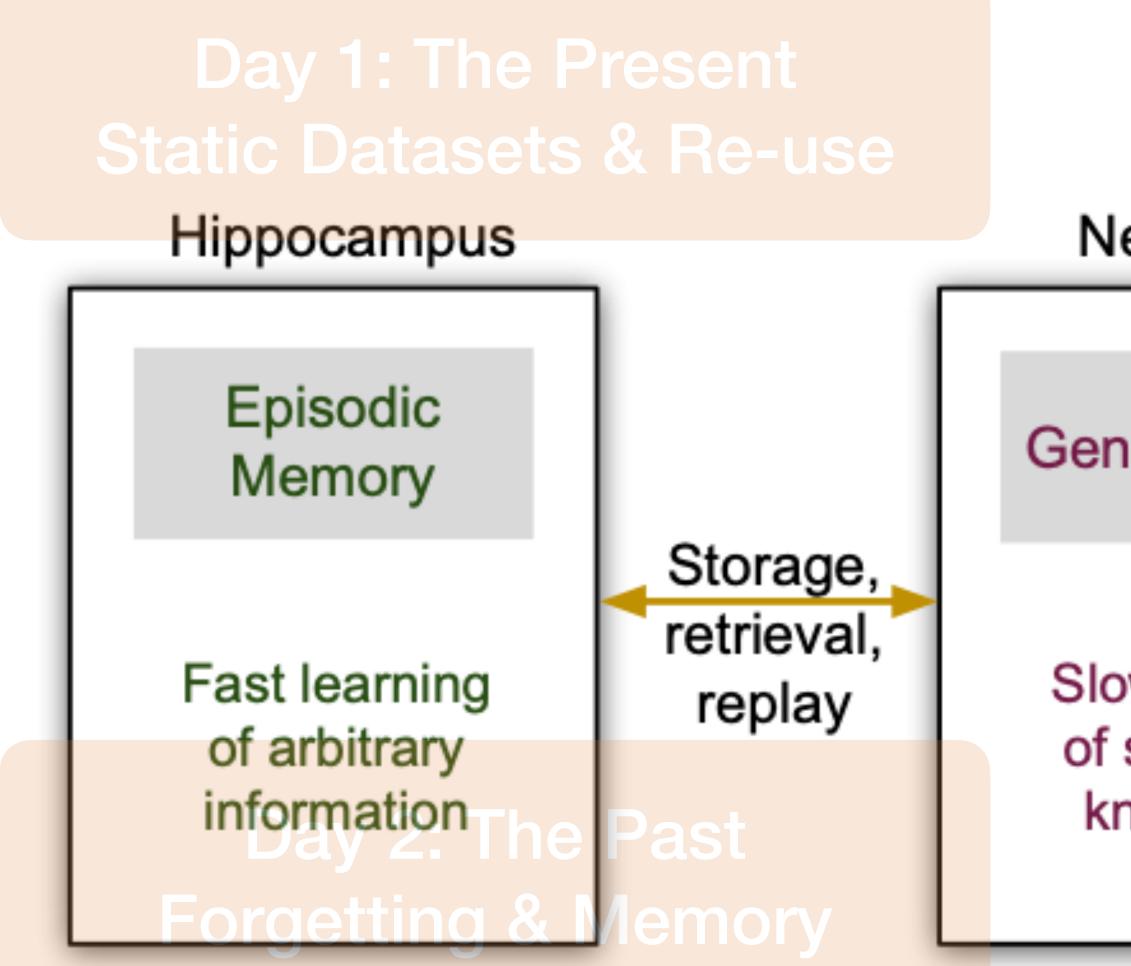


Figure from Parisi et al, "Continual Lifelong Learning with Neural Networks: A Review", Neural Networks 113, 2019

Day 3: From Past to Future Memory & Growth

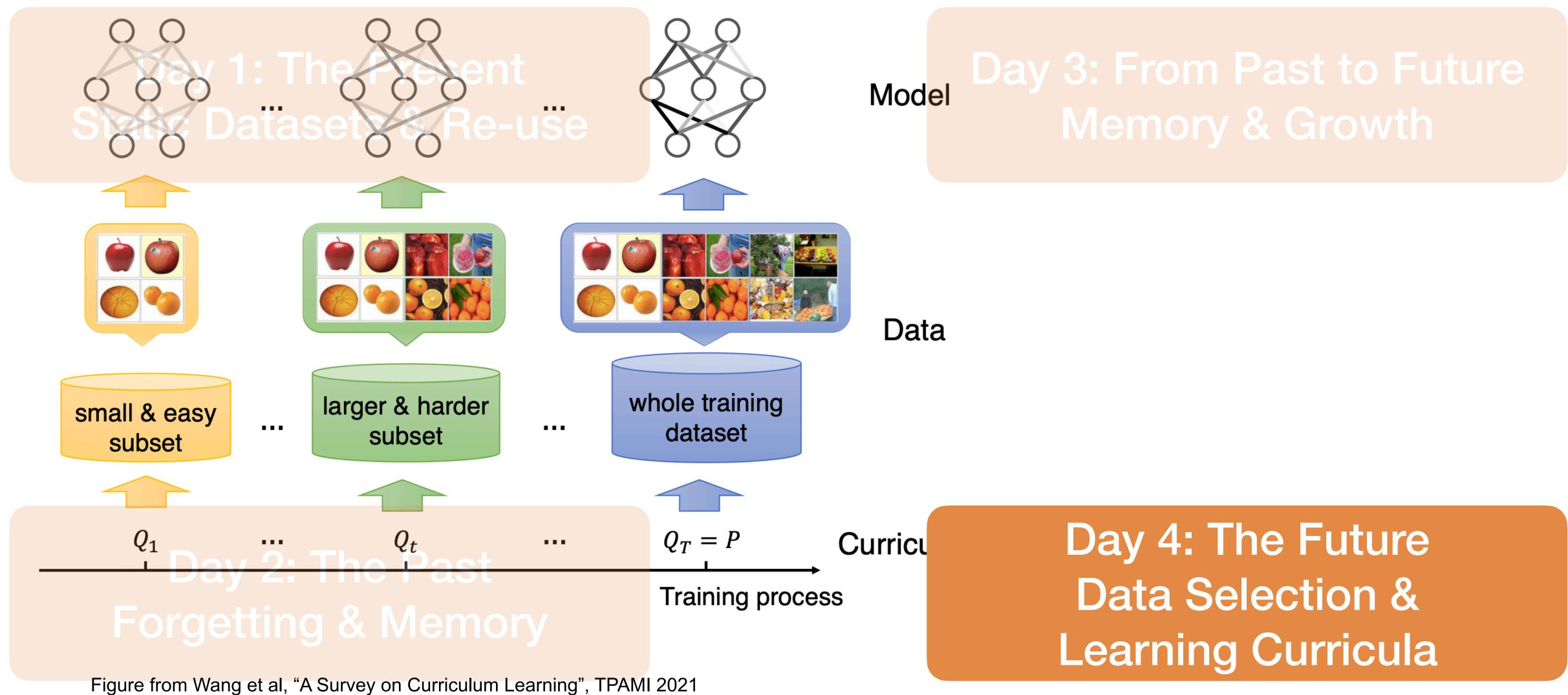
Neocortex

Generalization

Slow learning of structured knowledge







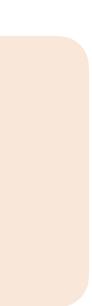


Day 5: The Unknown **Open World Learning & Evaluation**

The Problems! Why are we not there & what to do - Course Overview







Motivation: A step back - what is machine learning?



The static ML workflow

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E".

Machine Learning, T. M. Mitchell, McGraw-Hill, 1997



ML recap: train - test splits

- "The result of running the machine learning algorithm can be expressed as a *function.* The precise form of the function is determined during the *training* phase, also known as the *learning* phase, on the basis of the training data.
 - Once the model is trained it can then determine the identity of new instances, which are said to comprise a **test set**. The ability to categorize correctly new examples that differ from those used for training is known as generalization".
 - Pattern Recognition and Machine Learning, C. M. Bishop, Springer 2006, page 2





ML recap: error/loss & learning

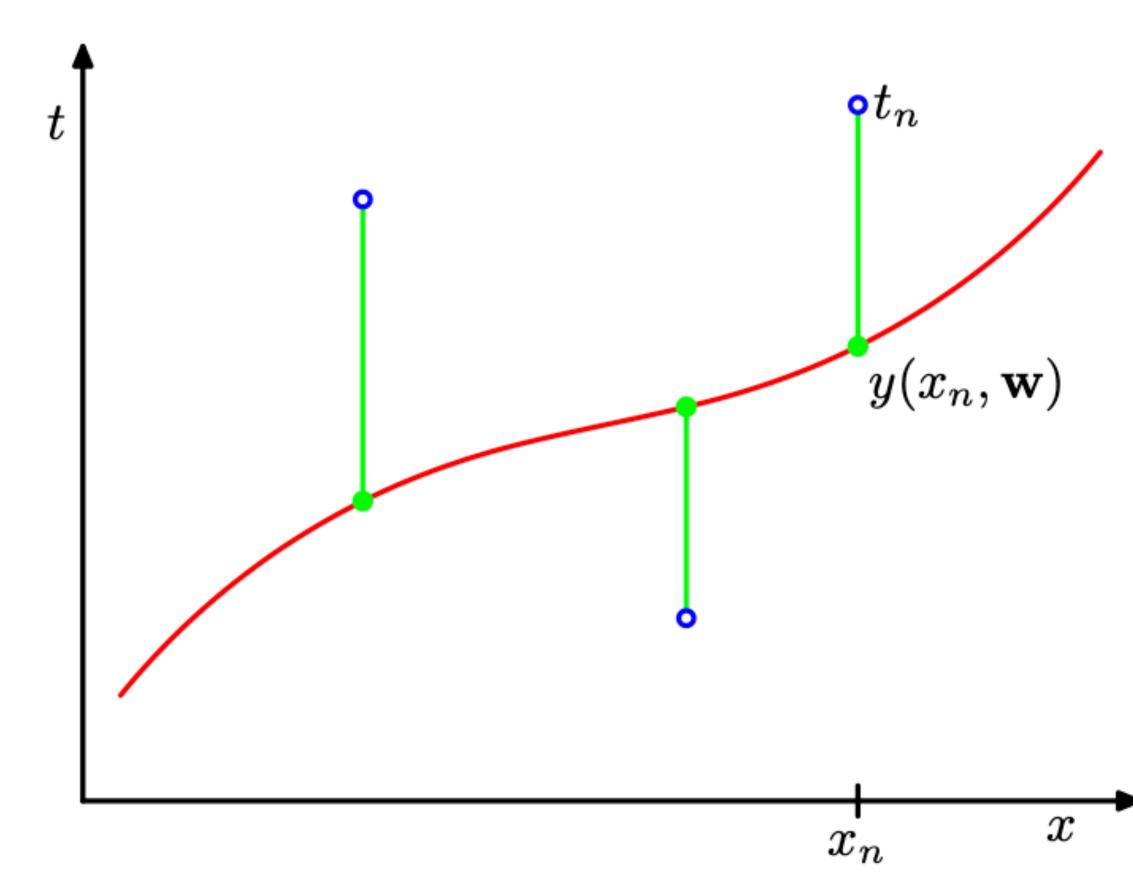


Figure 1.3 The error function (1.2) corresponds to (one half of) the sum of the squares of the displacements (shown by the vertical green bars) of each data point from the function $y(x, \mathbf{w}).$

Pattern Recognition and Machine Learning, C. M. Bishop, Springer 2006, example on polynomial curve fitting: intro page 6



ML recap: under & overfitting

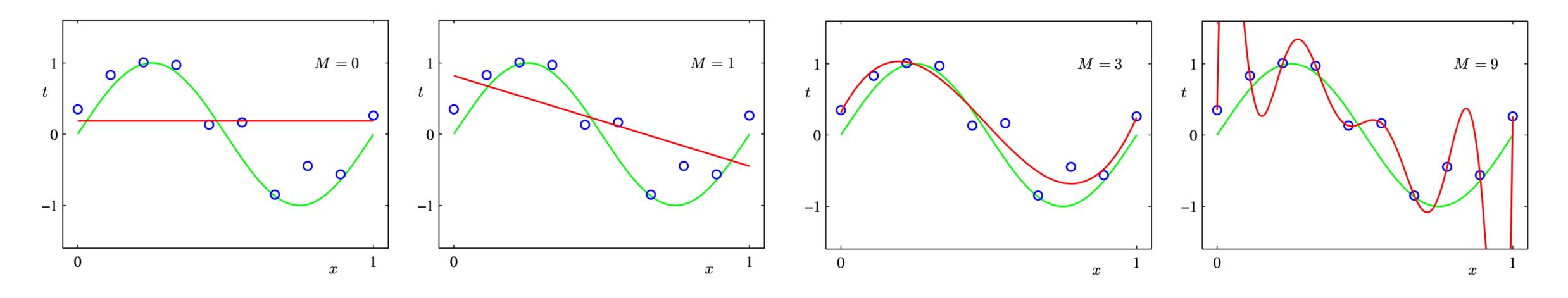
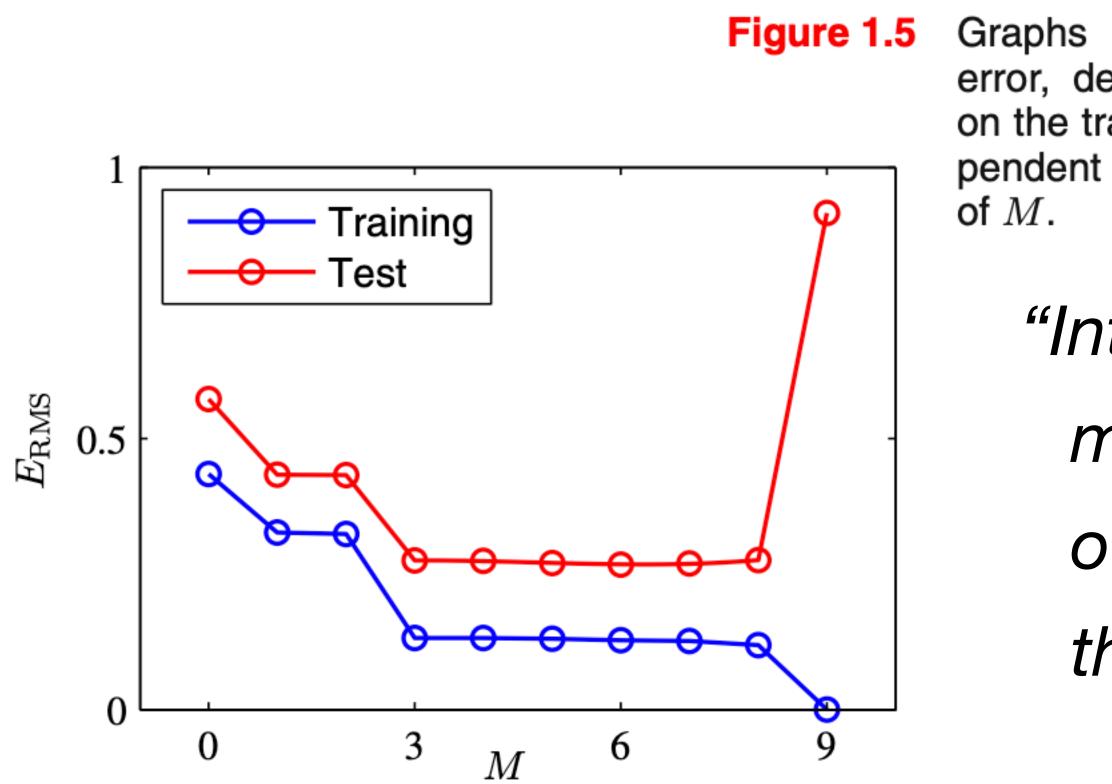


Figure 1.4 Plots of polynomials having various orders *M*, shown as red curves, fitted to the data set shown in Figure 1.2.

