Lecture 13: Semi-Supervised and Active Learning

COMP90049

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Semi-supervised Learning

Where we're at so far

- To date, we have talked a lot about **supervised learning** — where we have assumed (fully) labelled training data
- We also talked about **unsupervised learning** — where we have (fully) unlabelled training data
- What if we had a small amount of labelled training data, and lots of unlabelled training data?
- What if we had a small amount of labelled training data and a limited budget to label more training data?
- What if we can 'warm-start' our model by training it first on a (related) unsupervised task and then on the supervised target task?

Why bother? (I)

“Most Research in Deep Learning is a Total Waste of Time”

Watch this short clip (in your own time) to get the gist of active learning (and some pieces of wisdom about scientific resarch vs. solving the world’s real problems!)

https://www.youtube.com/watch?v=Bi7f1JSSlh8

Human learning

- humans can use from labelled and unlabelled data, e.g., concept learning in children: x =animal, y =concept (e.g., dog)
- You point to a brown animal and say “dog!”
- Children also observe animals by themselves

Why bother? (II)

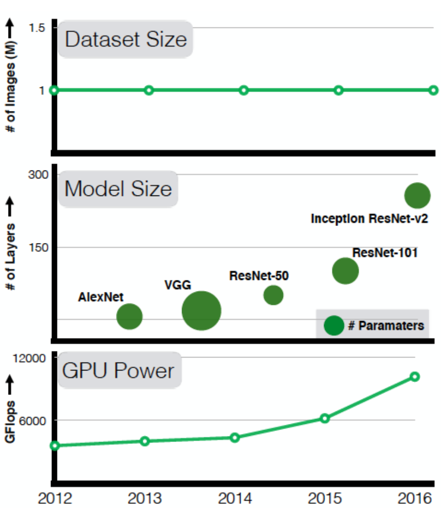
- “Simple models and a lot of data trump more elaborate models based on less data!”[1]
- (Labelled) data is a bottleneck for machine learning
  - labels may require human experts
  - labels may require special devices
- unlabelled data is often cheap and available in large quantity

[1] Halevy, Norvig, & Pereira (2009) “The Unreasonable Effectiveness of Data”

Example I

Image classification - Sun, Shrivastava, Singh, & Gupta (2017)

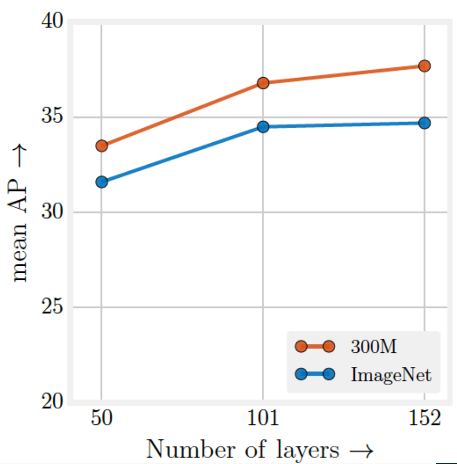
- model depth has increased dramatically
- AlexNet ≈ 10 layers → ResNet > 150 layers
- the size of "large scale" datasets has not kept pace
- 1 Million labelled images



Example II

Image classification - Sun, Shrivastava, Singh, & Gupta (2017)

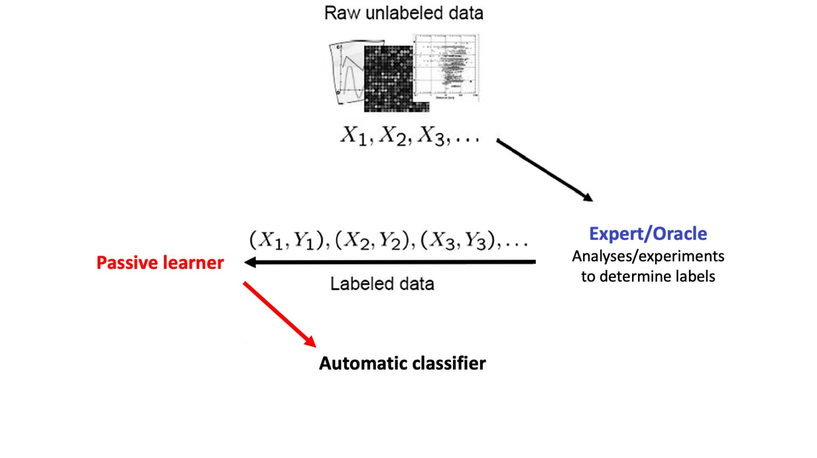
- Adding data is nearly as effective as adding layers
- There is a limit to what a network can learn on a smaller dataset – more parameters are not helpful unless you have more data



