Deep Learning for Image Analysis - Learning from fewer annotations

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2. Strategies
3. Contrastive Learning
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Deep Learning: there is just one catch ...

- Deep Learning is today the most powerful method for image classification, segmentation and object detecction.
- Deep Learning can achieve or even go beyond human performance for these tasks.
- There is a snag: deep learning relies on massive annotation.
- Example: ImageNet contains 1.4 million annotated images [Russakovsky et al., 2015].

Deep Learning: there is just one catch ...

- Manual image annotation is annoying.
- Manual image annotation is expensive.
- We need to address the need for massive image data sets, either by avoiding massive annotation or by making annotation cheap.

Two main strategies to overcome massive image annotation

1. Use cheap annotations.
2. Use different annotations.

Please note:

- We always need to consider what exactly we aim at predicting (e.g. the value of a pixel or the class of an image)
- For instance, in segmentation, annotations are expensive at the image level, but not at the pixel level: a single stroke annotates hundreds of pixels.

Image segmentation: cheap annotations?

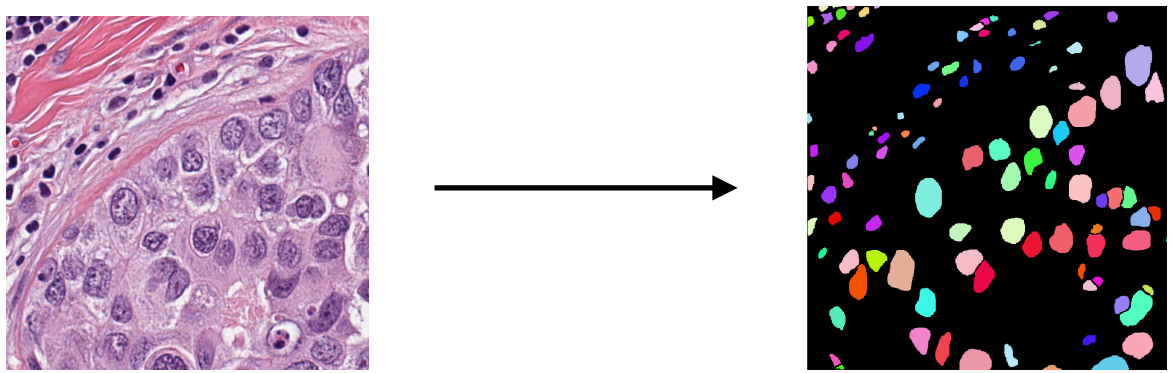

Image *Binary map*

Figure: Segmentation is tedious, but provides rapidly many samples.

- Providing pixel-level annotations is extremely tedious.
- But as we are classifying pixels, we can rapidly provide hundreds of thousands of samples.
- In practice however, we need to **cover the variability** to be expected at prediction time.
- For this reason, we still need a reasonable amount of images (depending on the variability).

Massive image annotation by crowd sourcing

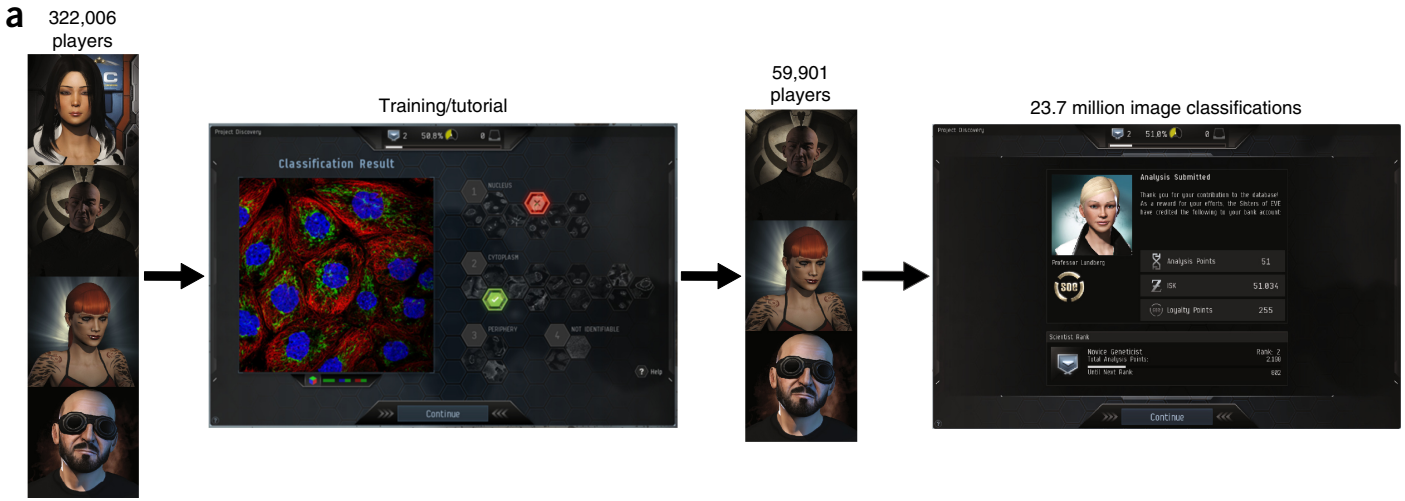

Figure: Gamification for the annotation of protein localization patterns: the actual annotation task is "disguised" as a computer game. Image taken from [Sullivan et al., 2018]

- Crowd sourcing: generate massive annotated data sets by recruiting more people to do the annotations.
- This requires the implication of untrained experts (citizen science).
- Several strategies to reach many people, e.g. gamification.