Pattern Recognition and Machine Learning, C. M. Bishop, Springer 2006, example on polynomial curve fitting: page 7



ML recap: under & overfitting



Pattern Recognition and Machine Learning, C. M. Bishop, Springer 2006, example on polynomial curve (over-)fitting in the introduction on page 8

Graphs of the root-mean-square error, defined by (1.3), evaluated on the training set and on an independent test set for various values

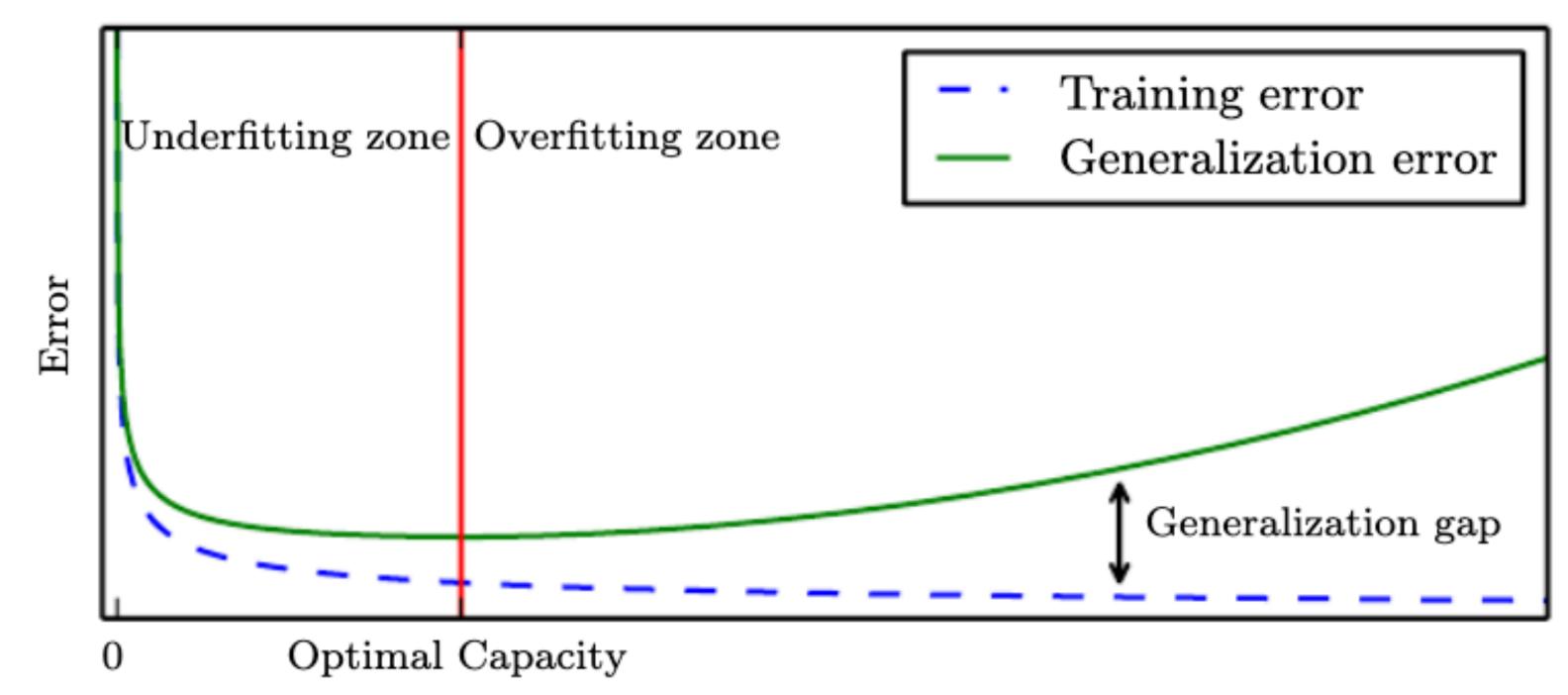
> "Intuitively, what is happening is that the more flexible polynomials with larger values of M are becoming increasingly tuned to the random noise on the target values".





ML recap: under & overfitting

This picture is still very much the same in the "deep learning era"



- Capacity
- Deep Learning, Goodfellow, Bengio, Courville, MIT Press 2016,
 - Machine Learning Basics chapter, page 112.



What do you think are the goals of ML?



The static ML workflow: goals

"Of course, when we use a machine learning algorithm, we do not fix the parameters ahead of time, then sample both datasets. We sample the training set, then use it to choose the parameters to reduce training set error, then sample the test set.

The factors determining how well a ML algorithm will perform are its ability to: 1. Make the training error small.

2. Make the gap between training and test error small".

Deep Learning, Goodfellow, Bengio, Courville, MIT Press 2016,

Machine Learning Basics chapter, page 108.

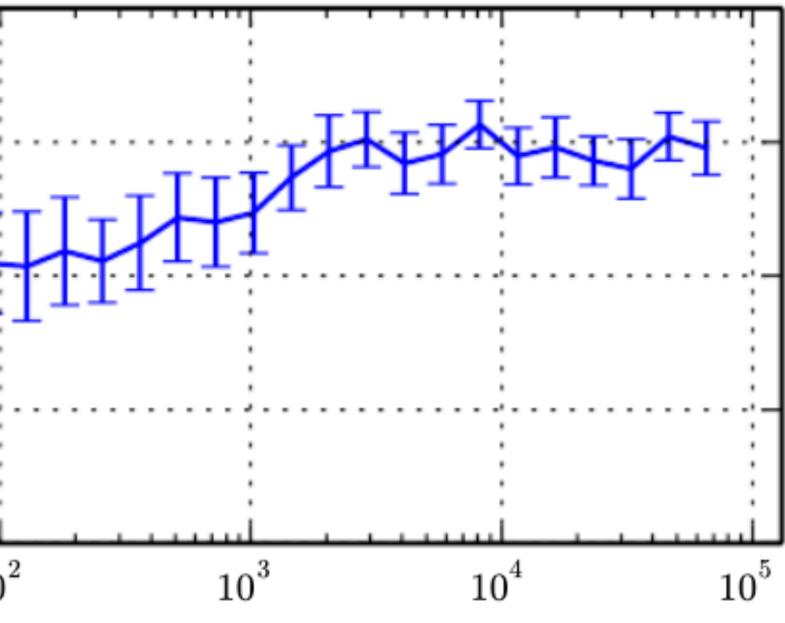






So is ML all about finding a large dataset & a right capacity model? Optimal capacity (polynomial degree 201510 10^{2} 10^3 10^{1} 10^{4} 10^{5} 10° Number of training examples

The static ML workflow: goals



- Deep Learning, Goodfellow, Bengio, Courville, MIT Press 2016,
 - Machine Learning Basics chapter, page 114.



How do you think datasets should be acquired?



Static datasets: controlled

Small scale, but (some) controlled acquisition parameters

Image	Object pose			Illumination direction		
number	Frontal	22.5 ° right	22.5 ° left	Frontal	$pprox$ 45 $^{\circ}$ from top	$pprox$ 45 $^{\circ}$ from side
1	X			X		
2	X				X	
3	X					X
4		x		X		
5		x			X	
6		x				X
7			x	X		
8			x		X	
9			X			X

Table 3: The labeling of images within each scale in the KTH-TIPS database.

Hayman et al, "On the significance of real-world conditions for material classification", ECCV 2004 & Fritz, Hayman et al, "The KTH-TIPS database", technical report 2004





Image #1



Image #4



Image #2



Image #5



Image #3



Image #6



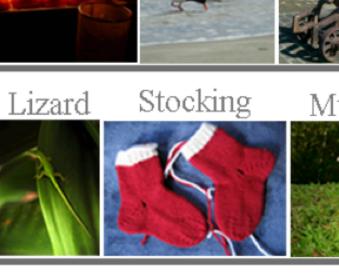
Static datasets: large scale

A big focus of modern dataset has been on large scale & diversity Spider Web Candle Oyster Cannon

Object Scale

Number of Instances

Image Clutter



Racket

Compass





Minivan



Pill BottleHorse-cart Monkey Canoe Deformability

Russakovsky & Deng et al, "ImageNet Large Scale Visual Recognition Challenge, IJCV 2015, (challenges since 2010)



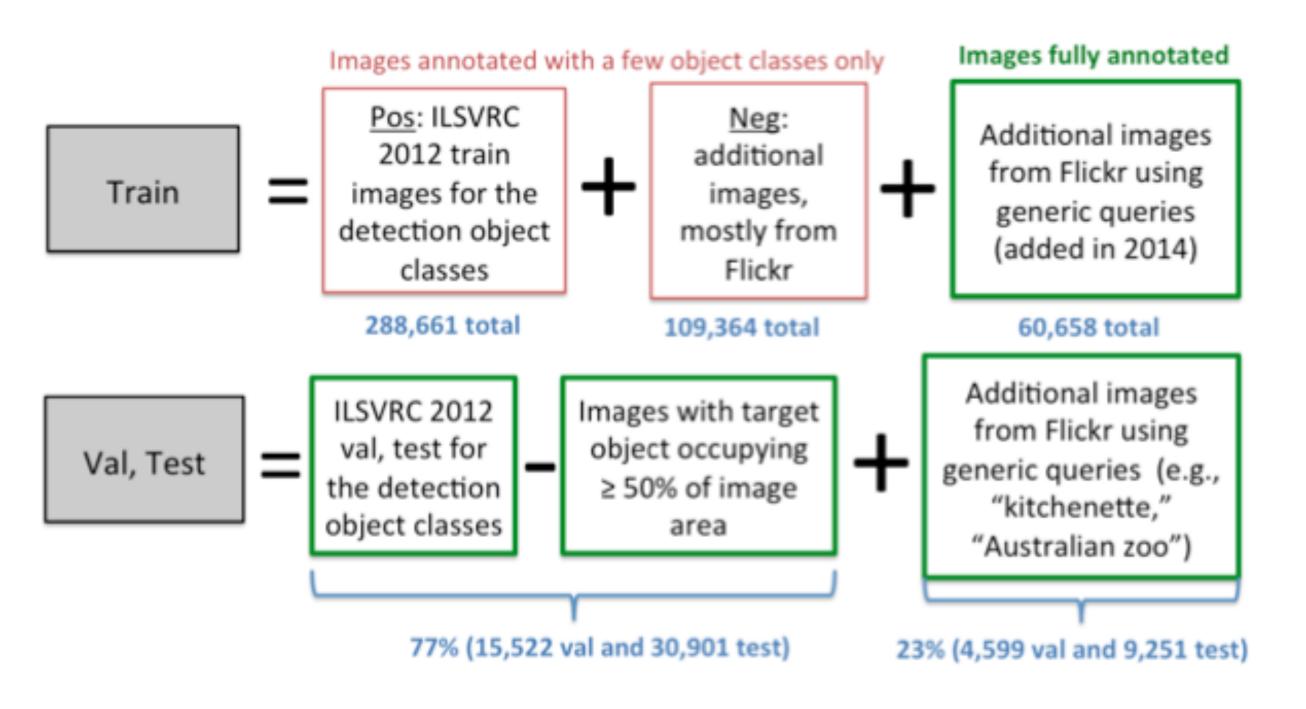




And trying to ensure reasonable train, validation, test splits through complex collection processes

Russakovsky & Deng et al, "ImageNet Large Scale Visual Recognition Challenge, IJCV 2015, (challenges since 2010)

