DS 4400

Machine Learning and Data Mining I
Spring 2021

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Announcements

- Final exam will start at 11:45am on Tuesday, April 6
  - It will be up for 6 hours
  - You can pick up a time frame of 2 hours
- Ethics of AI: Thu, April 8, by Kevin Mills
  - Over Zoom
  - Please fill in survey before class

Outline

- Final exam review
- Transfer learning
  - Using pre-trained models for new tasks
- Training Neural Networks
  - Backpropagation
  - Parameter Initialization
  - Stochastic Gradient Descent

Exam Review

DS-4400 Course objectives

- Become familiar with machine learning tasks
  - Supervised learning vs unsupervised learning
  - Classification vs Regression
- Study most well-known algorithms and understand their details
  - Regression (linear regression)
  - Classification (Naïve Bayes, decision trees, ensembles, neural networks)
- Learn to apply ML algorithms to real datasets
  - Using existing packages in R and Python
- Learn about security challenges of ML
  - Introduction to adversarial ML

What we covered

Ensembles

- Bagging
- Random forests
- Boosting
- AdaBoost

Deep learning

- Feed-forward Neural Nets
- Architectures
- Forward propagation

Linear classification

- Perceptron
- Logistic regression
- LDA
- SVM

Non-linear classification

- kNN
- Decision trees
- Naïve Bayes
- Kernel SVM

- Bias-variance tradeoff
- Metrics
- Evaluation
- Cross-validation
- Regularization
- Gradient Descent

Linear Regression

Linear algebra

Probability and statistics

Bias-Variance Tradeoff

- Why learning is hard
- What overfitting means
- How to avoid it
  - Regularization
  - Cross validation to report performance
- How different models improve generalization
  - Decision trees: limit tree depth
  - Ensembles randomize the training data in each model (bootstrap samples)
  - Neural networks use dropout or weight decay

ML Models

- Categorization
  - Is it a linear or non-linear?
  - Is it generative or discriminative?
  - Is it an ensemble?
- For each ML model
  - Understand how training is done
  - Take a small example and train a model
  - Once you have a model know how to evaluate a point and generate a prediction
    - Example: predict output by Naïve Bayes, decision tree, SVM, or neural network

Naïve Bayes Classifier

- For each class label k
  1. Estimate prior $\pi_k = P[Y = k]$ from the data
  2. For each value v of attribute X_j
     - Estimate $\mathrm{P}[X_j = v | Y = k]$

- Classify a new point via:

$$h(\mathbf{x}) = \arg\max_{y_k} \log P(Y = k) + \sum_{j=1}^{d} \log P(X_j = x_j \mid Y = k)$$