Massive image annotation by leveraging routinely acquired data

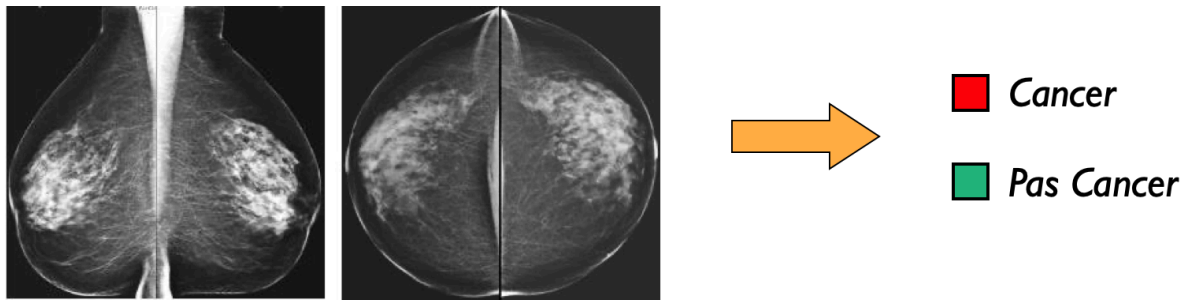

Figure: Radiology: mammographies are acquired routinely by physicians.

- In many fields, image data is routinely acquired (e.g. medical examinations).
- Origins of the image labels:
  - Routine annotation by a medical doctor.
  - Future evolution of the disease.
- Problem: we are limited in the tasks, i.e. in the variables that we can predict.

Massive image annotation by experimental setup

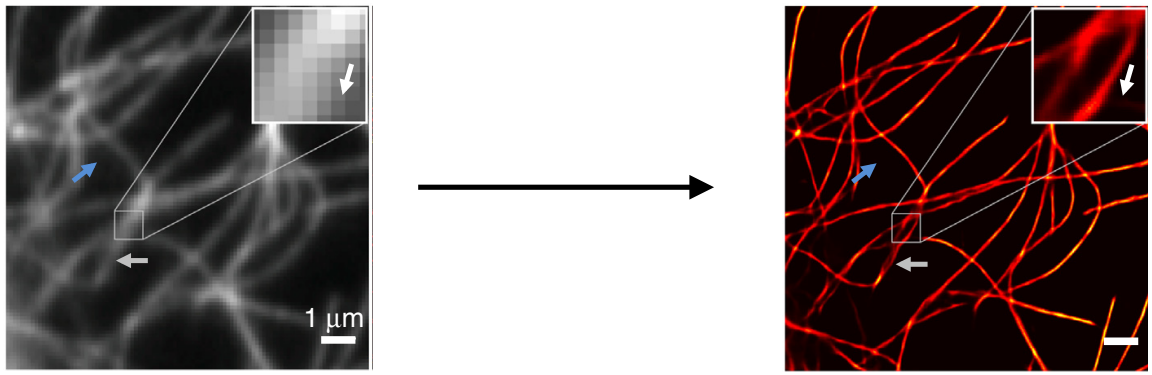

Figure: A high resolution image can be predicted from a low resolution image. Image adapted from [Ouyang et al., 2018]

- In image restoration, we aim at predicting a high quality image from a lower quality image.
- Here, the ground-truth is entirely generated by the experimental setup (pairs of images are acquired).

Massive image annotation by experimental setup

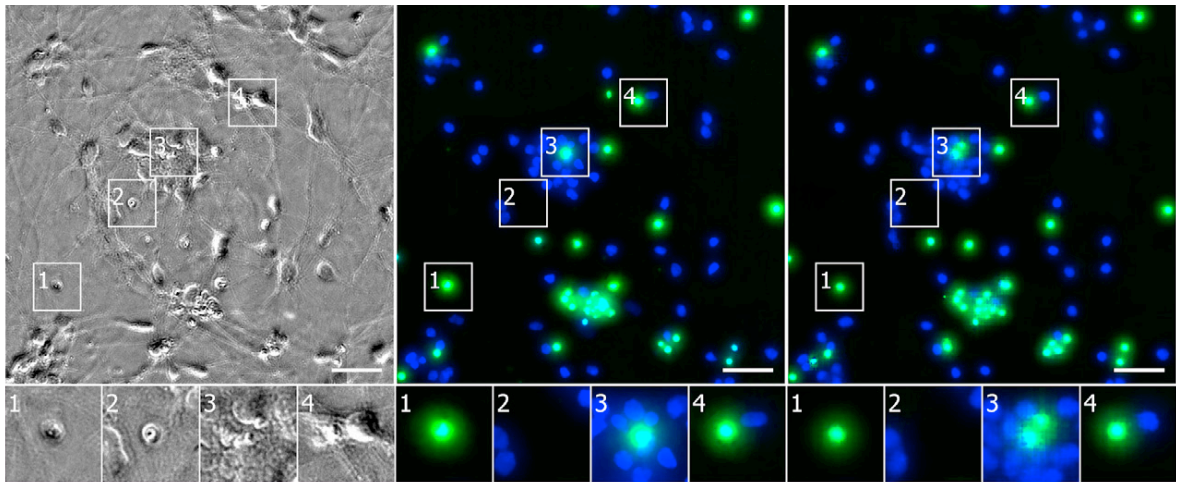

Figure: Amn image taken with a different modality can be predicted. Here, we show an example for a fluorescent microscopy image predicted from a phase contrast microscopy image. Image adapted from [Christiansen et al., 2018]

- We can also predict images taken with different modalities.
- This is interesting if one technique is more expensive or more invasive.
- Similarly, we can also use different experimental techniques to generate ground truth experimentally [J. Boyd et al., 2020].