Semi-supervised learning

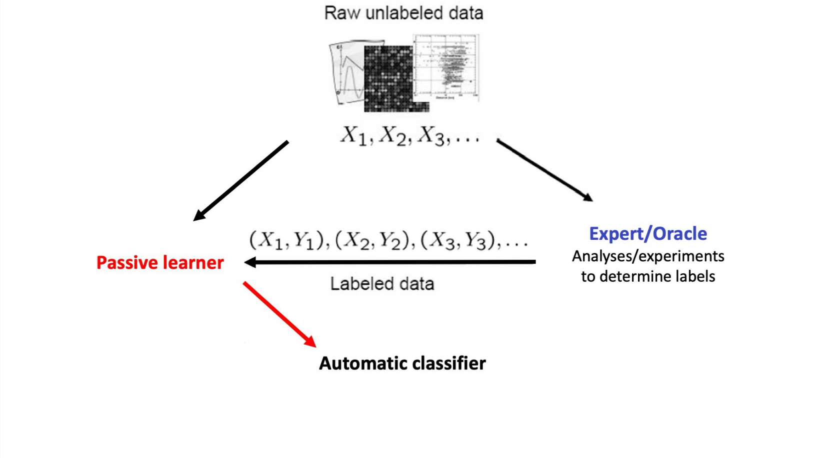
Supervised vs. Semi-supervised learning I

"Supervised" Learning:



Supervised vs. Semi-supervised learning I

“Semi-supervised” Learning:



Semi-supervised learning II

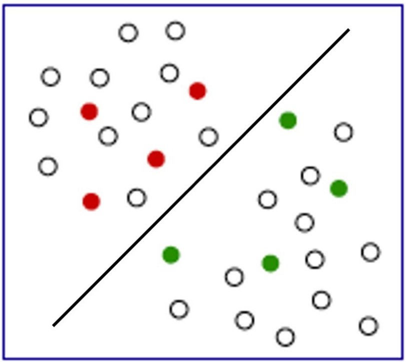
- Semi-supervised learning is learning from both labelled and unlabelled data

- **Semi-supervised classification**:
  - L is the set of labelled training instances $\{x_i, y_i\}_{i=1}^{l}$
  - U is the set of unlabelled training instances $\{x_i\}_{i=l+1}^{l+u}$
  - Often $U \gg l$
  - Goal: learn a better classifier from $L \cup U$ than is possible from L alone

Semi-Supervised Learning Approach I

Clustering + Majority-voting

- A simple approach: combine a supervised and unsupervised model
- For example, Find clusters, choose a label for each (most common label?) and apply it to the unlabelled cluster members



Semi-Supervised Learning Approach II

Self-Training (Also known as "Bootstrapping")

Creating *something* out of *nothing*.

- Assume you have $L = \{x_i, y_i\}_{i=1}^{l}$ labelled and $U = \{x_i\}_{i=l+1}^{l+u}$ unlabelled training instances

- Repeat
  - Train a model f on L using any supervised learning method
  - Apply f to predict the labels on each instance in U
  - Identify a subset U' of U with "high confidence" labels
  - Remove U' from U and add it to L with the classifier predictions as the "ground-truth" labels ($U \leftarrow U \setminus U'$ and $L \leftarrow L \cup U$)
  - Until L does not change