Learning Decision Trees

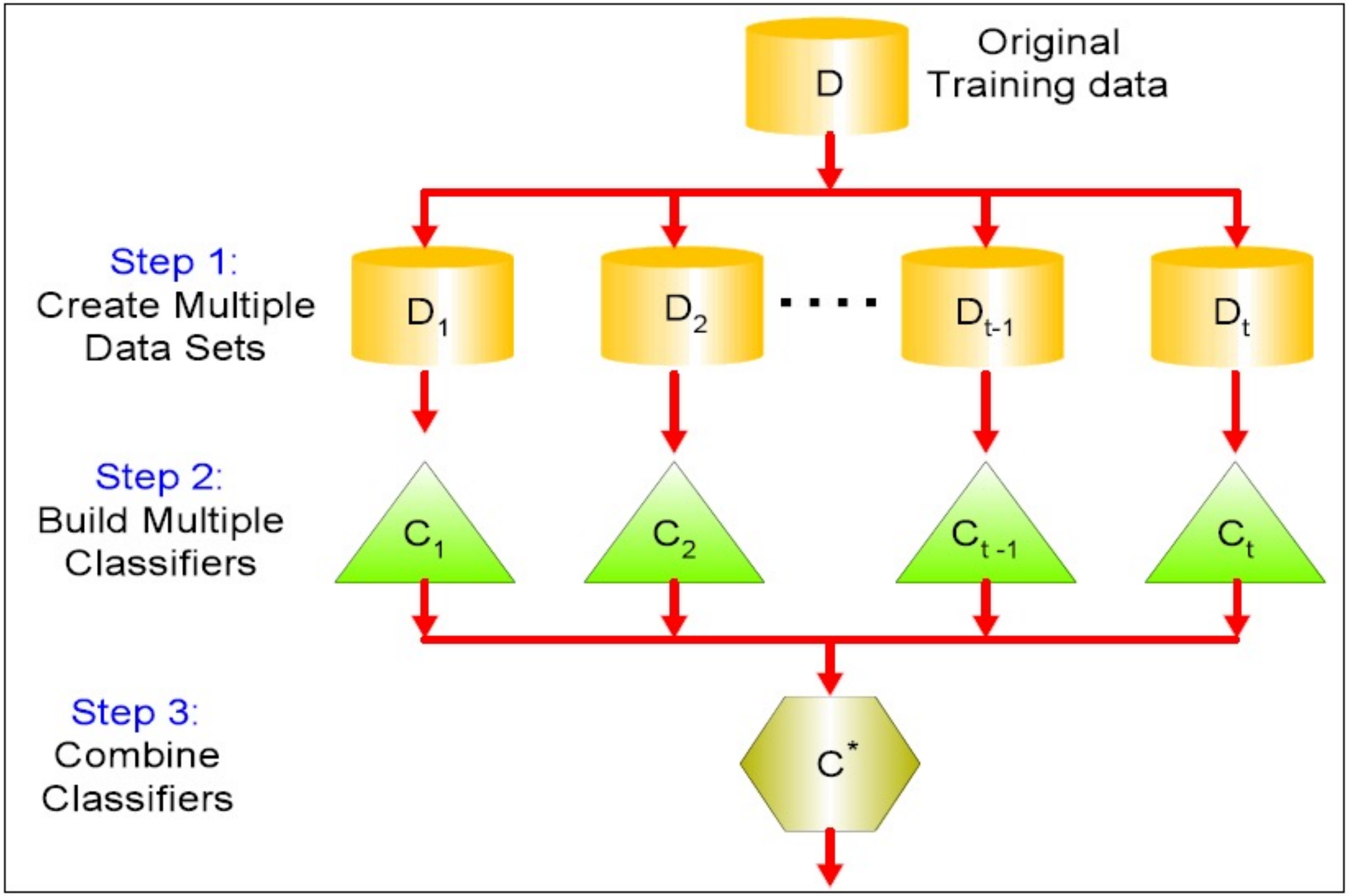
- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

- Recurse

Information Gain reduces uncertainty on Y
Can use Gini index

Bagging



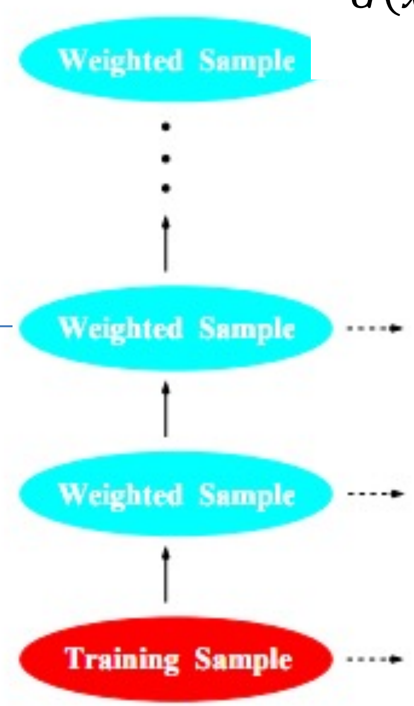
Majority Votes

Boosting

$$G(x) = sign(\sum_{i=1}^{T} \beta_t h_t(x))$$

Better classifiers will get higher weights

- Mis-classified examples get higher weights
- Correct examples get lower weights