Overcoming massive image annotation: simulation

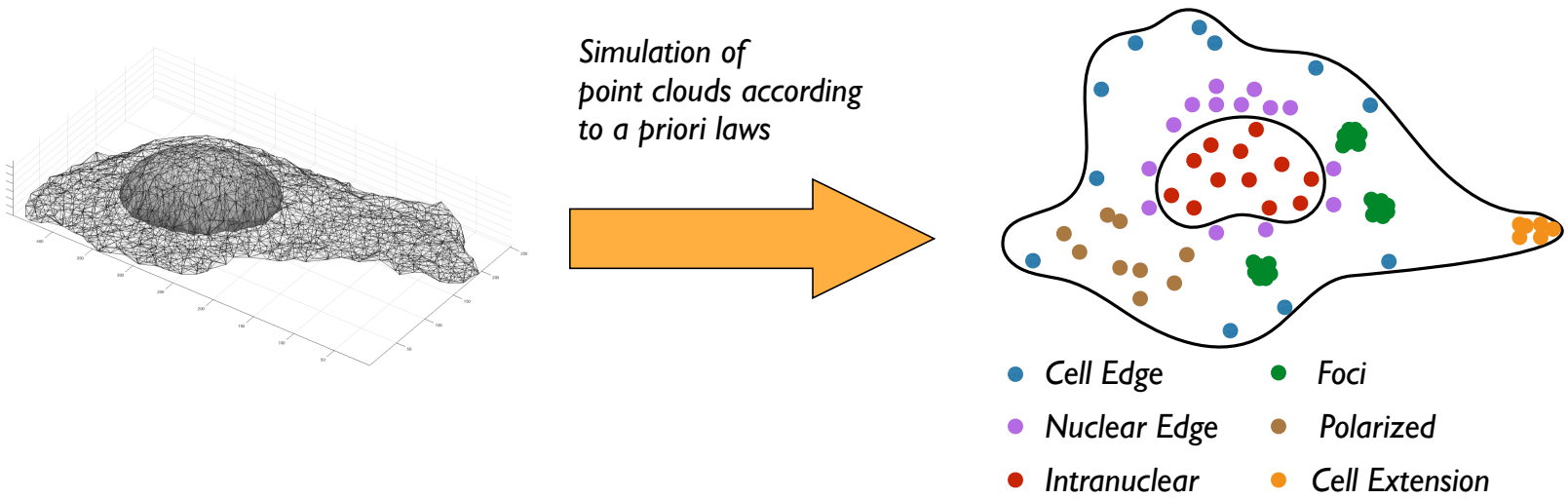

Figure: Simulated RNA localization in cells

- Simulation of large amounts of data with known ground truth.
- Train networks on simulated data.
- Problem: the data distributions between simulated and real data usually differ.

Overcoming massive image annotation: transfer learning

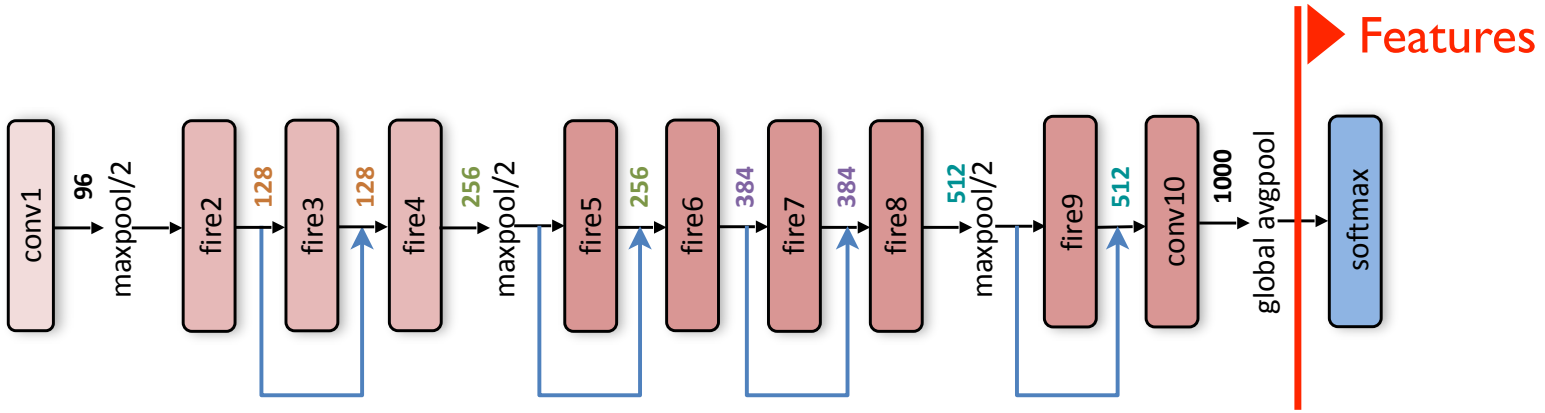

Figure: Image representations for transfer learning. Image adapted from [Iandola et al., 2017]

- Train a network on large annotated image bases.
- Use the learned representations to solve small scale problems (with or without fine-tuning) with few annotations.

Subject of today

In this lecture, we will learn about three strategies to address the problem of massive datasets required for training of deep neural networks:

1. Contrastive Learning
2. Learning in a weakly supervised setting (typically coarse annotations)
3. Learning from simulations with domain adaptation

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Idea

- Transfer Learning: transferring learned representation from one data set (with potentially different tasks) to a new data set.
- If we can define pretext tasks with known labels, we can also leverage unlabeled data to learn representations, which might also be transferable.
- Pretext task: learn the identity of transformed images.
- Here, we present the paper "A simple framework for Contrastive Learning of Visual Representations" (SimCLR) [Chen et al., 2020].

SimCLR [Chen et al., 2020]

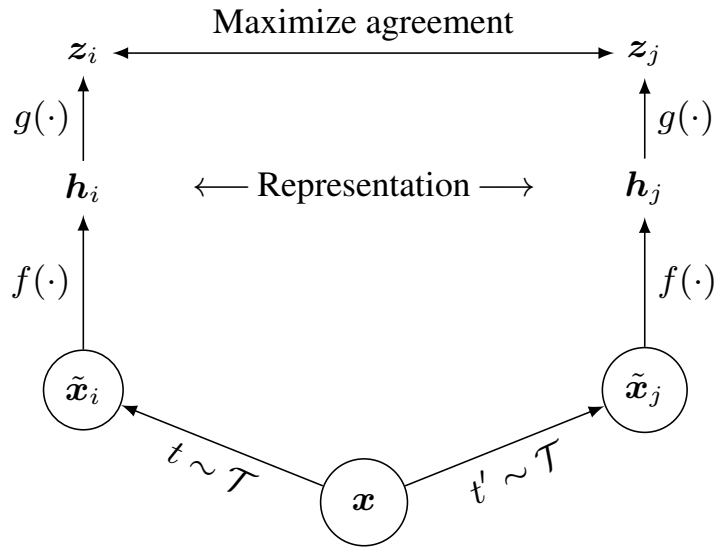


Figure: SimCLR workflow as defined in [Chen et al., 2020]

- For each image x, we calculate two transformed versions $\tilde{x}_i$ and $\tilde{x}_j$ by two transformations t and t' drawn from a set of parametrized transformations.
- For $\tilde{x}_i$ and $\tilde{x}_j$, we calculate the representations h_i and h_j, respectively. $f(\cdot)$ is the neural network we want to learn.