Static datasets: large scale

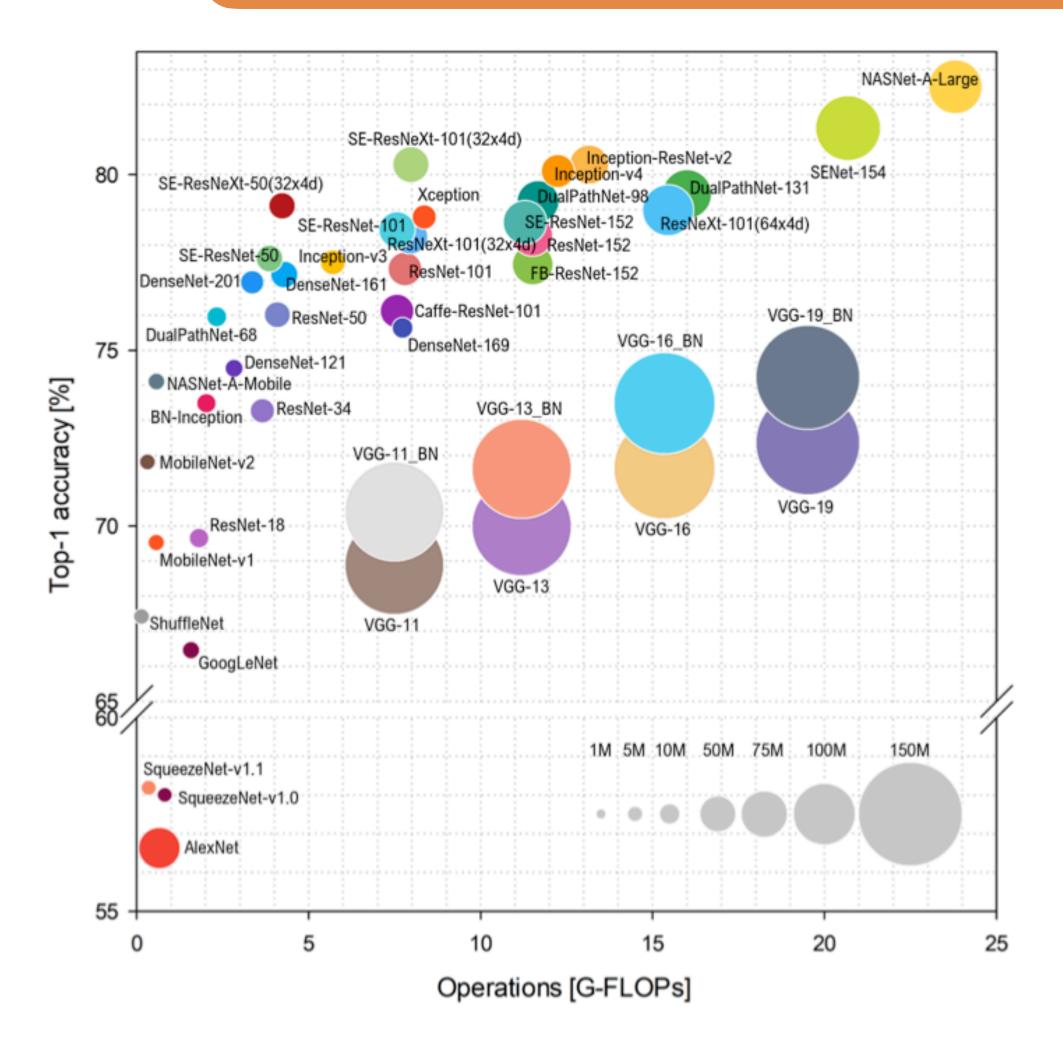




What do you think: should our primary goal be the solution to such benchmarks?



Static models



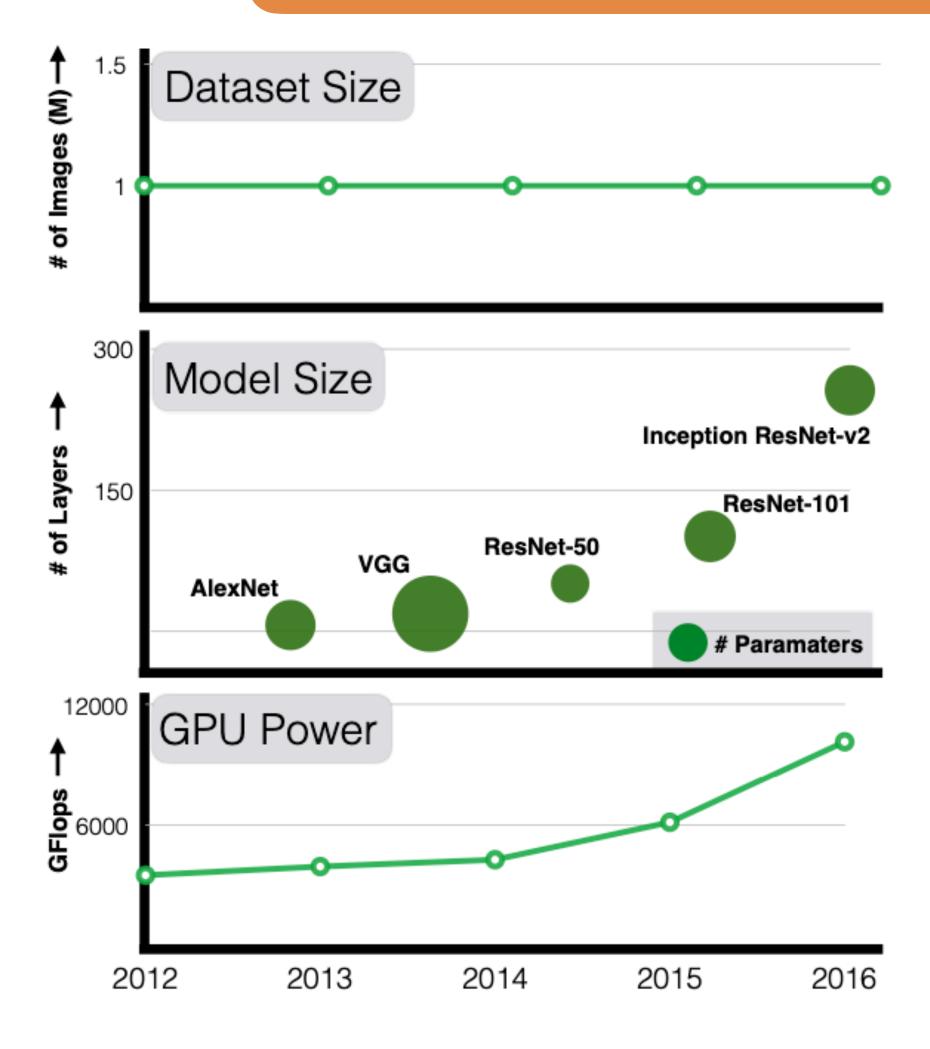
Bianco et al, "Benchmark Analysis of Representative Deep Neural Network Architectures", IEEE Access, 2018

A very big emphasis has then been on "solving" such benchmarks

ImageNet is a prime example, where models & compute got bigger and more accurate over time







Sun et al, "Revisiting Unreasonable Effectiveness of Data in Deep Learning Era", ICCV 2017

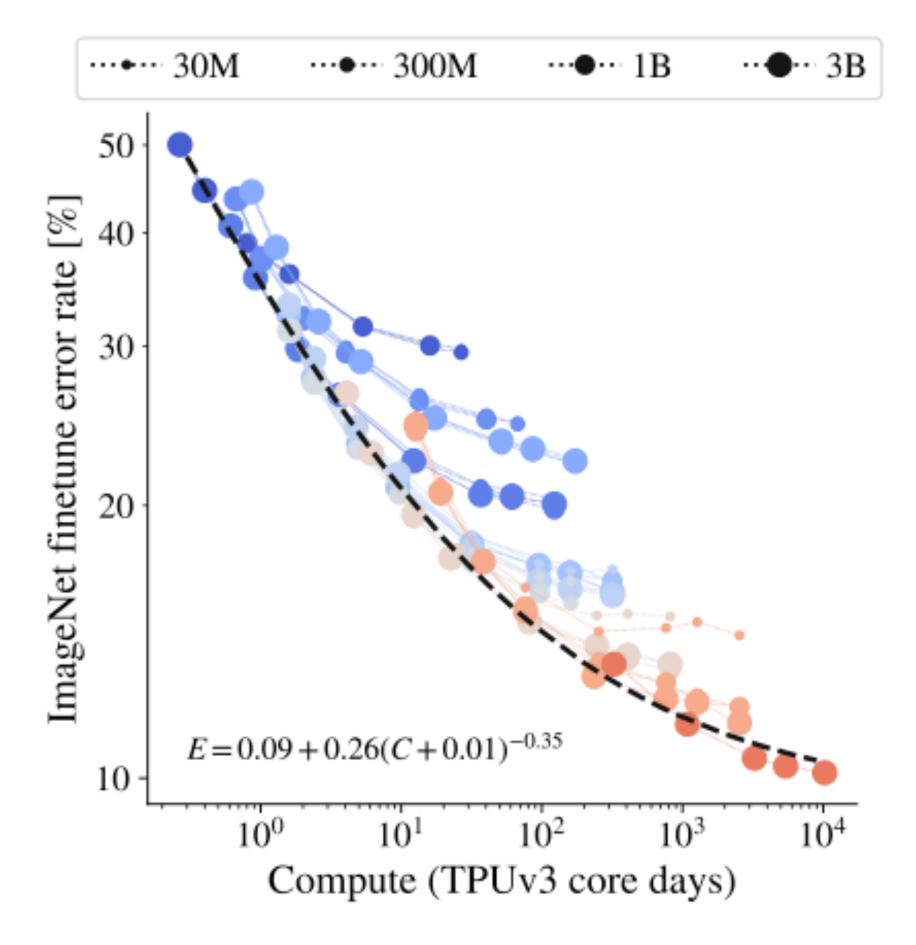
Data and model centrism

At the same time, it's often "either" models or data

For example, ImageNet has remained largely static* over time * (excluding some concerns over fair representation)







Zhao et al, "Scaling Vision Transformers", preprint 2021

Data and model centrism

Or conversely, a model is picked (here a transformer) and datasets are extended

Example from ImageNet to the (nonpublic) JFT 300M & JFT-3B

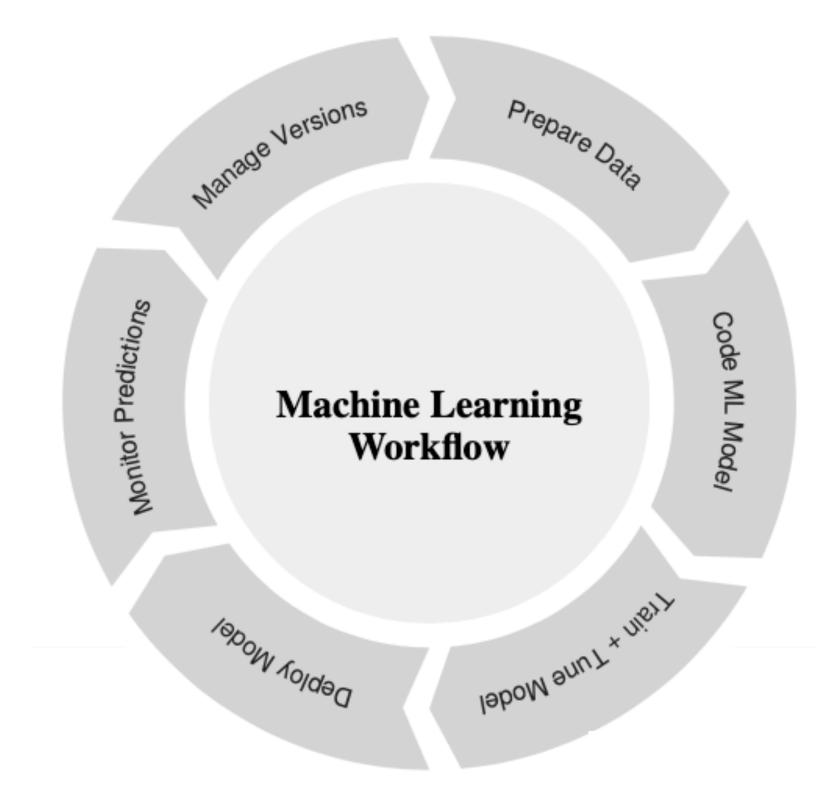




Let's start moving beyond static datasets + models







Mundt et al, "CLEVA-Compass: A Continual Learning Evaluation Assessment Compass to Promote Research Transparency and Comparability", ICLR 2022

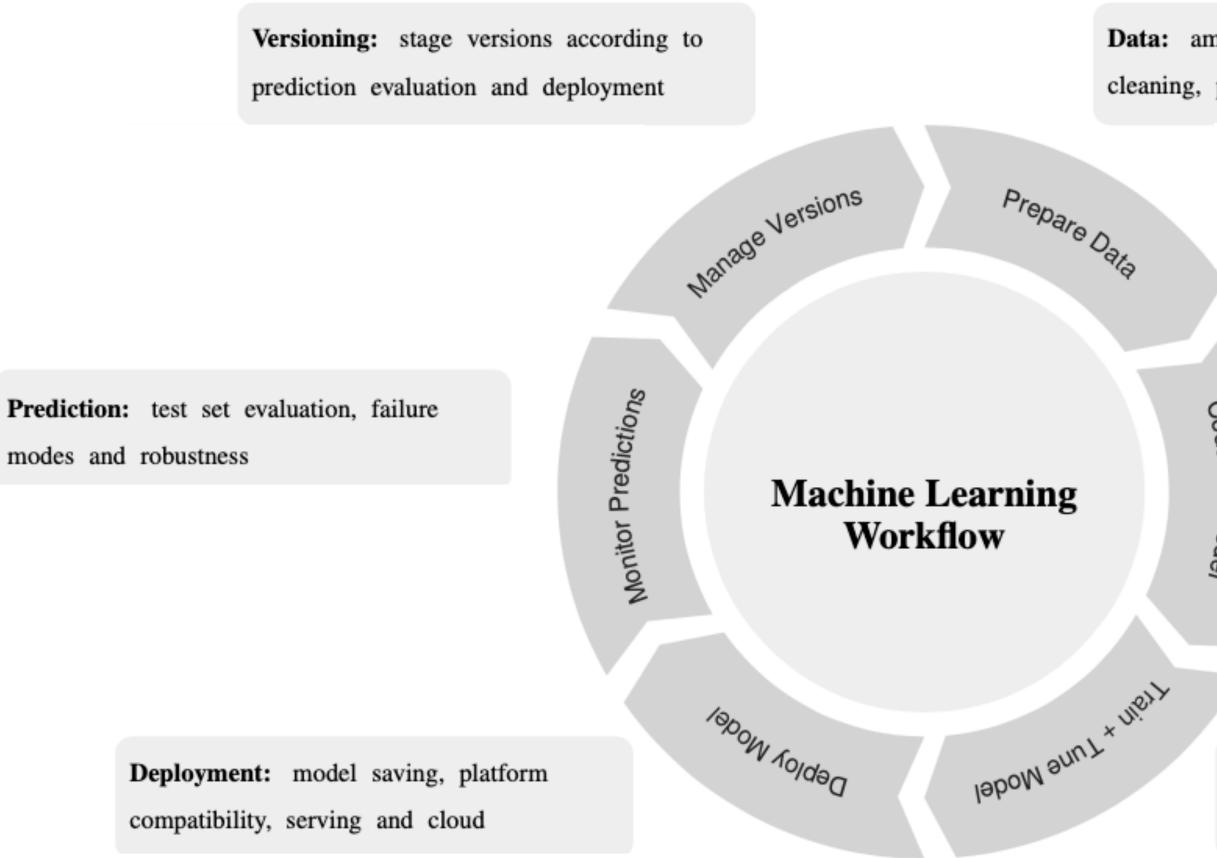
Can we just iterate?