$h_3(x)$

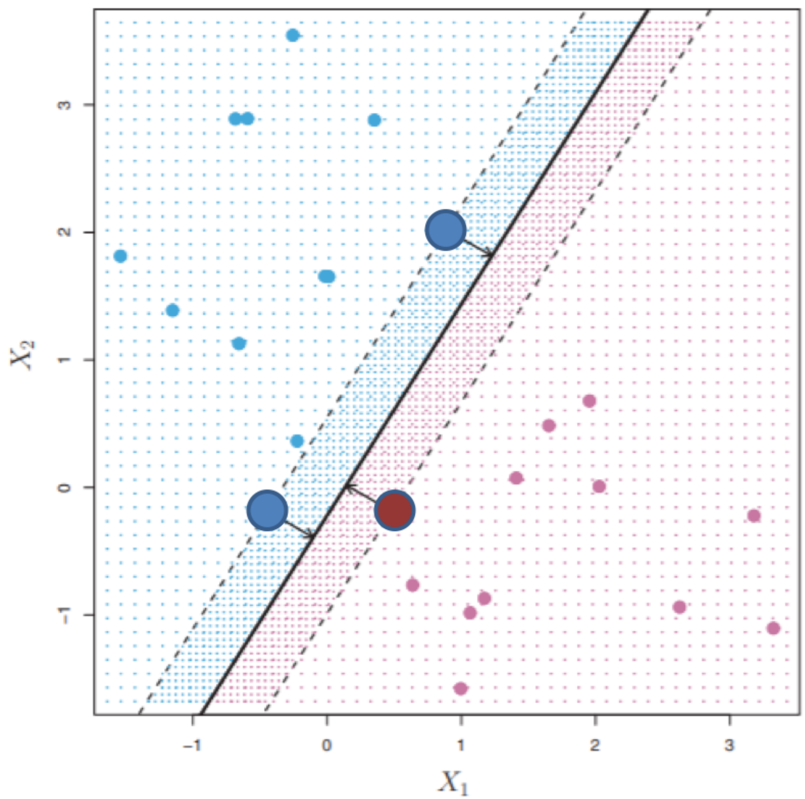
$h_2(x)$

$h_1(x)$

Uniform weights

FIGURE 10.1. *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

Support Vector Machines



- Support vectors = points “closest” to hyperplane
- Linear SVM: maximum margin
- Kernel SVM: radial basis, polynomial