SimCLR [Chen et al., 2020]

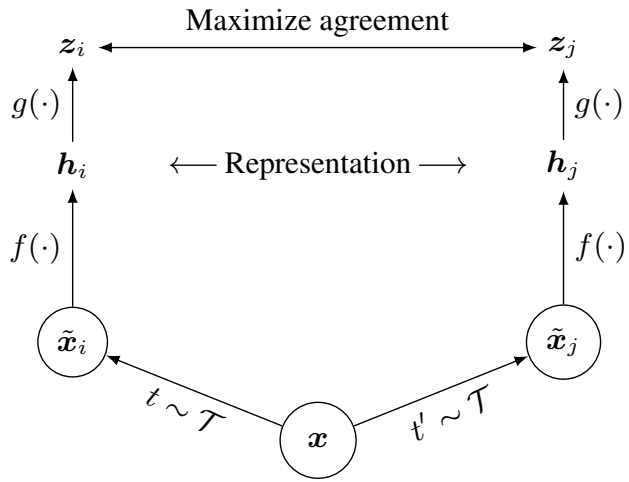


Figure: SimCLR workflow as defined in [Chen et al., 2020]

- The representations h_i and h_j are mapped to a space where contrastive loss is applied, by a small neural network $g(\cdot)$.
- The classification task is to identify among all transformed images for each transformed image x_i the transformed image x_j that originates from the same image.

SimCLR [Chen et al., 2020]

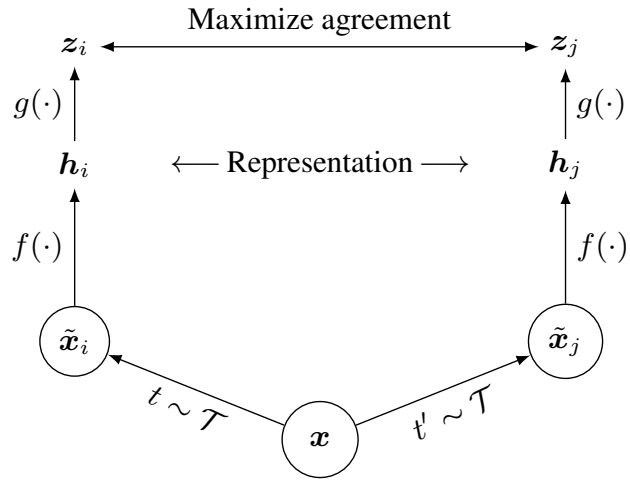


Figure: SimCLR workflow as defined in [Chen et al., 2020]

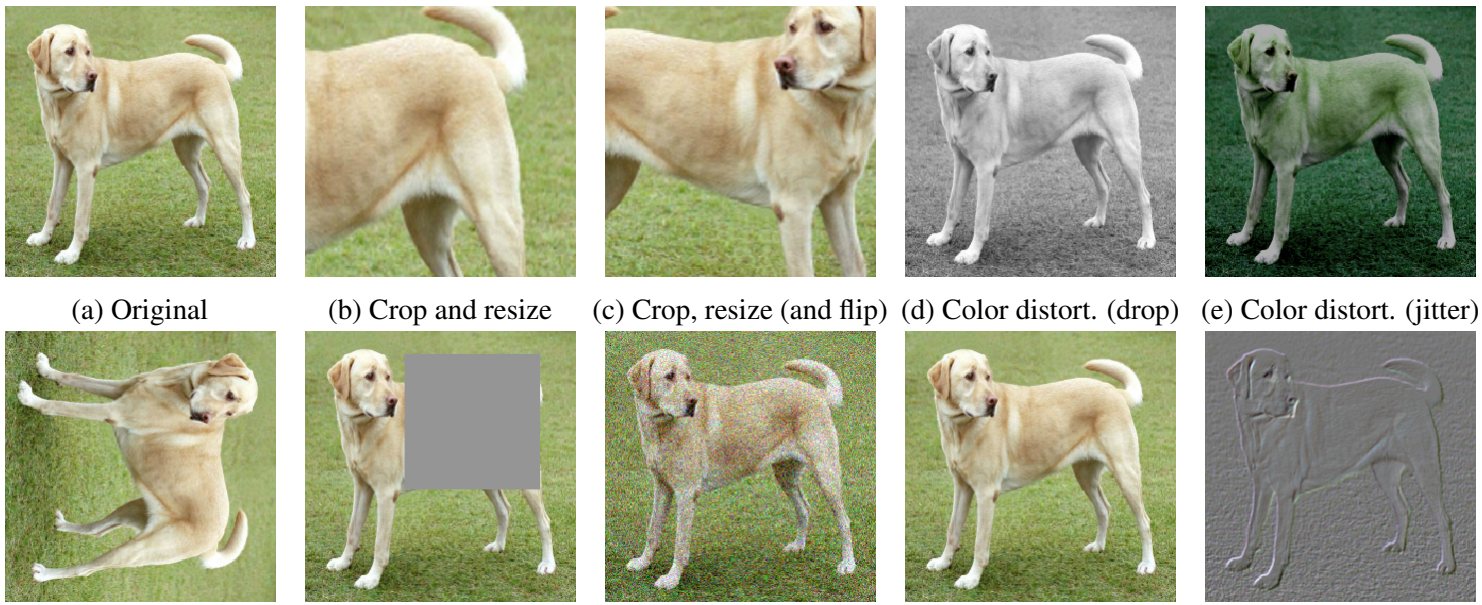
- We define the similarity of two representations as follows:

$$s(u, v) = \frac{u^T v}{\|u\|\|v\|} \tag{1}$$

- With this, we can define the contrastive loss as follows:

$$l_{i,j} = -\log \frac{\exp \frac{s(z_i, z_j)}{\tau}}{\sum_{k=1}^{2N} \mathbb{1}_{k \neq i} \exp \frac{s(z_i, z_k)}{\tau}} \tag{2}$$