Turns out that this will be much harder than you perhaps expect now!



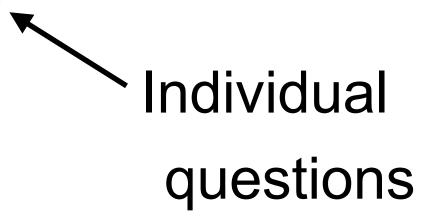
Why? From static ML workflow ...

Code ML Mode/



Mundt et al, "CLEVA-Compass: A Continual Learning Evaluation Assessment Compass to Promote Research Transparency and Comparability", ICLR 2022

Data: amount, redundancy vs. diversity, cleaning, preprocessing

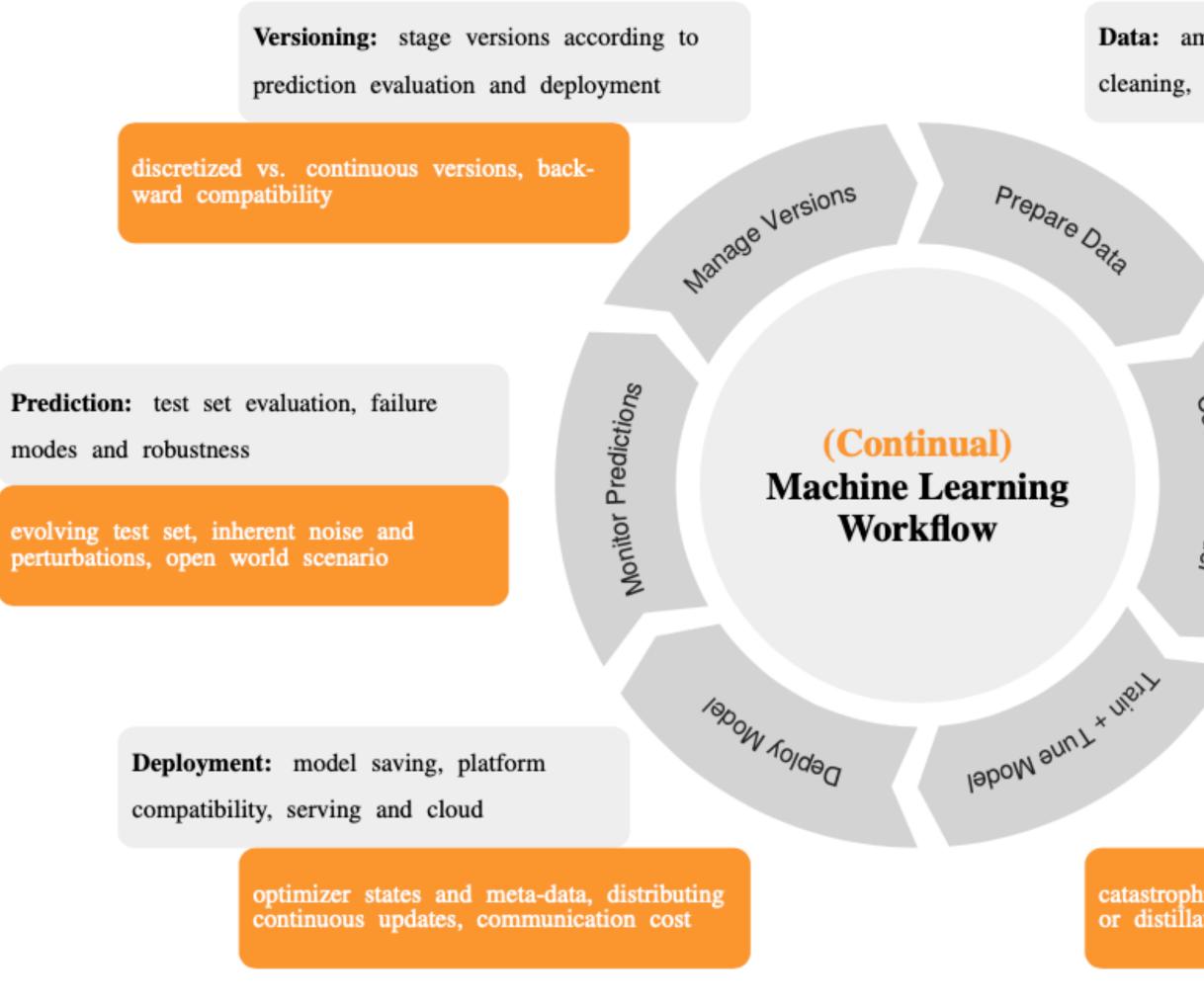


Model: architecture, inductive bias, discriminative/generative, functions, parameters

Training: loss function, optimizer, hyperparameters, convergence



... to continual/lifelong ML ...



Mundt et al, "CLEVA-Compass: A Continual Learning Evaluation Assessment Compass to Promote Research Transparency and Comparability", ICLR 2022

Data: amount, redundancy vs. diversity, cleaning, preprocessing

data selection and ordering, task similarity, noisy streams, distribution shifts

Continual dependencies & synergies

{Co}de ML Mod{e/}

Model: architecture, inductive bias, discriminative/generative, functions, parameters

model extensions, task-specific parameter identification

Training: loss function, optimizer, hyperparameters, convergence

catastrophic forgetting, knowledge transfer or distillation, selective updates, online



The first in a chain of questions: can we transfer our models?



Early definition: lifelong ML

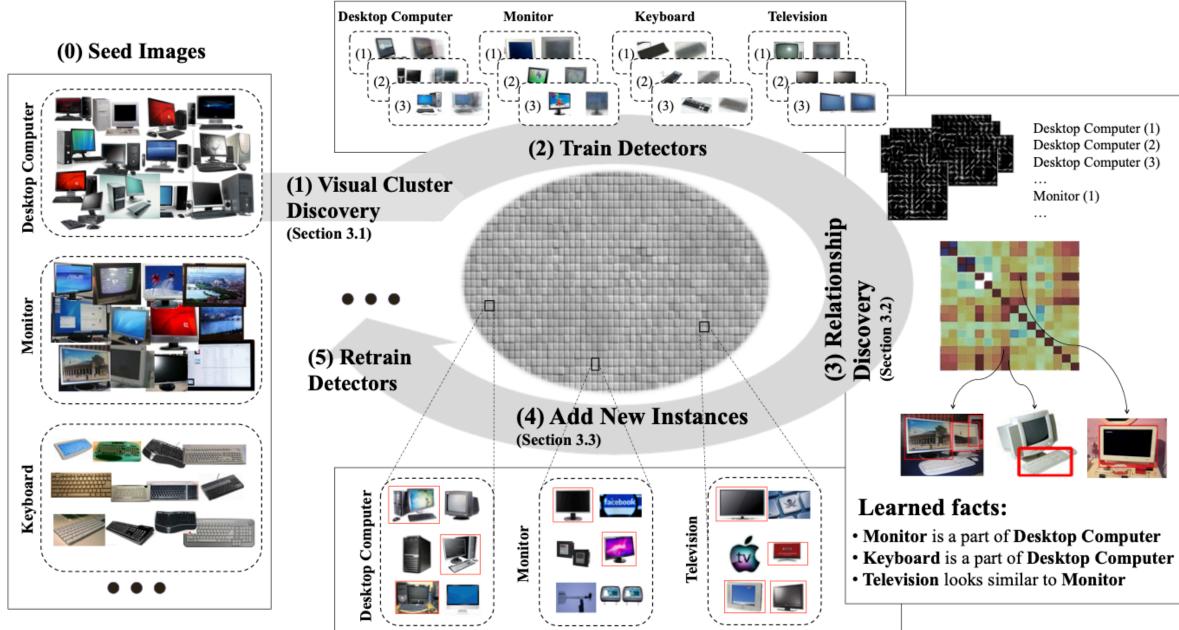
Definition - Lifelong Machine Learning - Thrun 1996: "The system has performed N tasks. When faced with the (N+1)th task, it uses the knowledge gained from the N tasks to help the (N+1)th task."

"Is Learning The n-th Thing Any Easier Than Learning the First?" (NeurIPS 1996) & "Explanation" based Neural Network Learning A Lifelong Learning Approach", Springer US, 1996



What is *knowledge* in a machine learning system?





"Towards an Architecture for Never-Ending Language Learning", Carlson et al, AAAI 2010 "NEIL: Extracting Visual Knowledge form Web Data", X. Chen et al, ICCV 2013 "Never-Ending Learning", T. Mitchell et al, AAAI 2015

Never-ending (language/image) learner

Knowledge is more than params

- (NELL) Ran 24/7 from 2010-2018
- Accumulated over 50 million candidate "beliefs" by reading the web
- Relational database
- Facts: barley is a grain
- Beliefs: sportUsesEquip (soccer, balls) ${ \bullet }$



Early definition: lifelong ML

Definition - Lifelong Machine Learning - Thrun 1996: "The system has performed N tasks. When faced with the (N+1)th task, it uses the knowledge gained from the N tasks to help the (N+1)th task."

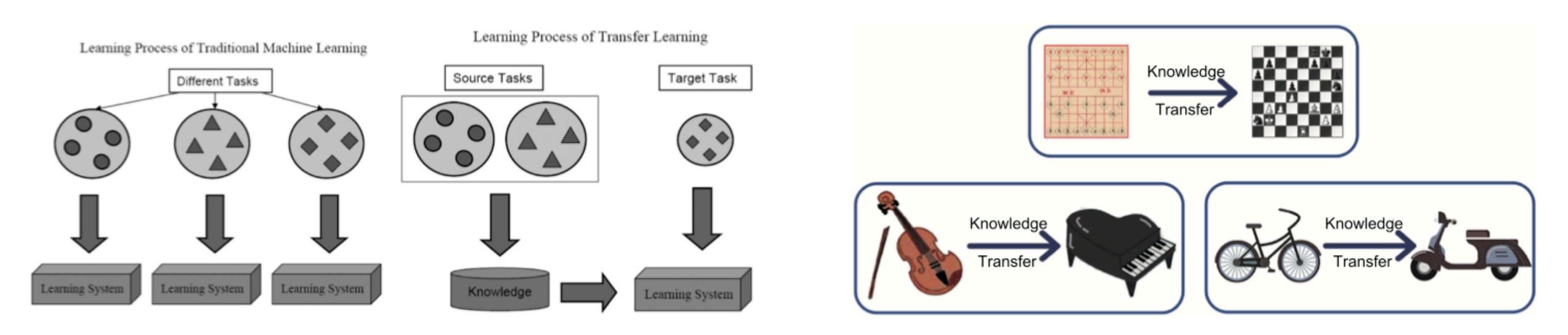
Is data accumulated? Stored?

- What are the ways to "help" the (N+1)th task?
- What is knowledge? What is a task?

"Is Learning The n-th Thing Any Easier Than Learning the First?" (NeurIPS 1996) & "Explanation based Neural Network Learning A Lifelong Learning Approach", Springer US, 1996



Transfer learning



"A Survey on Transfer Learning", Pan and Yang, IEEE Transactions on Knowledge & Data Engineering, 2010

model based on initial task(s) \rightarrow the essence of transfer learning

"A Comprehensive Survey on Transfer Learning", Zhuang et al, Proceedings of IEEE, 2020

"Help the (N+1th) task!": Assume that we already have "knowledge"/ a



What types of data shifts can you think of?