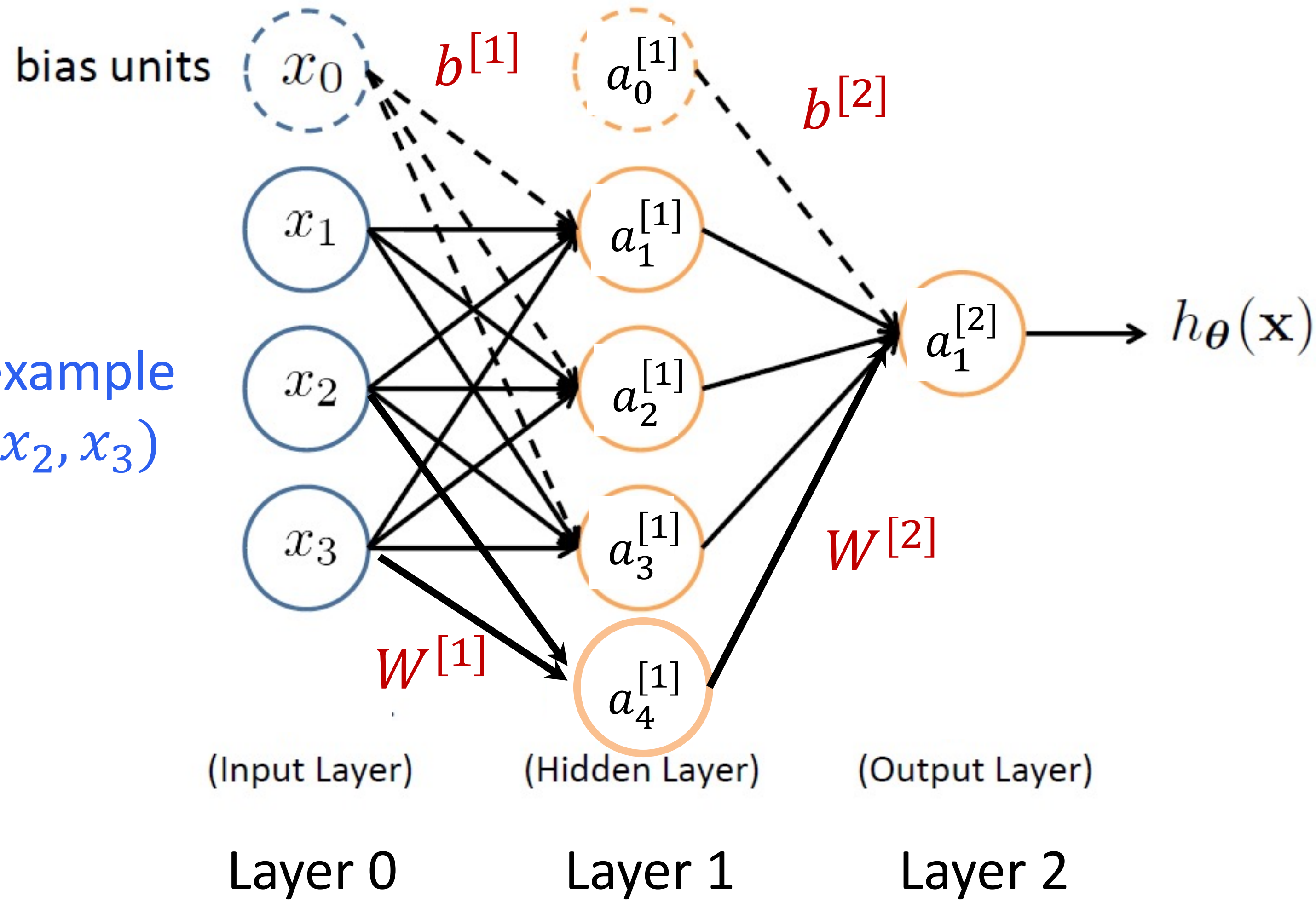
Online Perceptron

Let $\theta \leftarrow [0,0,\ldots,0]$
Repeat:
    Receive training example (x_i, y_i)
    If $y_i \theta^T x_i \leq 0$ // prediction is incorrect
        $\theta \leftarrow \theta + y_i\, x_i$
Until stopping condition

Online learning – the learning mode where the model update is performed each time a single observation is received

Batch learning – the learning mode where the model update is performed after observing the entire training set

Feed-Forward Neural Network

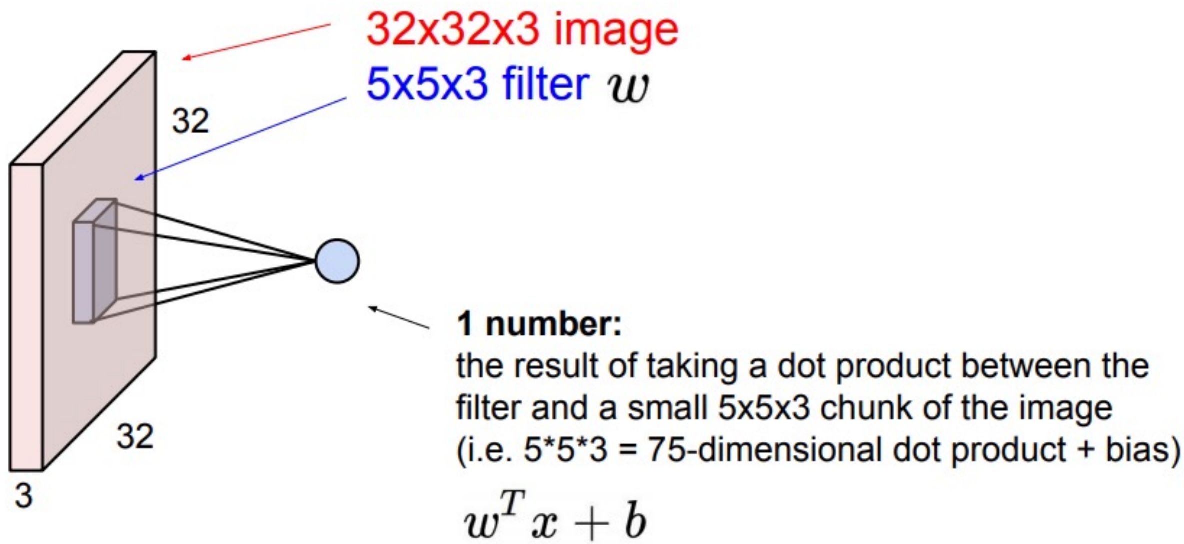


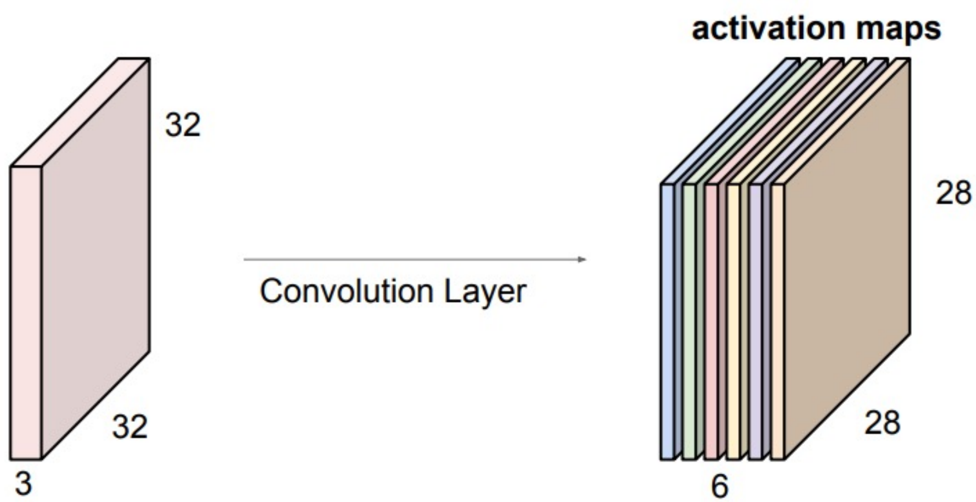
Training example
$x = (x_1, x_2, x_3)$

No cycles

$\theta = (b^{[1]}, W^{[1]}, b^{[2]}, W^{[2]})$

Convolution Layer





When to use each model

- Assumptions:
  – Naïve Bayes assumes conditional independence between features given class
- Linear models work well for linearly separable data
  – SVM results in linear model of max margin
  – Logistic regression estimates a probability
- Decision trees work well for categorical data
- Ensembles are powerful models
  – Need a lot of training data available
  – Reduce variance of single models