SimCLR: transformations



(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

(f) Rotate $\{90°, 180°, 270°\}$ (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

Figure: Transformations used in SimCLR [Chen et al., 2020]

SimCLR: results

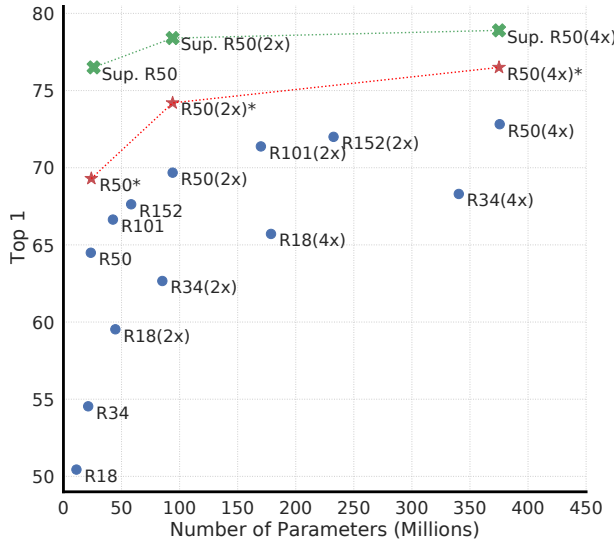


Figure: Results (linear evaluation) obtained by SimCLR [Chen et al., 2020]

- Evaluation of representations by *linear evaluation* (result obtained by a linear classifier trained with the representation as features): the unsupervised approach comes reasonably close to a fully supervised approach.
- Transfer-learning results (not shown): Fine-tuning the obtained representations is on par with fine-tuning pretrained networks.

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What is weak supervision?

- Weak supervision refers to a situation, where the ground truth data we build our model on is in some sense imperfect [Zhou, 2018].
- Three types of weak supervision:
  1. **Incomplete supervision:** only a subset of training data are labeled (semisupervised setting).
  2. **Inexact supervision:** training data are labeled but not as exact as required by the task we would like to perform
  3. **Inaccurate supervision:** training data are labeled, but may contain mistakes ().
- Here, we treat the case of inexact supervision.

The Multiple Instance Learning framework (MIL)

- MIL deals with problems with incomplete knowledge of labels in training sets.
- MIL assumes that instead of disposing of individual labels y_i for each sample x_i, we only have labels for subsets of samples, called "bags":

$$\begin{aligned} T &= \{(B_i, y_i)\} \\ B_i &= \{x_j\} \end{aligned} \tag{3}$$

- A bag is positively labeled if at least one instance in it is positive, and is negatively labeled if all instances in it are negative.
- Examples:
  - An image is labeled as "contains humans", if at least one region contains a human.
  - A tissue slide is labeled cancerous, if at least one region is cancerous.