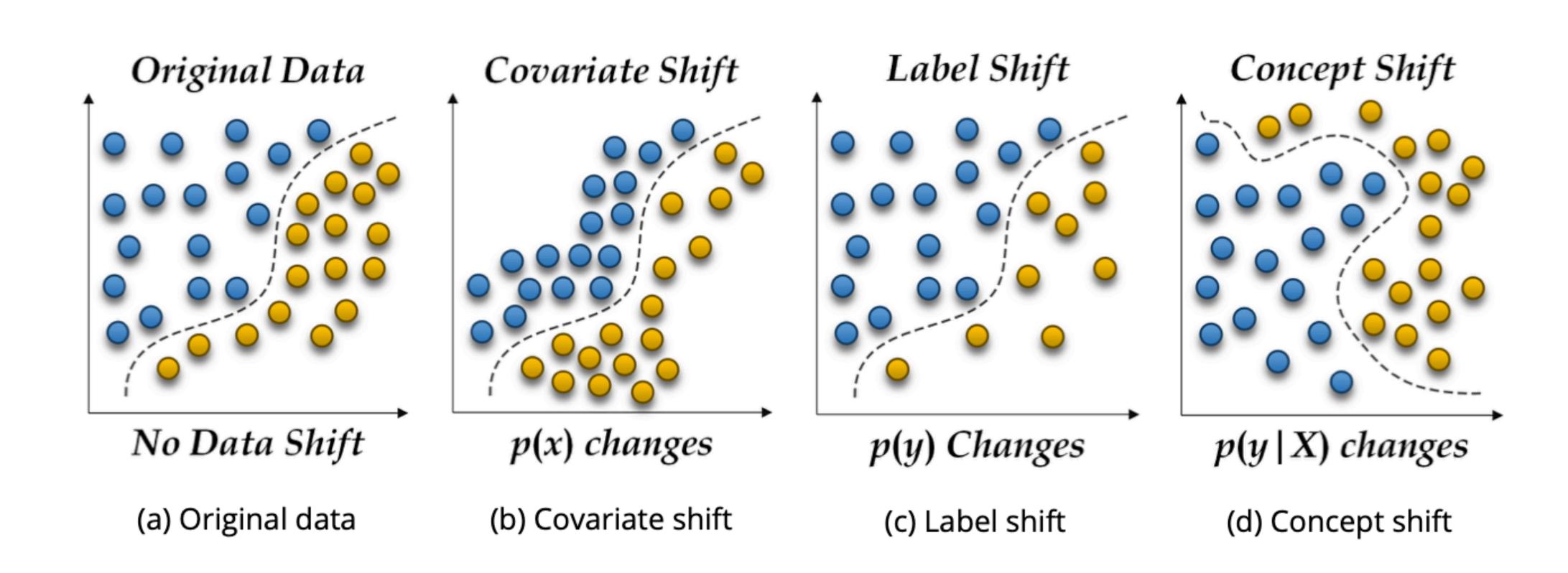


Figure from "Understanding Dataset Shift and Potential Remedies", Vector Institute Technical Report, 2021 See also: "Dataset Shift in Machine Learning" book, MIT Press 2009

Dataset shifts



Transfer learning: definition

Definition - Transfer Learning - Pan & Yang 2009: "Given a source domain D_S and learning task \mathcal{T}_S , a target domain D_T and $D_{S} \neq D_{T} \text{ or } \mathcal{T}_{S} \neq \mathcal{T}_{T}$."

- Domain D
- Task T
- Source S
- Target T

"A Survey on Transfer Learning", Pan & Yang, IEEE Transactions on Knowledge and Data Engineering 22(10), 2009

learning task \mathcal{T}_{T} , transfer learning aims to help improve the learning of the target predictive function $f_T(.)$ in D_T using the knowledge in D_S and \mathcal{T}_S , where



Transfer learning: definition

Definition - Domain & Task - Pan & Yang 2009: "Given a specific domain, $D = \{\mathcal{X}, p(x)\}$, a task consists of two components: a label space Y and an objective predictive function f() (denoted by $T = \{Y, f()\}$, which is not observed but can be learned from the training data, which consist of pairs $\{x^{(n)}, y^{(n)}\}$, where $x^{(n)} \in X$ and $y^{(n)} \in Y$."

- Task \mathcal{T} : find a function f() (to map to labels in the case of supervision)
- Where generally $\mathscr{X}_{S} \neq \mathscr{X}_{T}$ or $p_{S}(x) \neq p_{T}(x)$

"A Survey on Transfer Learning", Pan & Yang, IEEE Transactions on Knowledge and Data Engineering 22(10), 2009

• Domain D: a pair of data distribution p(x) and corresponding feature space \mathcal{X}





Transductive transfer

Definition - Transductive Transfer Learning - Pan & Yang 2009: "Given a source domain D_{S} and learning task \mathcal{T}_{S} , a target domain D_{T} and learning task \mathcal{T}_{T} , transductive transfer learning aims to help improve the learning of the target predictive function $f_T(.)$ in D_T using the knowledge in D_S and \mathcal{T}_{S} , where $D_{S} \neq D_{T}$ and $\mathcal{T}_{S} = \mathcal{T}_{T}$."

- Feature spaces between the source and target are different $\mathscr{X}_S \neq \mathscr{X}_T$

"A Survey on Transfer Learning", Pan & Yang, IEEE Transactions on Knowledge and Data Engineering 22(10), 2009

• Feature spaces between source and target are the same, but $p_S(x) \neq p_T(x)$ Frequently encountered as domain adaptation or sample selection bias





Inductive transfer

Definition - Inductive Transfer Learning - Pan & Yang 2009: "Given a source domain D_{S} and learning task \mathcal{T}_{S} , a target domain D_{T} and where $\mathcal{T}_{s} \neq \mathcal{T}_{T}$."

"A Survey on Transfer Learning", Pan & Yang, IEEE Transactions on Knowledge and Data Engineering 22(10), 2009

learning task \mathcal{T}_{T} , inductive transfer learning aims to help improve the learning of the target predictive function $f_T(.)$ in D_T using the knowledge in D_S and \mathcal{T}_S ,

(Labeled) data points are required to "induce" the target predictive function





What do you think are the central questions & measures of success for transfer learning?



(Some) central questions

- 1. What to transfer: some knowledge is domain or task specific or may be more general/ transferable
- 2. When to transfer: when does transfer help or when does it even hurt?
- 3. How to transfer: algorithms to actually include, transfer/combine knowledge

(Some) central objectives

- Improved loss/more accurate function in direct comparison to learning just on the target
- 2. Accelerate learning
- 3. Reduce data dependence (of target)



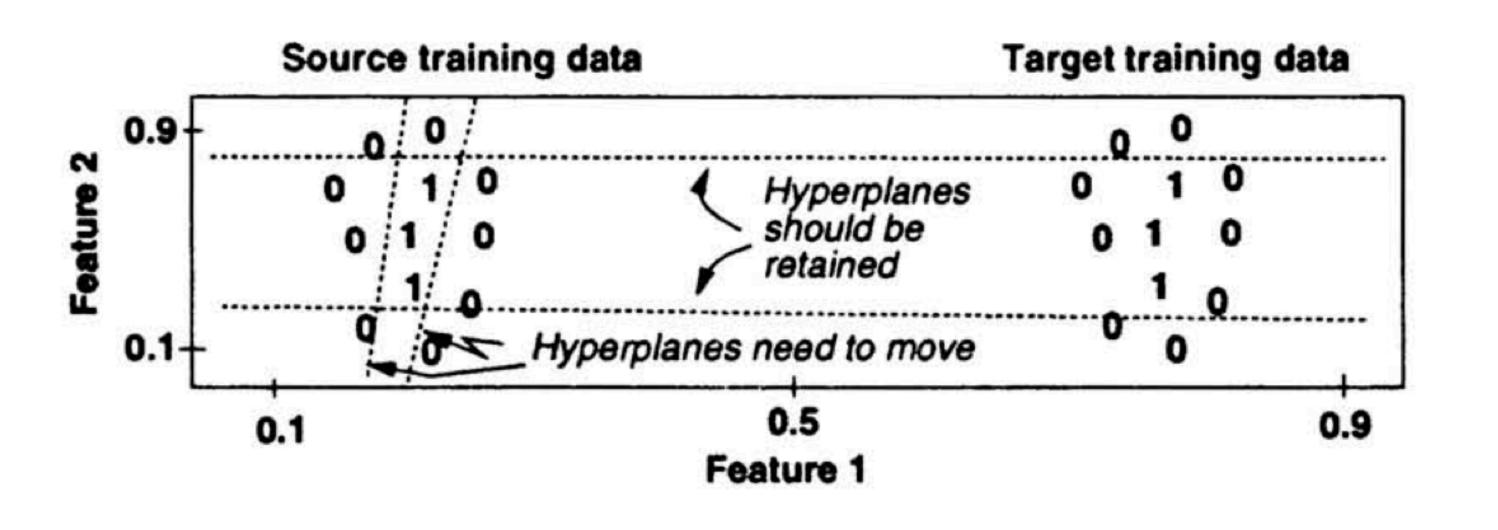




Examples of transfer learning approaches



Transductive transfer



"Discriminability-Based Transfer between Neural Networks", L. Y. Pratt, NeurIPS 1992

Early approaches transfer by identifying the amount that a specific hyperplane helps to separate the data into different classes (& then reweighting/reinitializing).

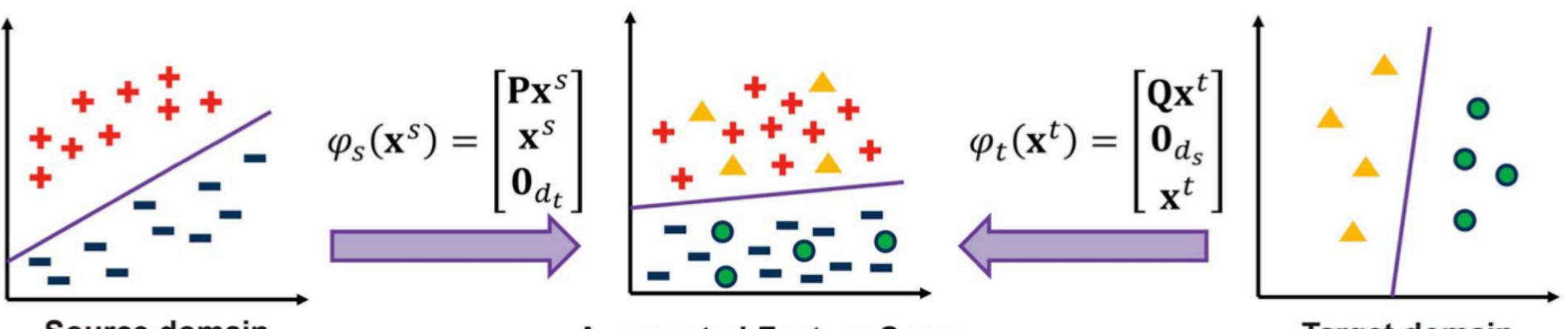






Transductive transfer

A domain adaptation example through feature transformation



Source domain

Augmented Feature Space

Fig. 1. Samples from different domains are represented by different features, where red crosses, blue strips, orange triangles and green circles denote source positive samples, source negative samples, target positive samples and target negative samples, respectively. By using two projection matrices P and Q, we transform the heterogenous samples from two domains into an augmented feature space.

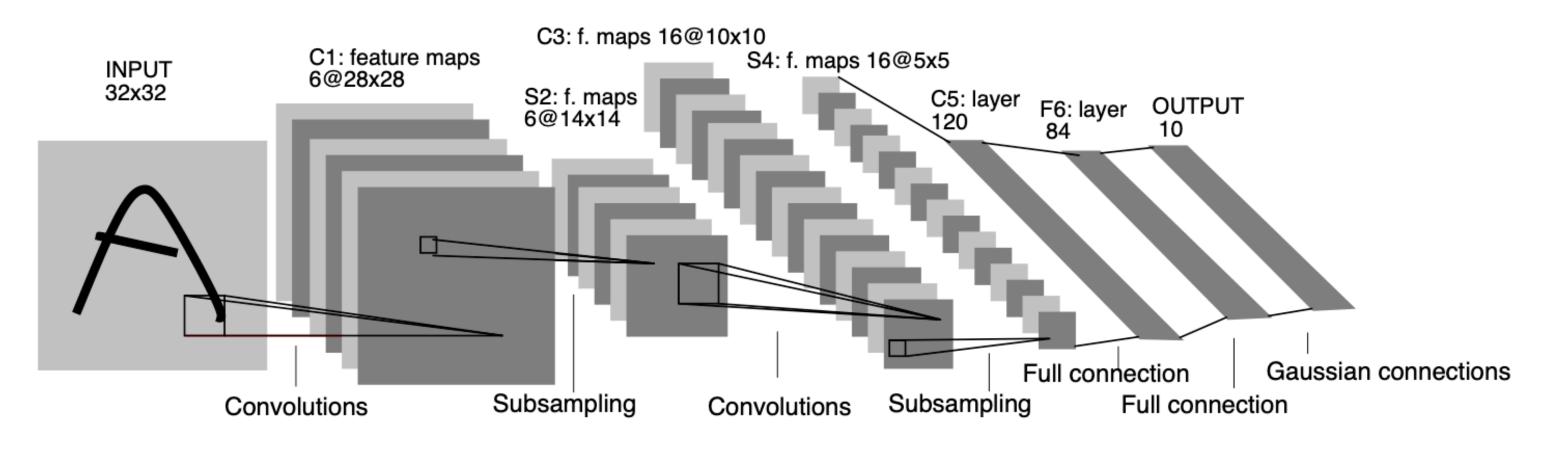
"Learning with augmented Features for Supervised and Semi-Supervised Heterogeneous Domain Adaptation", Wen Li et al, TPAMI 2014

Target domain

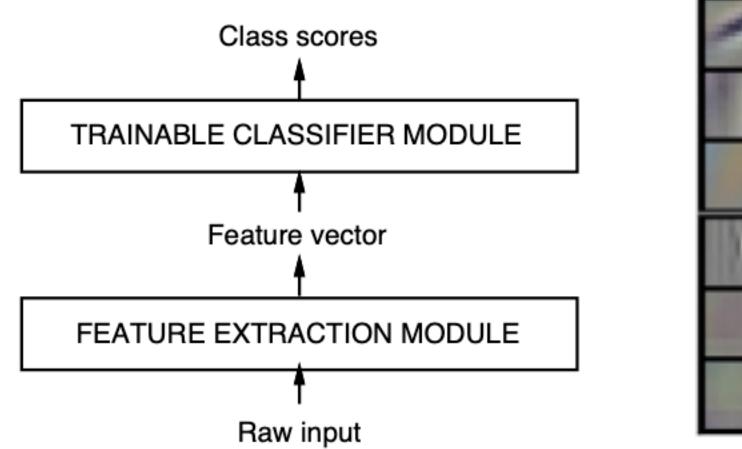


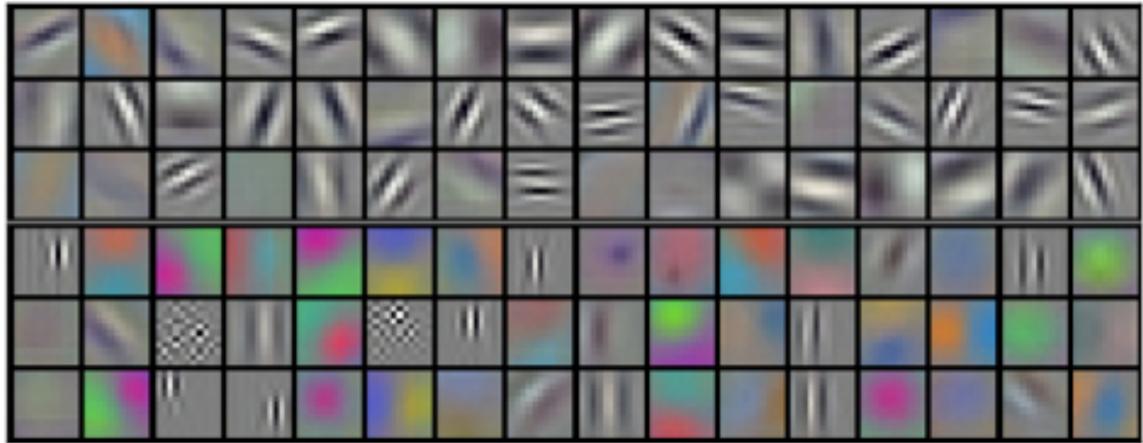


"Gradient-Based Learning Applied to Document Recognition", LeCun et al, Proceedings of the IEEE, 1998