Comparing classifiers

Algorithm	Interpretable	Model size	Predictive accuracy	Training time	Testing time
Logistic regression	High	Small	Lower	Low	Low
kNN	Medium	Large	Lower	No training	High
LDA	Medium	Small	Lower	Low	Low
Decision trees	High	Medium	Lower	Medium	Low
Ensembles	Low	Large	High	High	High
Naïve Bayes	Medium	Small	Lower	Medium	Low
SVM	Medium	Small	Lower	Medium	Low
Neural Networks	Low	Large	High	High	Low

Type I: Conceptual

- Example 1: Describe difference between generative and discriminative models
- Example 2: Given some dataset with certain properties, what is the best model
- Example 3: Provide advantages and disadvantages, and compare the following:
  - Linear classifiers compared to non-linear ones
  - Naïve Bayes versus LDA
  - FFNNs versus CNNs
- Important: write short answers

Type II: Computational

- Example 1: Given a small dataset, train a particular ML model
  - E.g., decision tree, Naïve Bayes, etc.
  - Evaluate model on some small training and testing data
- Example 2: Given a particular model, describe the training process and count the number of parameters
- Example 3: Compute different metrics: true positives, false positives, precision, recall, accuracy, error

Type III: Constructive

- Example 1: Given a function, construct a FFNN to compute it

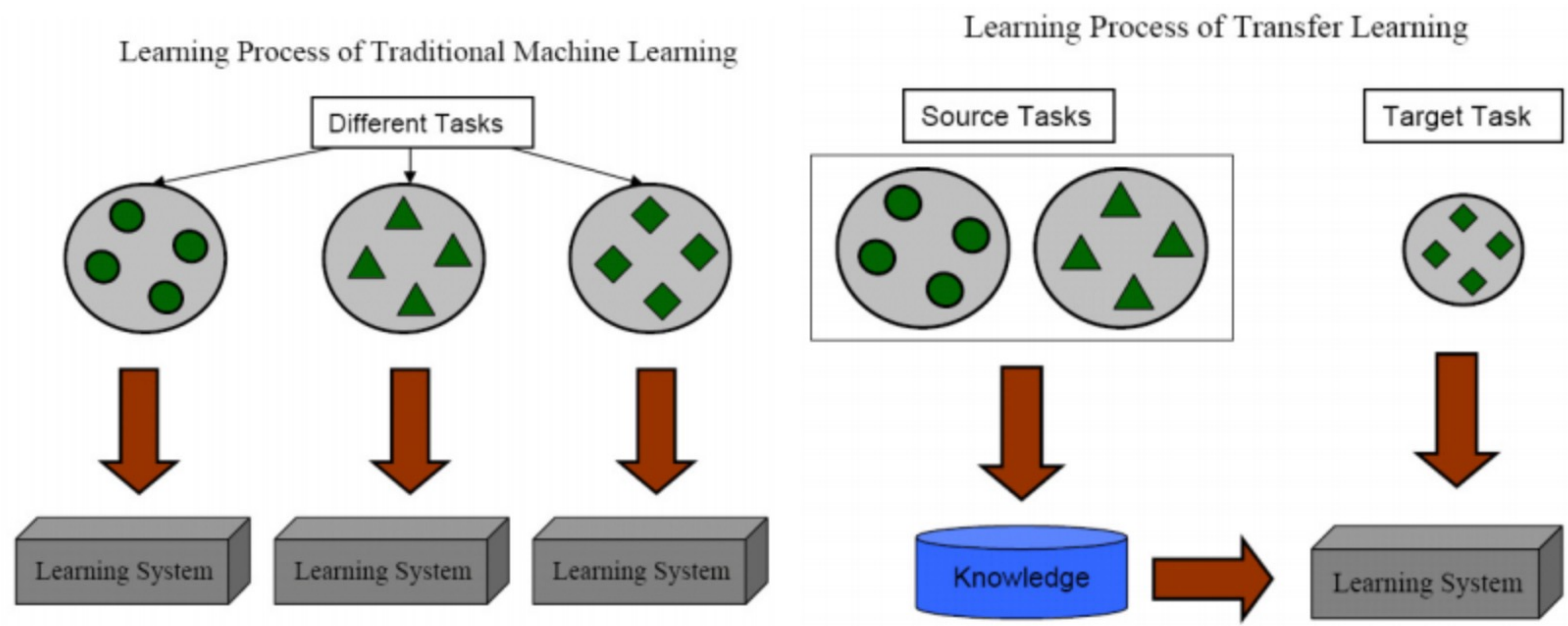
- Example 2: Construct a small NN architecture for a particular problem