A deep learning approach to MIL

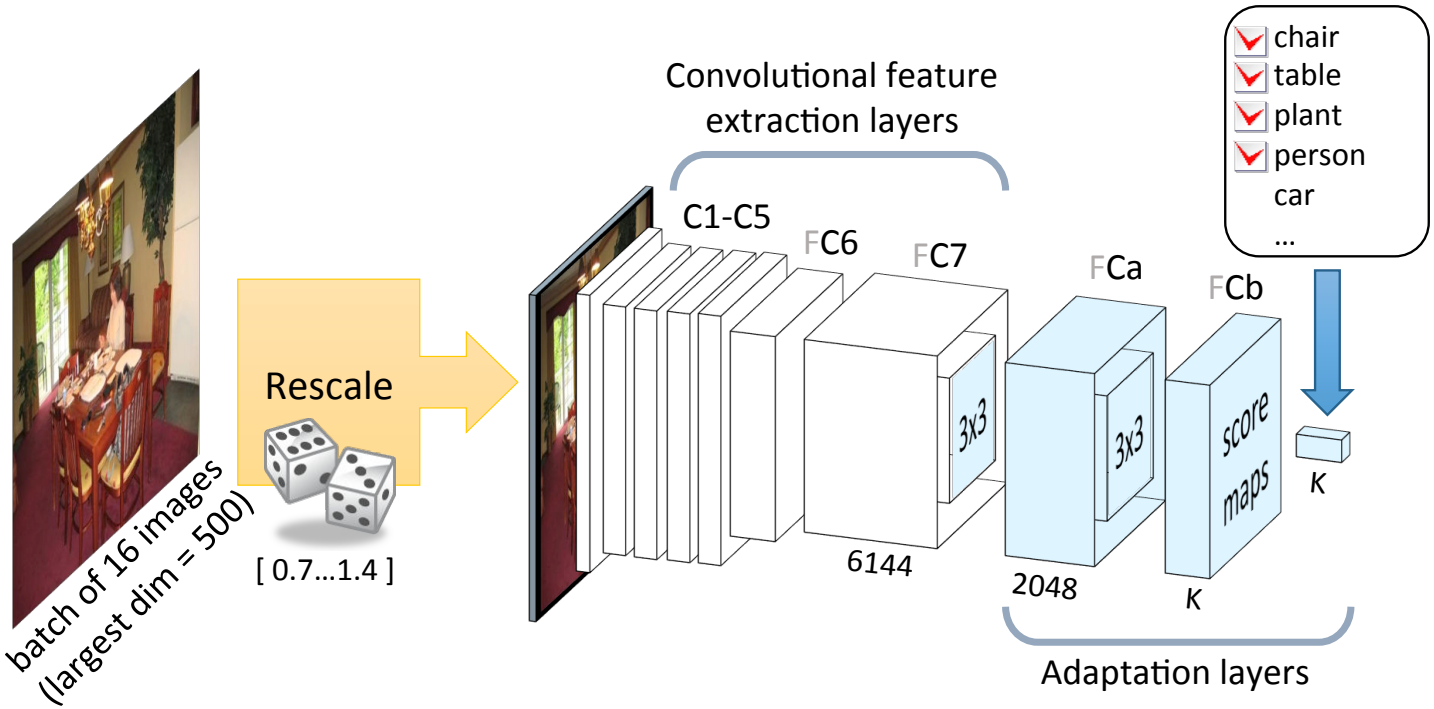

Figure: CNN architecture for Multiple Instance Learning. Image taken from [Oquab et al., 2015]

First, a standard CNN is applied as feature extractor (without fully connected layers). This maps an image X to a $n \times m \times l$ layer (l feature maps of spatial dimensions $n \times m$).

A deep learning approach to MIL

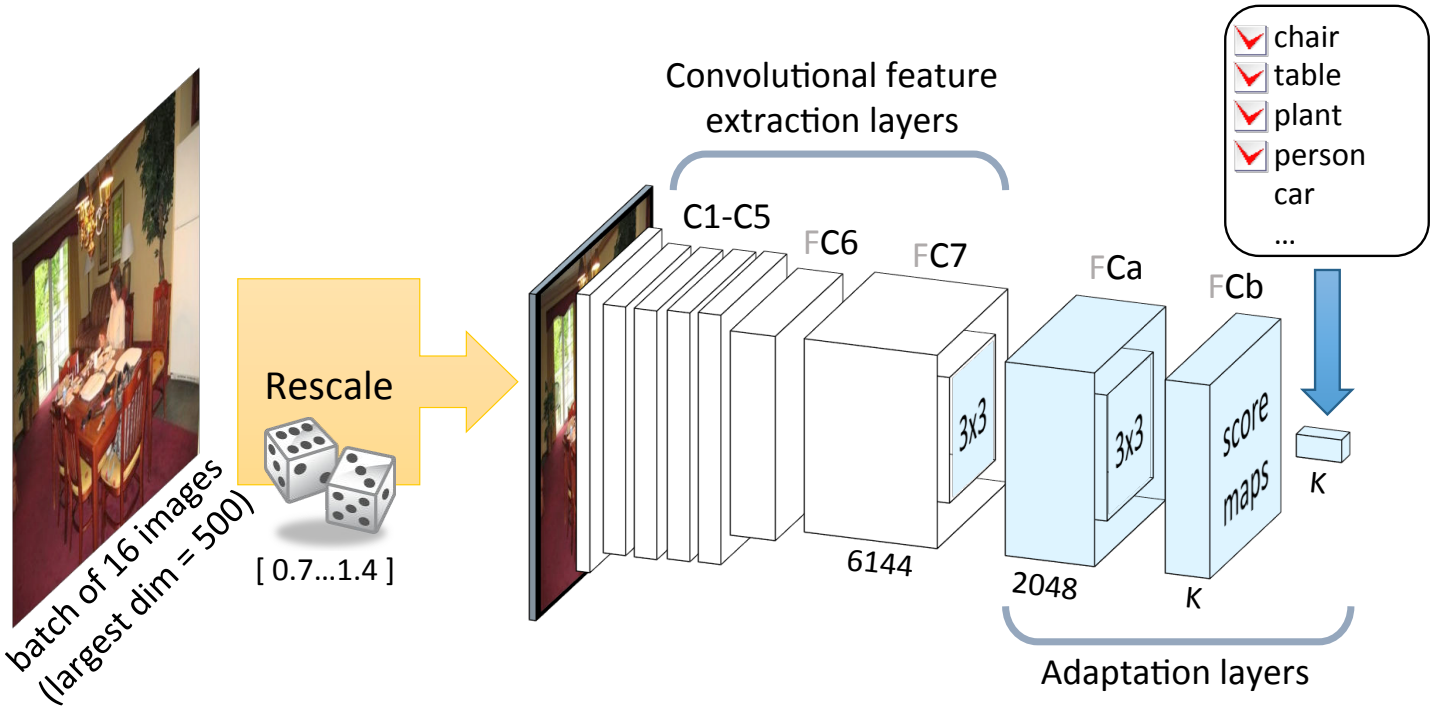

Figure: CNN architecture for Multiple Instance Learning. Image taken from [Oquab et al., 2015]

This layer is then mapped to a $n \times m \times K$ layer by 1×1 convolutions, where K is the number of output classes. Of note, a 1×1 convolutional layer is equivalent to a fully connected layer, if its input is a vector (spatial dimension 1). We can understand the 1×1 conv layer as parallel fully connected layers.