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Self-Training Assumptions

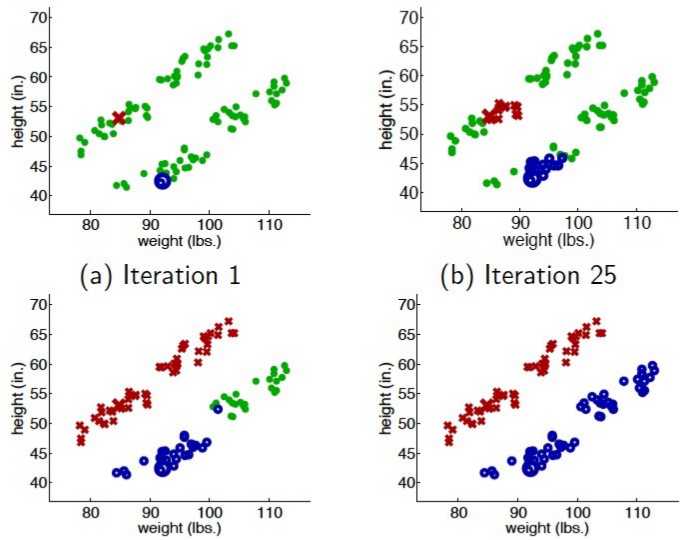
- Propagating labels requires some assumptions about the distribution of labels over instances:
  - Points that are nearby are likely to have the same label
- Classification errors are propagated
- Solution: Keep a kind of safety net...
  - Allow to move points back to the "unlabelled" pool if the classification confidence falls below a threshold

Self-Training Example: 1-NN

- 1-nearest neighbour with $L = \{x_i, y_i\}_{i=1}^{l}$ labelled and $U = \{x_i\}_{i=l+1}^{l+u}$ unlabelled training instances

- Repeat
  - Find neighbours for unlabelled instances in U
  - For instances x, whose nearest neighbour is in L, take the labels y' from 1-NN
  - $U \leftarrow U \setminus \{x\}$
  - $L \leftarrow L \cup \{x, y'\}$
  - Until L does not change

Self-Training Example: 1-NN



(a) Iteration 1 (b) Iteration 25

(c) Iteration 70 (d) Iteration 100

Self-Training Example: Naive Bayes

- Naive Bayes with $L = \{x_i, y_i\}_{i=1}^{l}$ labelled and $U = \{x_i\}_{i=l+1}^{l+u}$ unlabelled training instances
- Initialization: Train on L to learn $P(X|Y)$ and $P(Y)$ for all features X and all classes Y
- Repeat (EM algorithm)
  - **Expectation**: For each unlabelled instance, compute a probability distribution over classes
  - **Maximization**: Recompute $P(X|Y)$ and $P(Y)$ with all data, weighting the unlabelled instances by their probability of being in each class

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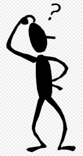
Self-Training Example: Naive Bayes

- **Problem**: if the unlabelled dataset is much larger than the labelled dataset, probability estimates will be based almost entirely on unlabelled data

- **Solution**:  Discuss!

Active Learning

Active Learning I

- Active learning builds off the hypothesis that a classifier can achieve higher accuracy with **fewer training instances** if it is allowed to have some say in the **selection** of the training instances

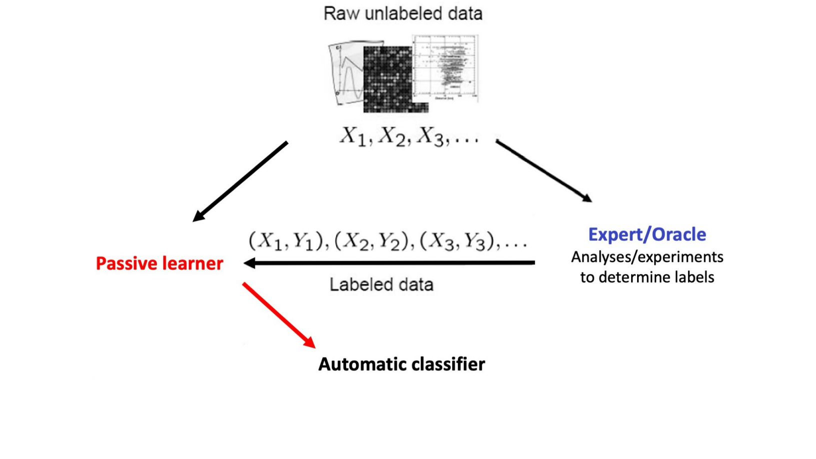
- The underlying assumption is that **labelling is a finite resource**, which should be expended in a way which optimises machine learning effectiveness

- Active learners pose **queries** (unlabelled instances) for labelling by an **oracle** (e.g. a human annotator)

Which instances are "most interesting"?