- Example 3: Given dataset, which features to select for particular prediction problem

Transfer Learning

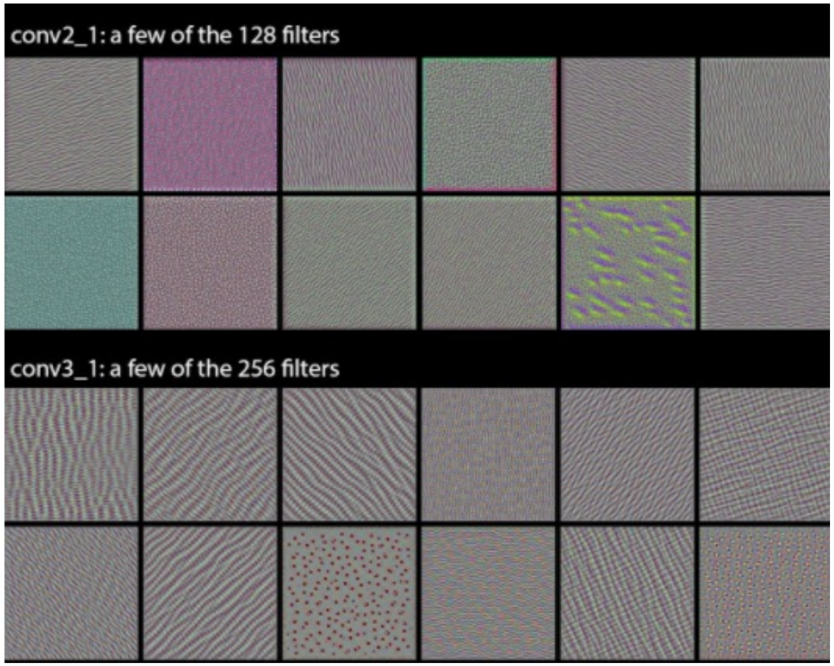
- Improvement of learning in a **new** task through the *transfer of knowledge* from a **related** task that has already been learned.
- Motivation: Reuse representations learned by expensive training procedures that cannot be easily replicated
  - Image classification on ImageNet is very expensive (VGG-16: 138 million, ResNet 50: 23 million parameters)
  - Generative language models very large (BERT: 110 million, GPT-2: 1.5 billion, GPT-3: 175 billion parameters)
- Two major strategies
  - Pretrained Neural Network as fixed feature extractor
  - Fine-tuning the Neural Network