Transfer learning in deep learning

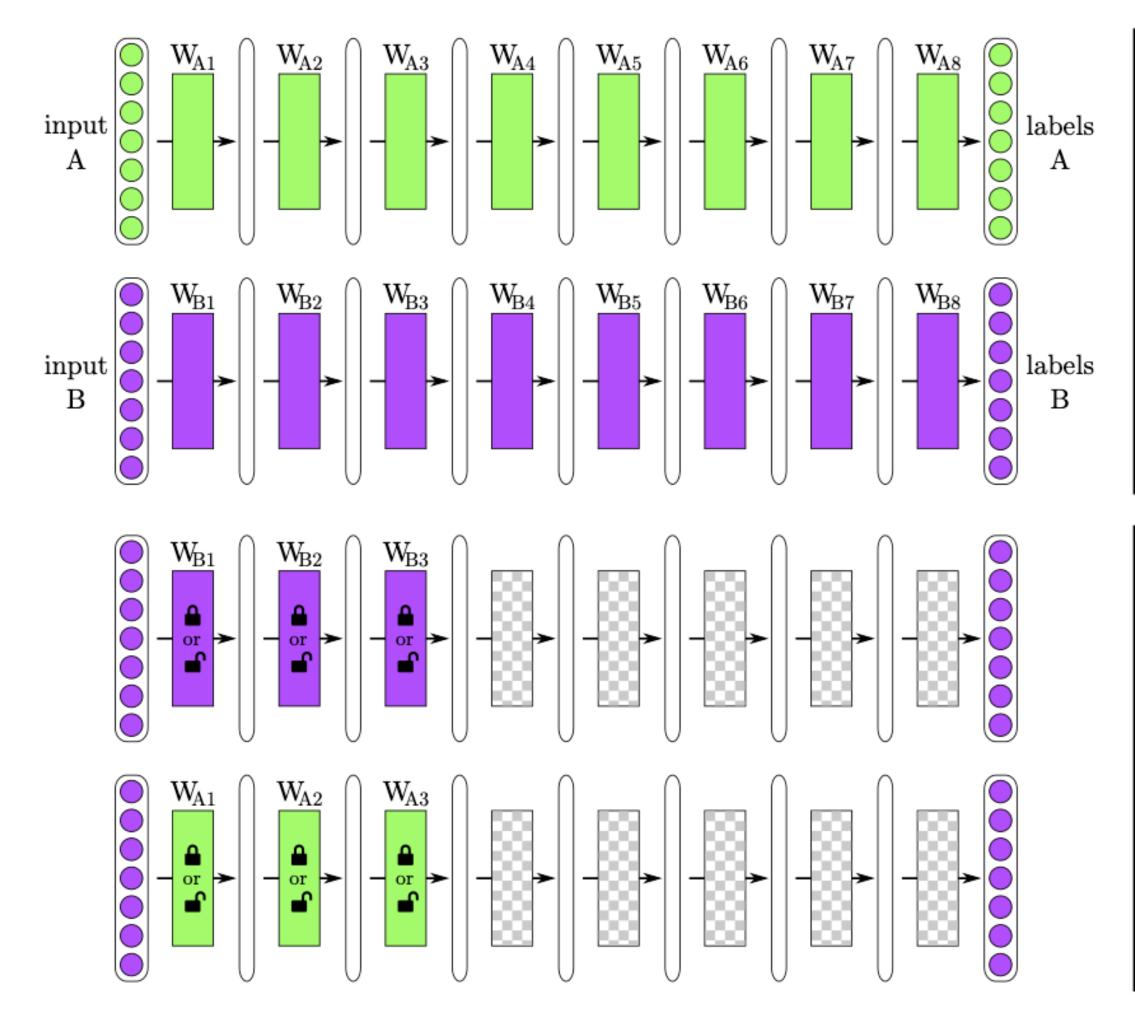




"ImageNet Classification with Deep Convolutional Neural Networks", Krizhevsky et al, NeurIPS 2012



(Inductive) ImageNet transfer



"How transferable are features in deep neural networks", Yosinski et al, NeurIPS 2014

- Split Imagenet into 2 sets of 500 baseA classes: A and B
- "Lock" different sets of layers/ baseBrepresentations & randomly initialize upper remaining layers B3B and Alternatively: continue training/ $B3B^+$ fine-tuning transferred layers A3B and $A3B^{+}$























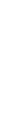


















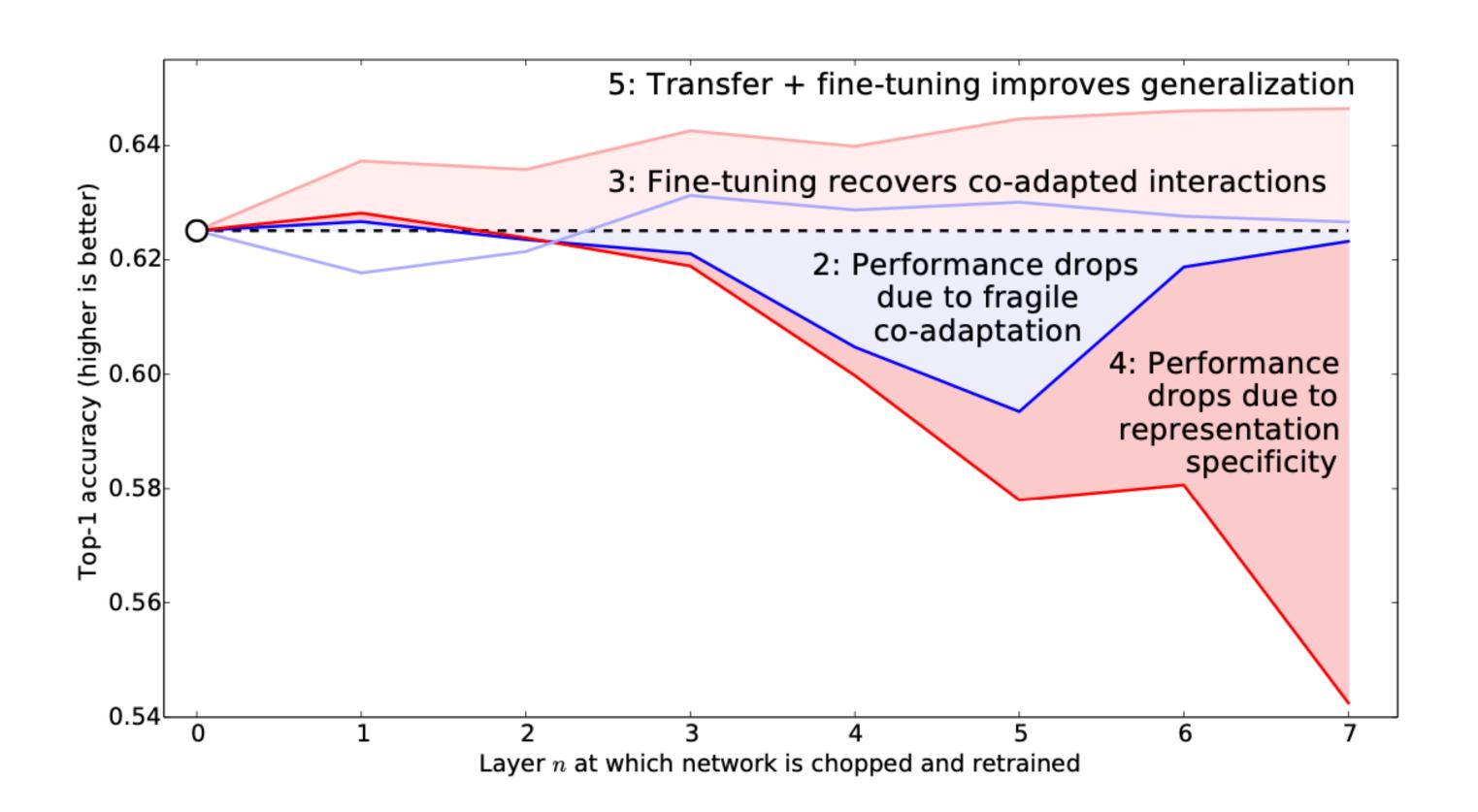








(Inductive) ImageNet transfer



"How transferable are features in deep neural networks", Yosinski et al, NeurIPS 2014

- 2. B-B: copied from B and frozen + random rest trained on B
- 3. B-B+: copied features are allowed to adapt/fine-tune
- 4. A-B: transfer from A to B with frozen layers
- 5. A-B+: transferring + fine-tuning from A to B