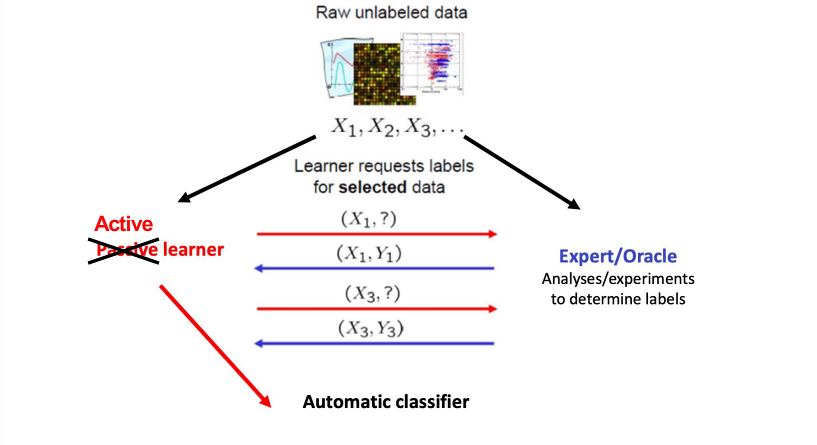
Semi-supervised learning vs. Active Learning

Semi-supervised Learning:



Semi-supervised learning vs. Active Learning

Active Learning:



Active Learning II

- Ideally, we want to select the instances that are most effective for distinguishing between competing models
  - Often, hard to do directly
  - E.g., because it requires comparison of likelihood functions of different models
- But, it is usually straightforward to identify instances on which a model is highly **uncertain**, e.g.:
  - Instances near the boundaries between classes
  - Instances in regions with few labels

Query Strategies

Which unlabelled instances will be most useful for learning?

1. One simple strategy: query instances where the **classifier is least confident** of the classification

$$x = \underset{x}{argmax}(1 - P_\theta(\hat{y}|x))$$

where $$\hat{y} = \underset{y}{argmax}(P_\theta(y|x)$$

Which unlabelled instances will be most useful for learning?

2. **Margin sampling** selects queries where the classifier is **least able to distinguish between two categories**, e.g.:

$$x = \underset{x}{argmin}(P_\theta(\hat{y}_1|x) - P_\theta(\hat{y}_2|x))$$

where $\hat{y}_1$ and $\hat{y}_2$ are the first- and second-most-probable labels for *x*

Query Strategies

Which unlabelled instances will be most useful for learning?

3. Use **entropy** as an uncertainty measure to utilize all the possible class probabilities:

$$x = \underset{x}{argmax} - \sum_{i} P_{\theta}(\hat{y}_i|x) \, log_2 \, P_{\theta}(\hat{y}_i|x)$$

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Query Strategies

Which unlabelled instances will be most useful for learning?

4. A more complex strategy, if you have multiple classifiers: **query by committee (QBC)**

   - Train multiple classifiers on a labelled dataset, use each to predict on unlabelled data, and select instances with the highest disagreement between classifiers

   - Assumes that all the classifiers learn something different, so can provide different information

   - Disagreement can be measured by entropy

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Active Learning Practicalities

Active learning is used increasingly widely, but must be handled with some care:

- empirically shown to be a robust strategy, but a theoretical justification has proven elusive
- active learning introduces bias: data with predicted labels no longer follows the true label distribution
- results to suggest that active learning is more highly reliant on “clean” labelling (error propagation)

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Data Augmentation

Data Augmentation

- There are various ways to **expand** a labelled training dataset
- **General:** re-sampling methods
- **Dataset-specific:** add artificial variation to each instance, without changing ground truth label

Bootstrap sampling

General Data Augmentation

- Bootstrap sampling: create “new” datasets by resampling existing data, with or without replacement
- Cross validation / repeated random subsampling are based on the same idea
- Each “batch” has a slightly different distribution of instances, forces model to use different features and not get stuck in local minima
- Also, common in perceptron and neural network training (“mini-batch”,“batch size”), methods that involve stochastic gradient descent (*much more on this over the coming weeks!*)

Data Manipulation

Problem-specific Data Augmentation

- Another option: add a small amount of “noise” to each instance to create multiple variations:
    - Images: adjust brightness, flip left-right, shift image up /down / left / right, resize, rotate
    - Audio: adjust volume, shift in time, adjust frequencies
    - Text: synonym substitution
- These perturbations should not change the instance’s label
- Generally, they should be the same kind of variations you expect in real-world data