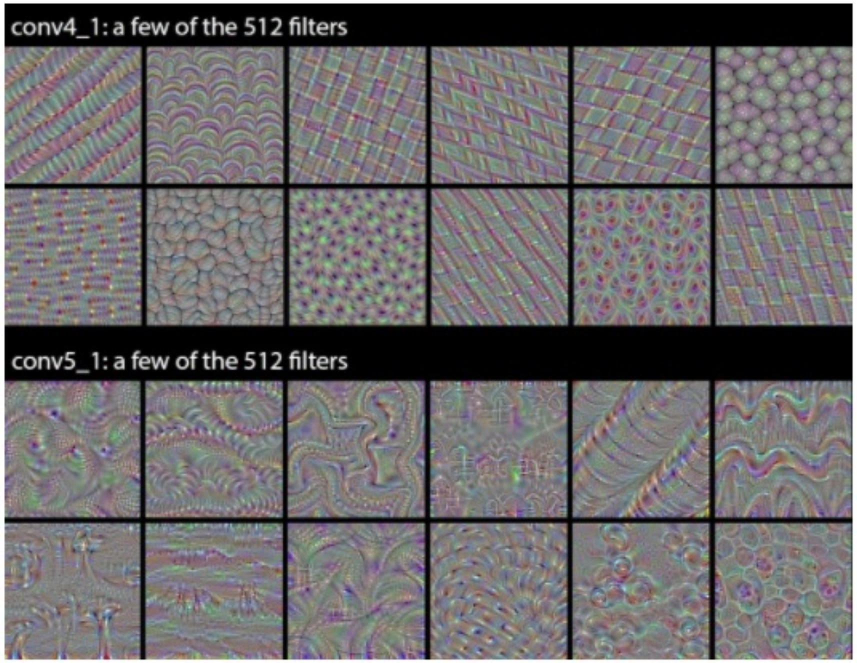
Transfer Learning



(a) Traditional Machine Learning (b) Transfer Learning

Visualizing Filters in VGG 16





- First layers: general learners
  - Low level notion of edges

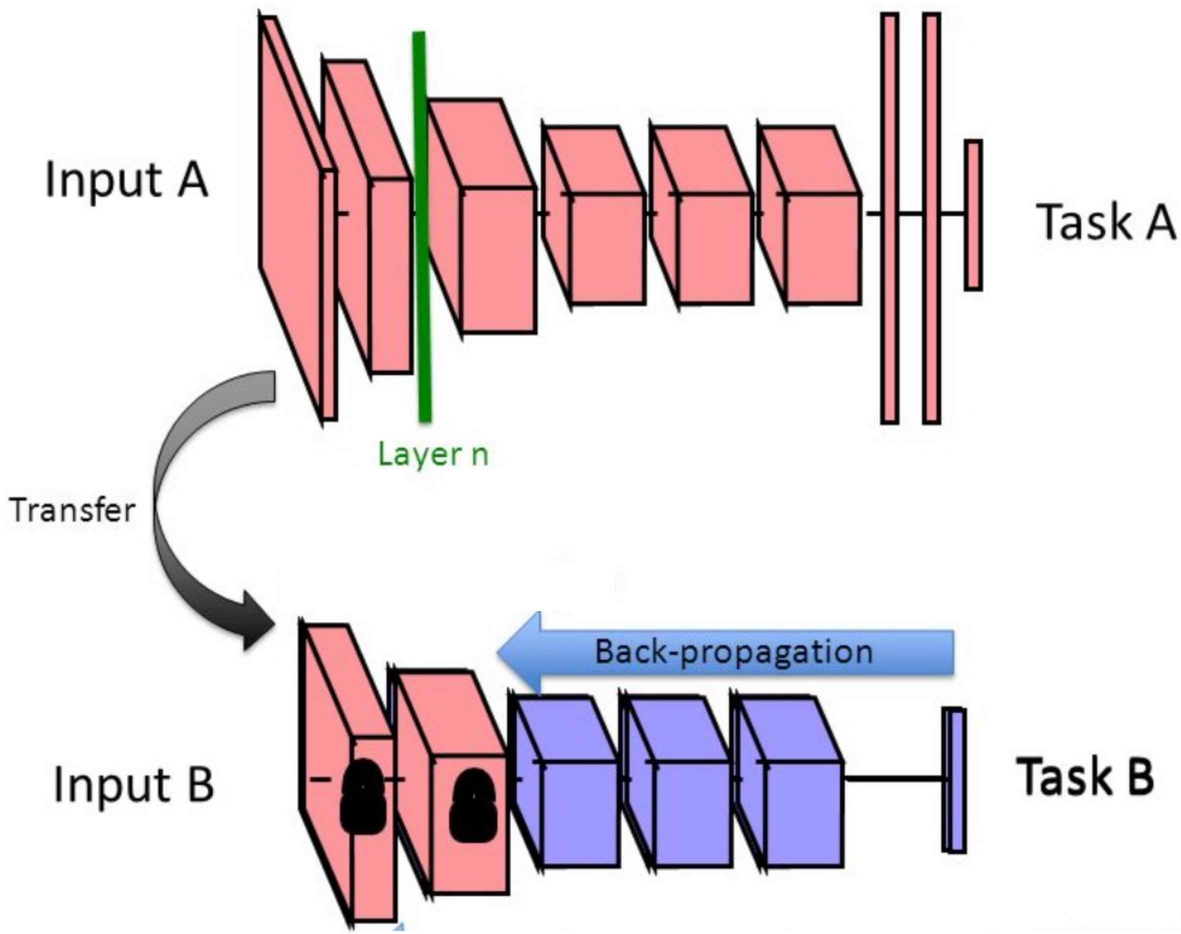
- Last layers: specific learners
  - High-level features: eyes, objects

Methods for Transfer Learning

- Use a pre-trained model
  - https://modelzoo.co/

1. Use Convolutional Nets as Feature Extractor
   - Take a ConvNet pretrained on ImageNet
   - Remove the last fully-connected layer
   - Train the last layer on new dataset (usually a linear classifier such as logistic regression or softmax)
2. Fine-tuning
   - Decide to freeze first n layers
   - Train the remaining layers and stop backpropagation at layer n
   - In the limit fine-tuning can be applied to all layers