A deep learning approach to MIL

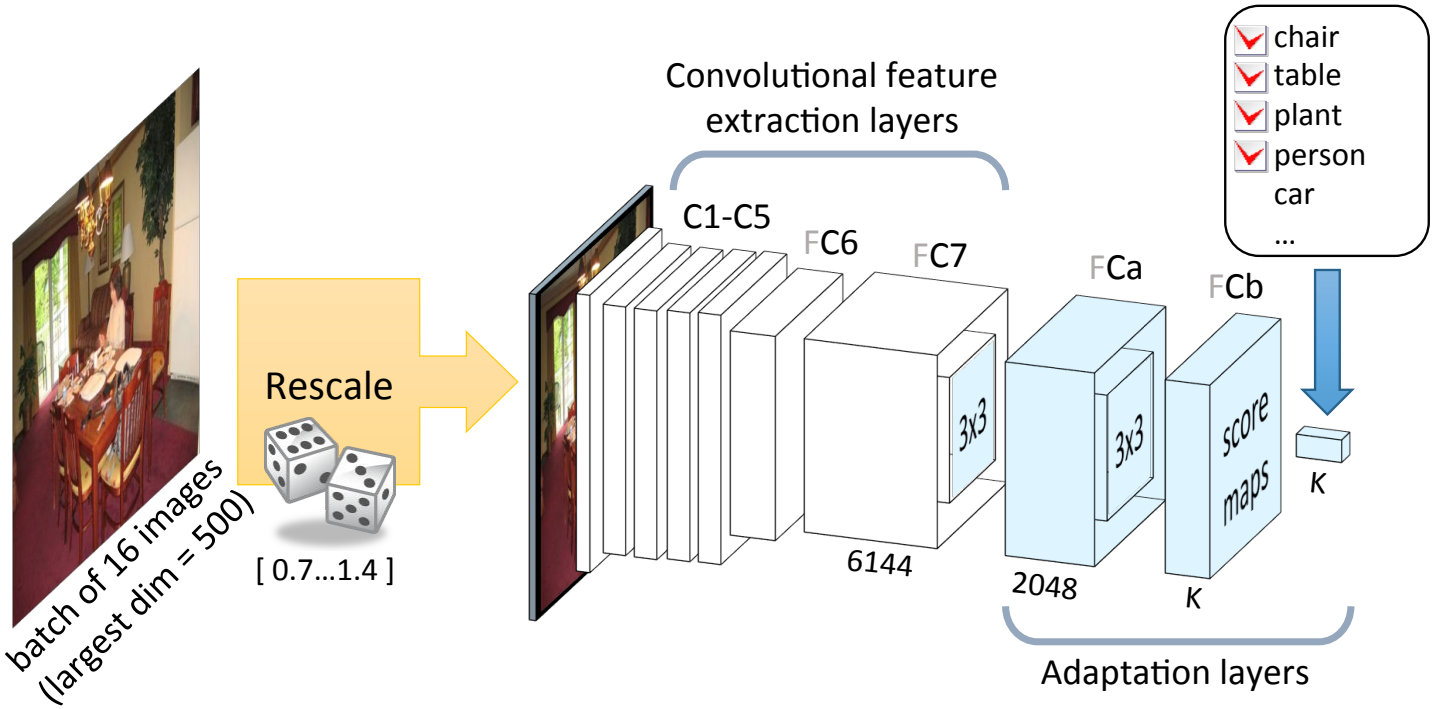

Figure: CNN architecture for Multiple Instance Learning. Image taken from [Oquab et al., 2015]

Each "pixel" in feature map *FCb* is thus the score vector for an input region. *FCb* therefore corresponds to a bag of image regions. We therefore maximize over the spatial dimensions:

$$s_k = \max_{i,j} f_{i,j}^k \tag{4}$$

A deep learning approach to MIL

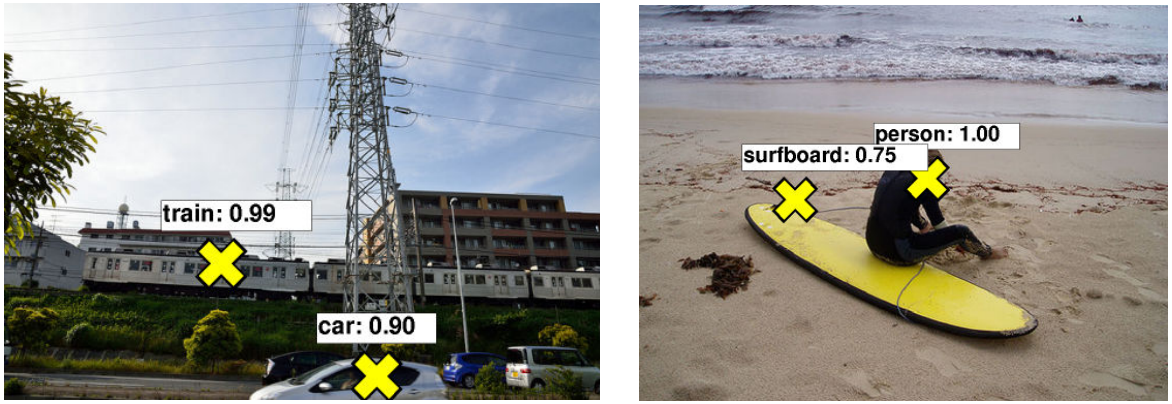

Figure: Example for MIL by deep learning. Image adapted from [Oquab et al., 2015]

- Maximization over the spatial dimensions corresponds exactly to the MIL-paradigm: for the decision on the image label, it is sufficient to have one single positive region.
- This is a typical situation, when we want to detect objects in crowded images.

Discussion

- Improvement of image classification, as only the relevant region is taken into consideration.
- This is particularly useful, if the size of the relevant region is comparatively small.
- Objects can also be detected and this without expensive annotation (bounding boxes or pixel-wise annotation).
- In addition, the detection of different classes is eased by the setup.
- Limitations:
  - Scale issue: the desired object might not fit into the considered regions.
  - Object extensions cannot be faithfully predicted.
  - The context is not taken into consideration.

Improvements on the WSL strategy

- Instead of taking the maximum score over all image regions [Durand et al., 2016]:
  - Select the s_{top} highest scoring regions
  - Select the s_{low} lowest scoring regions
- Intuition: taking $s_{top} > 1$ regions makes the algorithm more robust, taking s_{low} lowest scoring regions provides negative evidence for the class.