Data Augmentation Pros and Cons

Advantages

- More data nearly always improves learning
- Most learning algorithms have some robustness to noise (e.g., from machine-translation errors)

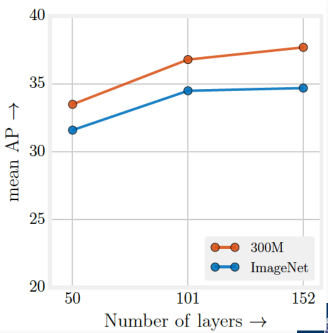
Disadvantages

- Biased training data
- May introduce features that don't exist in the real world
- May propagate errors
- Increases problems with interpretability and transparency

Unsupervised pre-Training: The secret sauce of (recent) deep learning success

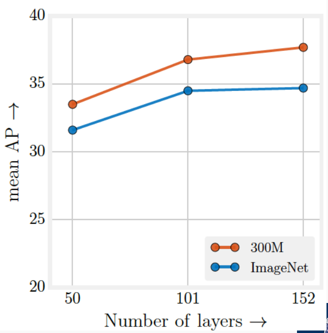
Why is deep learning so successful?

- Better models (recurrent models, convolutional, activation functions, ...)
- Bags of tricks (dropout, mini-batching, layer normalization, ...)
- More powerful machines (GPUs)
- **More data** – but we cannot label it all!



Why is deep learning so successful?

- Better models (recurrent models, convolutional, activation functions, ...)
- Bags of tricks (dropout, mini-batching, layer normalization, ...)
- More powerful machines (GPUs)
- **More data**
  - Pre-train (reuseable) parameters on some **unsupervised** task
  - Use the pre-trained weights to **initialize** your final model
  - Fine-tune the final model on a (usually) **supervised** target task.



Unsupervised Pre-training in NLP (taster)

Unsupervised pre-training in Natural Language Processing. Pre-training **word embeddings**.

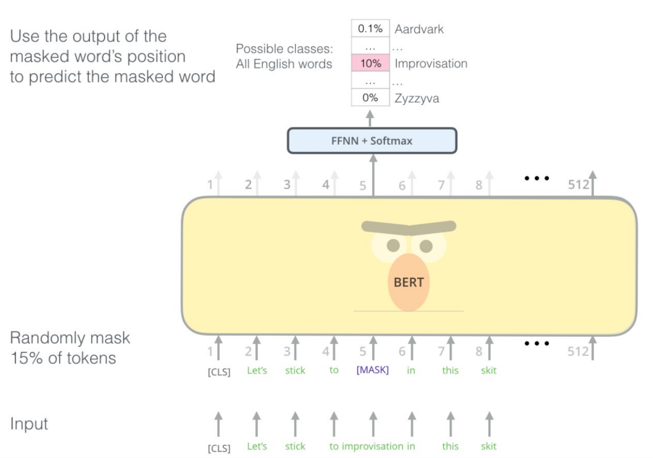


Image: http://jalammar.github.io/illustrated-bert/

Unsupervised Pre-training in NLP (taster)

Unsupervised pre-training in Natural Language Processing. Pre-training **word embeddings**.

- **Input**: “The girl is coding a [MASK] network using Python.”
- **Task**: Predict the hidden word given its context
- **Model**: Neural networks, increasingly complex (BERT, Sentence transformers,[2] GPT-2, ...)
- **Output**: A neural network which is a function: $f(\text{word}) \rightarrow$ feature vector

Use these feature vector to map language input $\rightarrow$ machine-readable representation. Use the representations in your **final** supervised text classification model.

[2]Which you’ll meet in Assignment 3!

Summary

Summary

Today

- What is semi-supervised learning?
- What is self-training, and how does it operate?
- What is active learning?
- What are the main sampling / query strategies in active learning?
- Pre-training in modern deep learning

Up next

- The Perceptron

References

- Burr Settles. Active learning literature survey. Technical report, Department of Computer Sciences, University of Wisconsin, Madison, 2010.
- Xiaojin Zhu. Semi-supervised learning literature survey. Technical Report Technical Report 1530, Department of Computer Sciences, University of Wisconsin, Madison, 2005.
- Xiaojin Zhu. Tutorial on semi-supervised learning.
- Devlin, Jacob, et al. ”BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding.” *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers). 2019.*