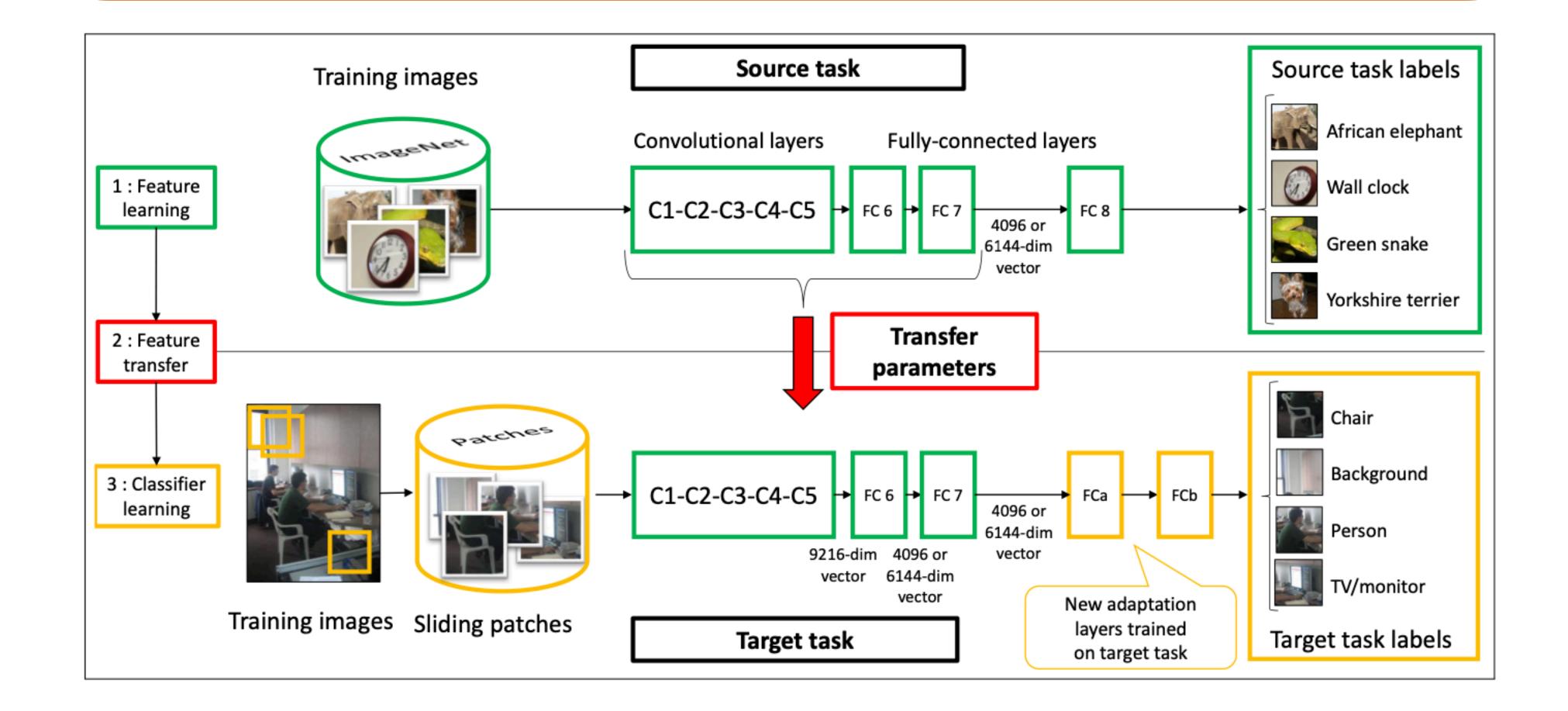








(Inductive) ImageNet transfer



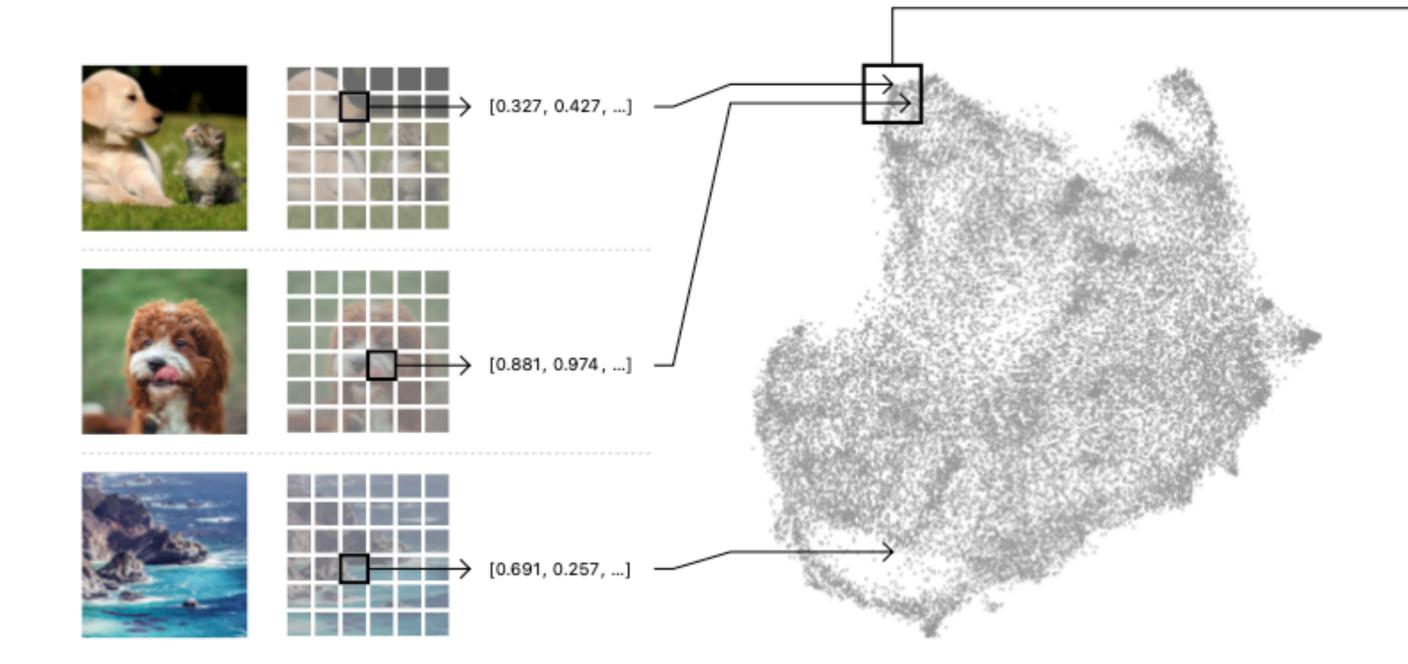
"Learning and Transferring Mid-Level Image Representations using Convolutional Neural Networks", Oquab et al, CVPR 2014



The role of embeddings: few-shot to one-shot transfer

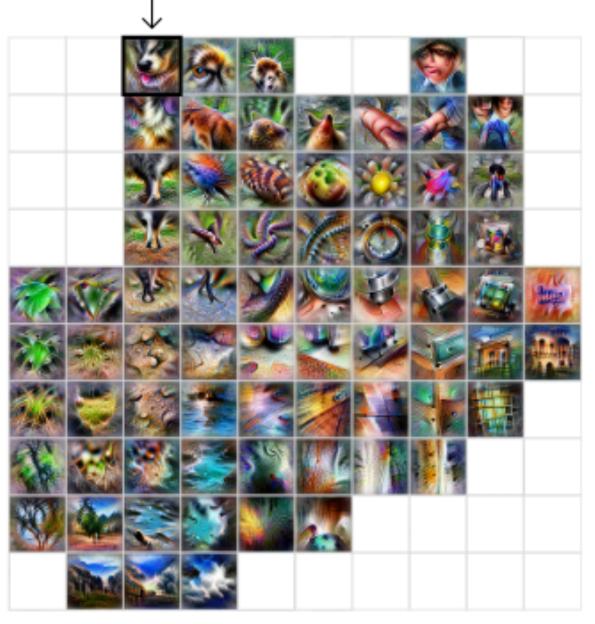


The role of embeddings



A randomized set of one million images is fed through the network, collecting one random spatial activation per image. The activations are fed through UMAP to reduce them to two dimensions. They are then plotted, with similar activations placed near each other.

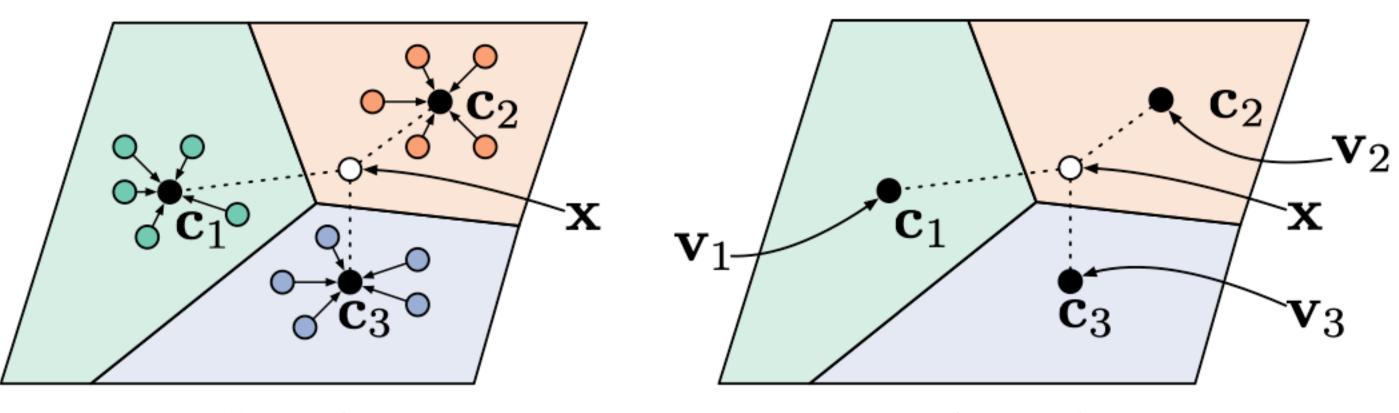
"Activation Atlas", Carter et al, Distill 2019



We then draw a grid and average the activations that fall within a cell and run feature inversion on the averaged activation. We also optionally size the grid cells according to the density of the number of activations that are averaged within.



Special cases of transfer: few-shot learning



(a) Few-shot

(b) Zero-shot

Figure 1: Prototypical networks in the few-shot and zero-shot scenarios. Left: Few-shot prototypes \mathbf{c}_k are computed as the mean of embedded support examples for each class. **Right**: Zero-shot prototypes c_k are produced by embedding class meta-data v_k . In either case, embedded query points are classified via a softmax over distances to class prototypes: $p_{\phi}(y = k | \mathbf{x}) \propto \exp(-d(f_{\phi}(\mathbf{x}), \mathbf{c}_k))$.

"Prototypical Networks for Few-shot Learning", Snell et al, NeurIPS 2017

See also "Object Classification from a Single Example Utilizing Class relevance Metrics", M. Fink, NeurIPS 2004 & "One-shot Learning of Object Categories", Fei-Fei et al, TPAMI 2006

Compute prototype c as the mean vector of each class with parametrized embedding function of a support set of labelled examples

Given a distance function d, classify according to softmax over distances to the prototypes in embedding space







Special cases of transfer: one-shot learning

function d if for any pair of examples belonging to the same class $d(x_1, x_1') \leq d(x_2, x_2') - \gamma$.

2. Learn a nearest neighbor classifier, where the classifier employs d

"Object Classification from a Single Example Utilizing Class relevance Metrics", M. Fink, NeurIPS 2004 See also "One-shot Learning of Object Categories", Fei-Fei et al, TPAMI 2006

"We say that a set of classes is $\gamma > 0$ separated with respect to a distance $\{(x_1, c), (x'_1, c)\}$, the distance $d(x_1, x'_1)$ is smaller than the distance between any pair of examples from different classes $\{(x_2, e), (x'_2, g)\}$ by at least γ :

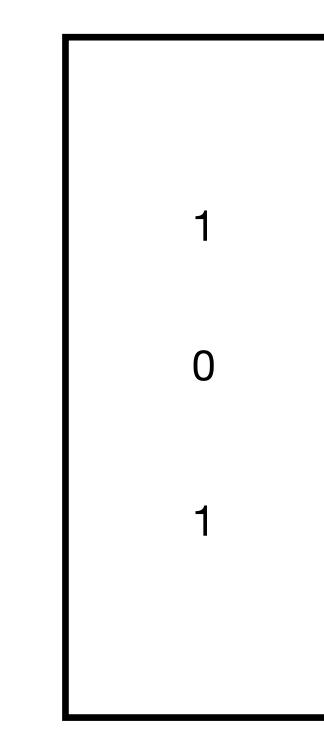
- 1. Learn from extra sample a distance function d that achieves γ separation



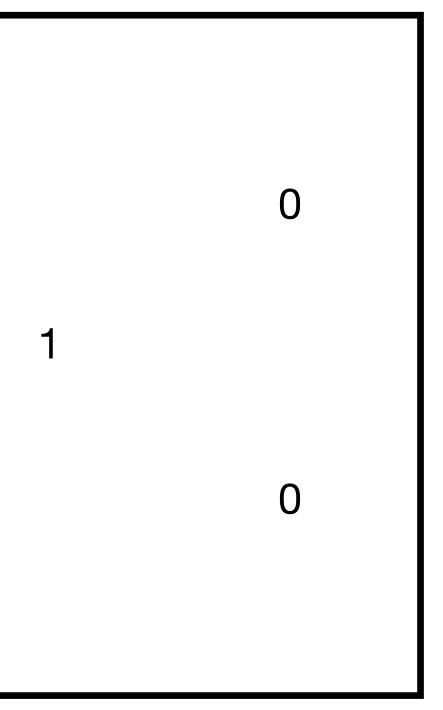
Why is transfer challenging?



How would you separate this data with a set of hyperplanes? (Try 3)

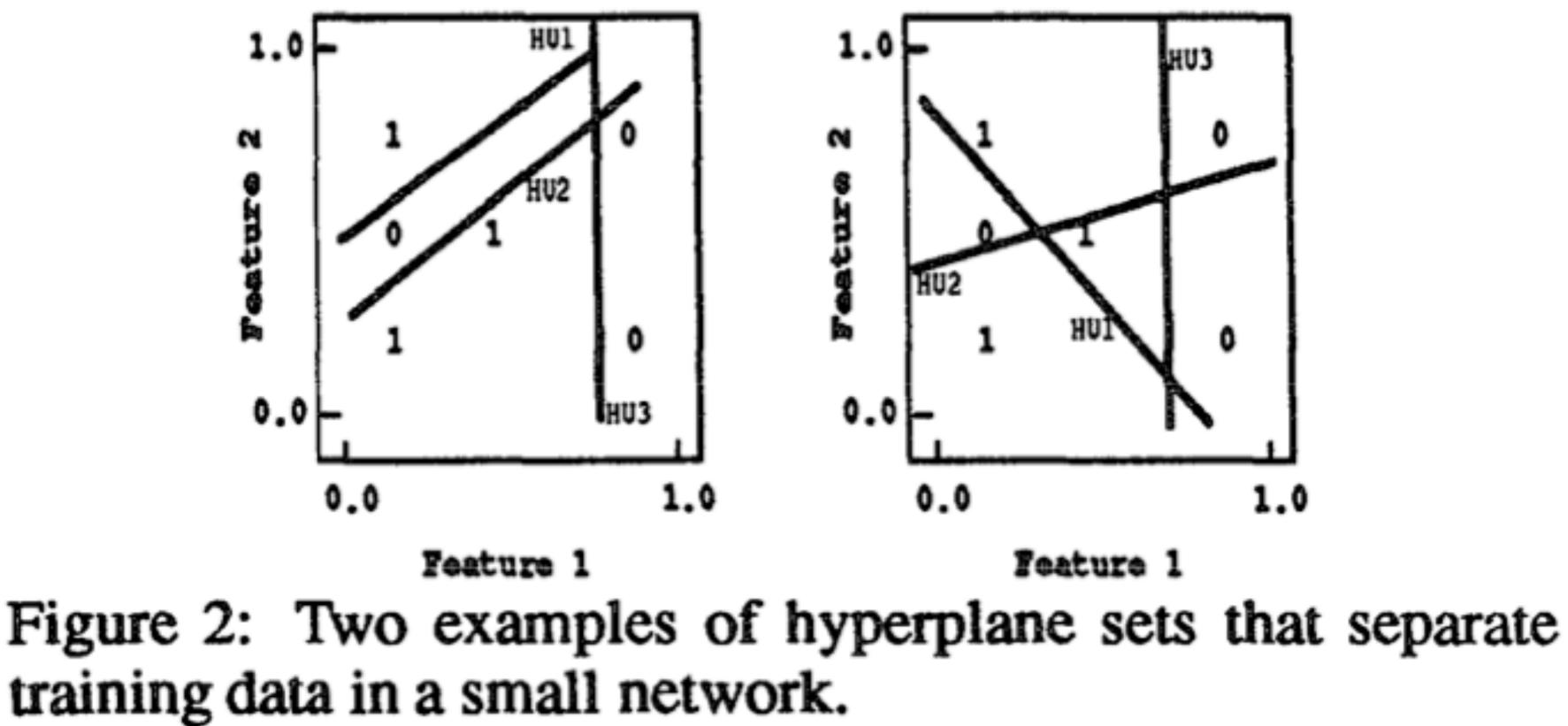




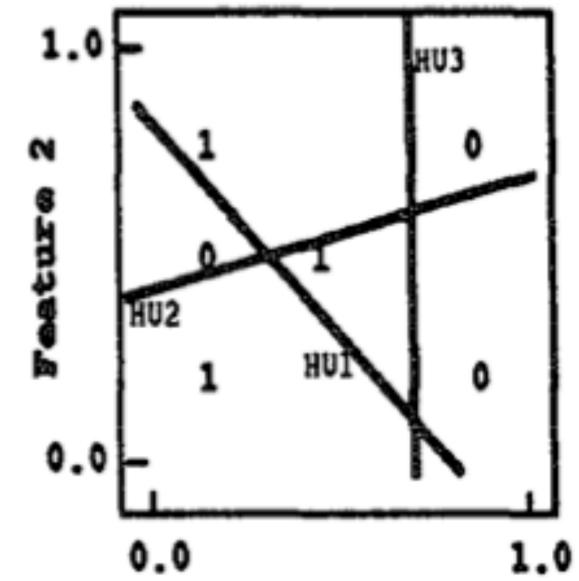




Transfer challenges



"Direct Transfer of Learned Information Among Neural Networks", L. Y. Pratt et al, AAAI 1991