Transfer Learning in NN: Freeze Layers



How to do Transfer Learning

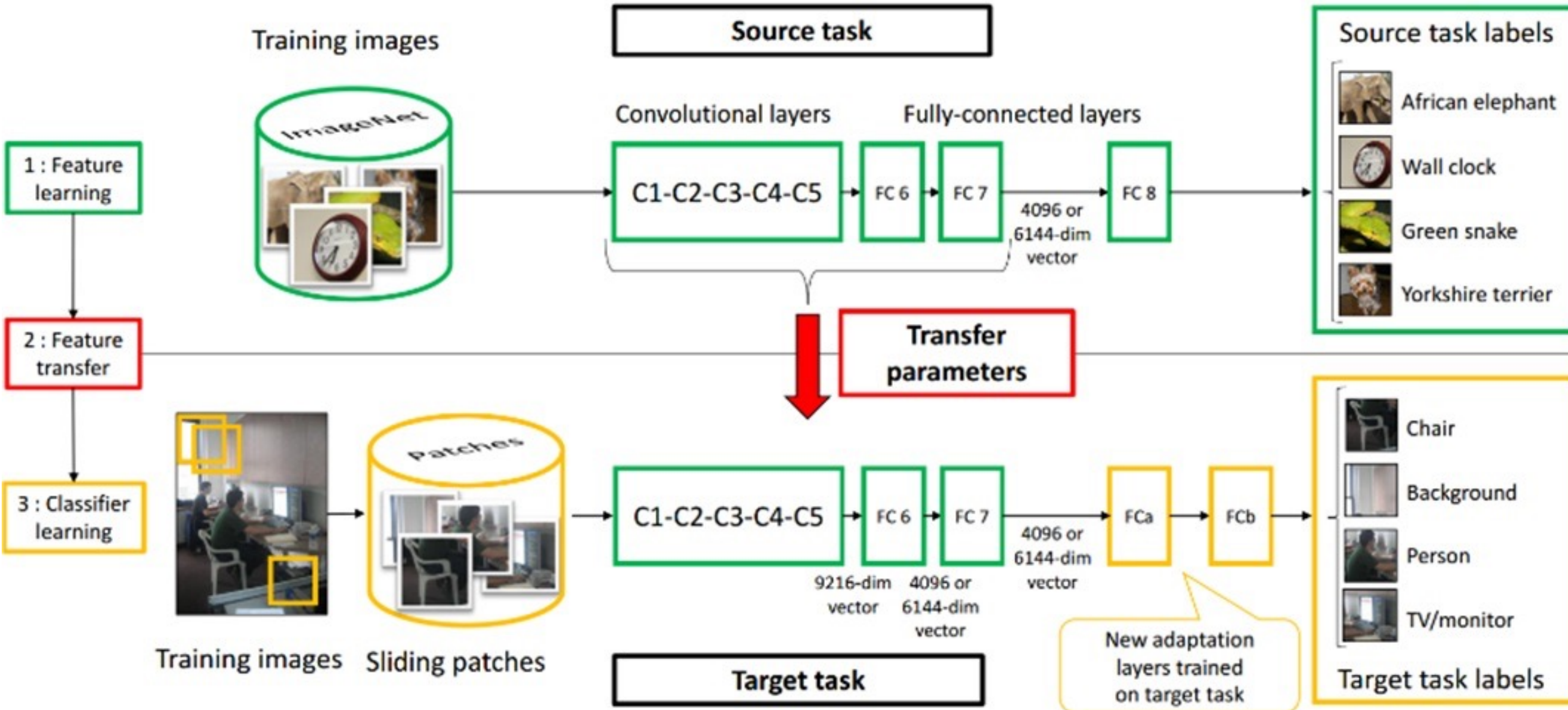
Dataset size	Dataset similarity	Recommendation
Large	Very different	Train model B from scratch, initialize weights from model A
Large	Similar	OK to fine-tune (less likely to overfit)
Small	Very different	Train classifier using the earlier layers (later layers won't help much)
Small	Similar	Don't fine-tune (overfitting). Train a linear classifier

Learning Rates

- Training linear classifier: typical learning rate
- Fine-tuning: use smaller learning rate to avoid distorting the existing weights

Transfer Learning Applications

- Image classification (most common): learn new image classes
- Text sentiment classification
- Text translation to new languages
- Speaker adaptation in speech recognition
- Question answering



Learning and Transferring Mid-Level Image Representations using Convolutional Neural Networks [Oquab et al. CVPR 2014]

Acknowledgements

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