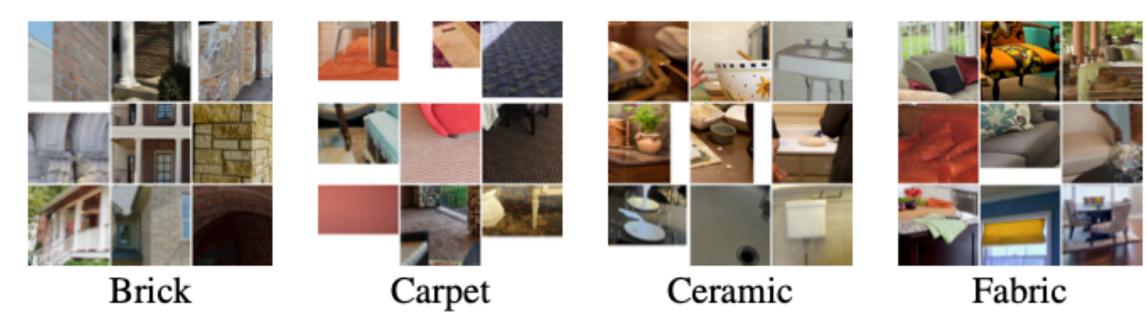


Not intuitive if transfer works





"Meta-learning Convolutional Neural Architectures for Multi-target Concrete Defect Classification with the Concrete Defect Bridge Image Dataset", Mundt et al, CVPR 2019



"Material Recognition in the Wild with the Materials in Context Database, CVPR 2015"

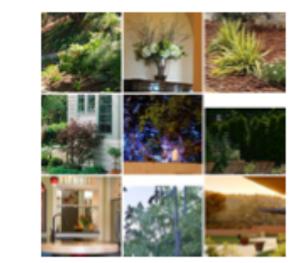
- Alexnet: 66.98 %
- VGG-A: 70.45%
- VGG-D: 70.61%

Transfer learning

Architecture

Source

Accuracy [%]



Foliage

Alexnet	ImageNet	62.87
VGG-A	ImageNet	66.35
VGG-D	ImageNet	65.56
Densenet-121	ImageNet	57.66
Alexnet	MINC	66.50
VGG-D	MINC	67.14

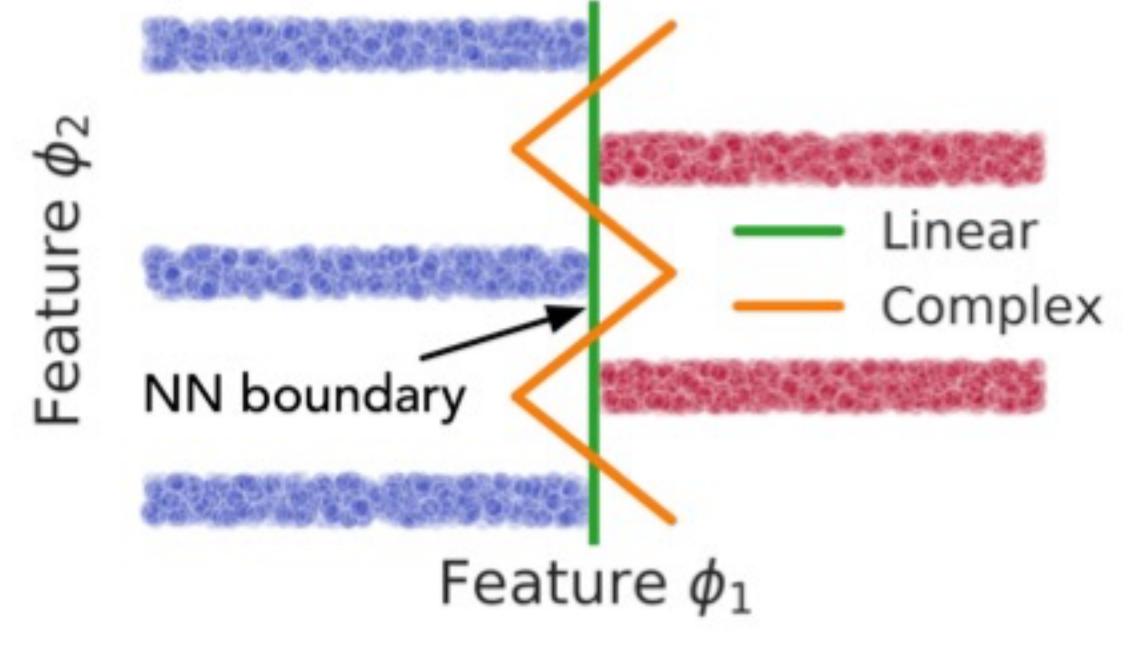




Simplicity bias

Representations are biased in ways that we don't anticipate: simplicity

Simplicity Bias in Neural Networks (NNs)



"The Pitfalls of Simplicity Bias in Neural Networks", Shah et al, NeurIPS 2020





Representations are biased in ways that we don't anticipate: texture bias





(a) Texture	image	(b) Conten	t in
81.4%	Indian elephant	71.1%	t
10.3%	indri	17.3%	g
8.2%	black swan	3.3%	S

"ImageNet-trained CNNS are biased towards texture", Geirhos et al, ICLR 2019

Representation Bias

mage tabby cat grey fox Siamese cat



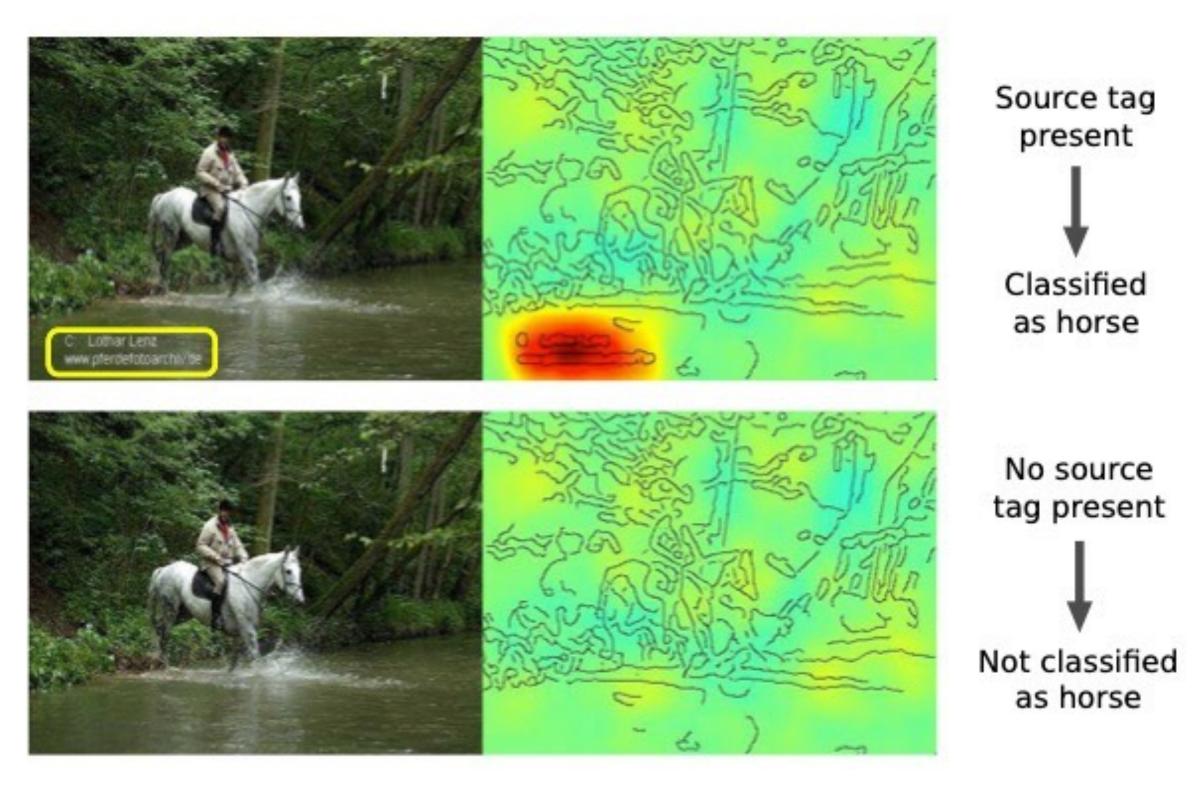
c) Texture-shape cue conflict		
63.9%	Indian elephant	
26.4%	indri	
9.6%	black swan	



Clever Hans predictors

Representations are biased in ways that we don't anticipate: confounders

Horse-picture from Pascal VOC data set

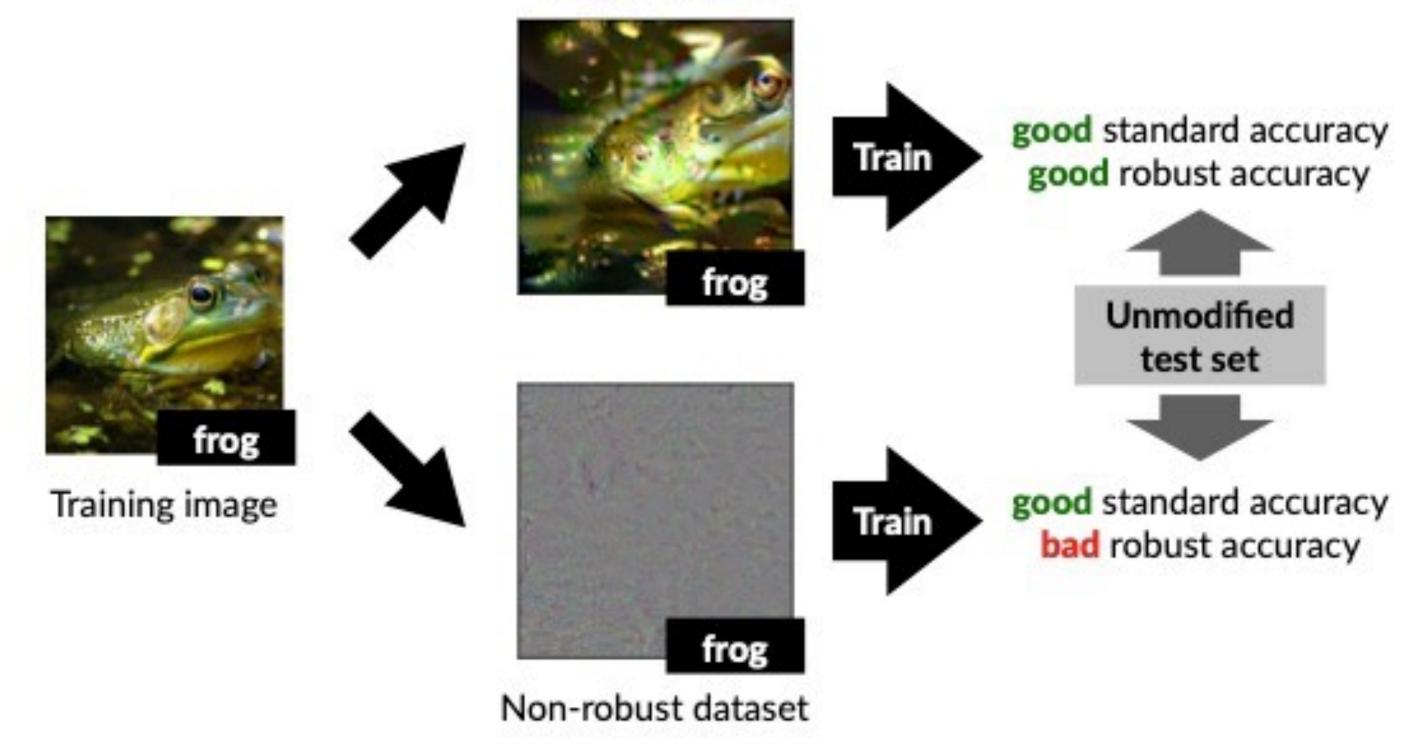


"Unmasking Clever Hans Predictors", Lapuschkin et al, Nature Communications 2019





Representations are biased in ways that we don't anticipate: adversarial



"Adversarial Examples are not Bugs, they are Features", Ilyas et al, NeurIPS 2019

Adversarial features

Robust dataset



Back to the earlier definition. It said "lifelong learning"! Not "transfer learning"



Early definition: lifelong ML

Definition - Lifelong Machine Learning - Thrun 1996: "The system has performed N tasks. When faced with the (N+1)th task, it uses the knowledge gained from the N tasks to help the (N+1)th task."

- We have looked primarily at (positive) forward transfer today
- Let us look at training & backward transfer (or forgetting) next

"Is Learning The n-th Thing Any Easier Than Learning the First?" (NeurIPS 1996) & "Explanation" based Neural Network Learning A Lifelong Learning Approach", Springer US, 1996



Later definition: lifelong ML

Definition - Lifelong Machine Learning - Chen & Liu 2017: performed a sequence of N learning tasks, $\mathcal{T}_1, \mathcal{T}_2, ..., \mathcal{T}_N$. These tasks can be of the same type or inconsistency checking, reasoning, and meta-mining of additional higher-level knowledge." "Lifelong Machine Learning", Chen & Liu, Morgan Claypool, 2017

- "Lifelong Machine Learning is a continuous learning process. At any time point, the learner
- different types and from the same domain or different domains. When faced with the (N+1)th task \mathcal{T}_{N+1} (which is called the new or current task) with its data D_{N+1} , the learner can leverage past knowledge in the knowledge base (KB) to help learn \mathcal{T}_{N+1} . The objective of LML is usually to optimize the performance on the new task \mathcal{T}_{N+1} , but it can optimize any task by treating the rest of the tasks as previous tasks. KB maintains the knowledge learned and accumulated from learning the previous task. After the completion of learning \mathcal{T}_{N+1} , KB is updated with the knowledge (e.g. intermediate as well as the final results) gained from learning \mathcal{T}_{N+1} . The updating can involve