Application example: histopathology

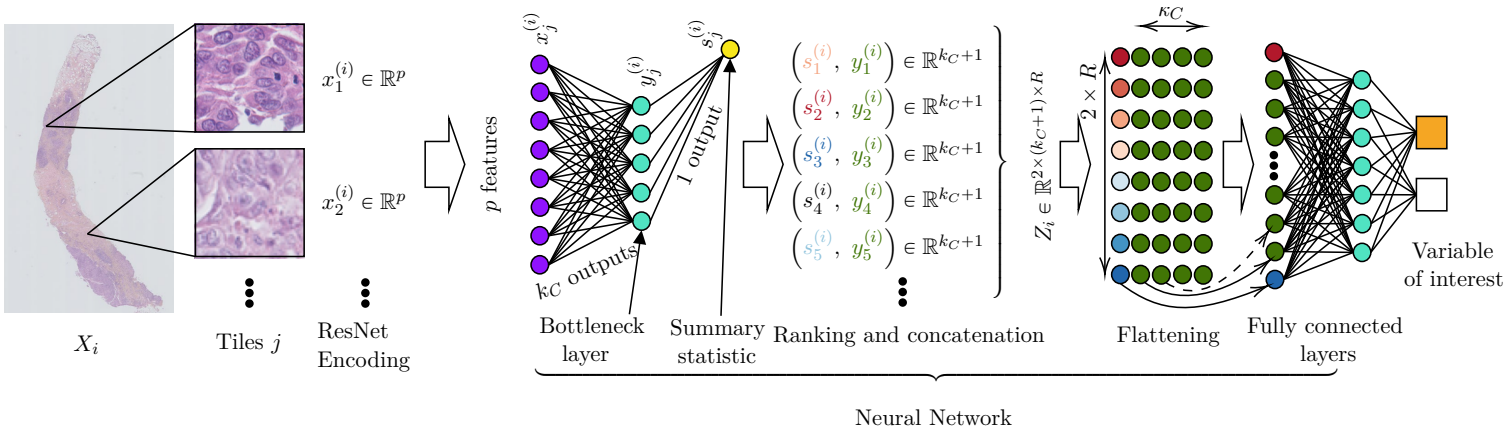

Figure: Example for WSL for tumor detection. Image provided by Peter Naylor.

- Histopathology images are extremely big.
- Sometimes, what we want to find can be small.
- There is slide-level annotation, but detailed annotation is scarce.

Application example: metastasis detection

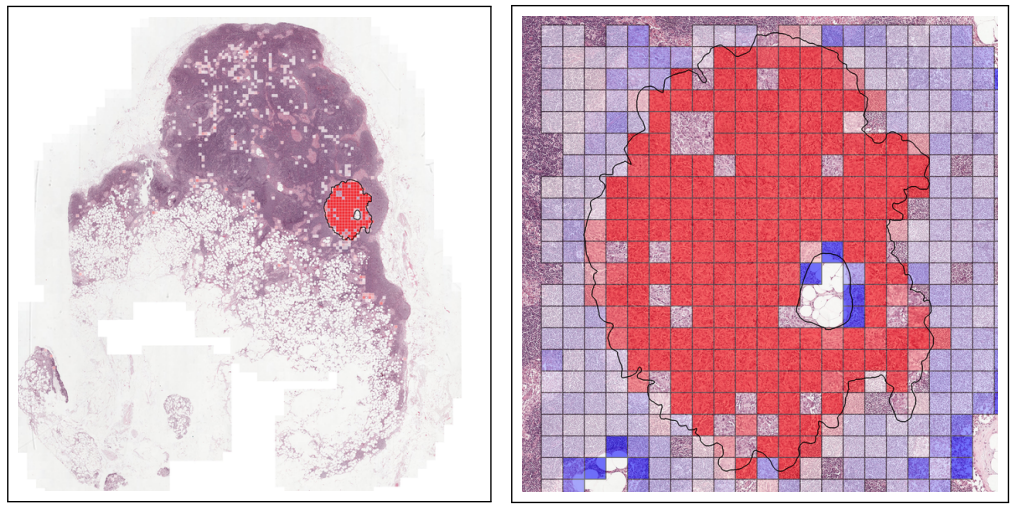

Figure: Example for WSL for tumor detection. Image adapted from [Courtiol et al., 2017]

Here, [Courtiol et al., 2017] use the WELDON algorithm to detect metastases. Only global annotation is used. The results are on par with classification / detection algorithms trained on detailed annotation.

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Simulation for the generation of training data

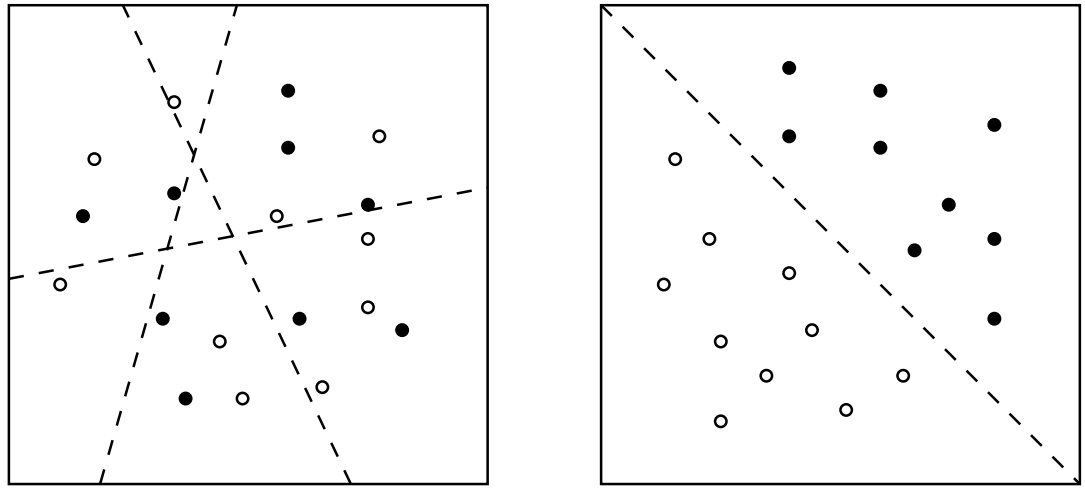
- With simulation, we can generate arbitrary quantities of data with known ground truth.
- Simulation is regularly used for benchmarking of methods.
- Usually, simulation provides us with data similar to real world data, but not identical.
- For this reason, the use of simulated data for training neural networks is limited.
- Idea: can we overcome the differences between simulated and real data by explicit algorithmic strategies?

Domains

- Domain adaptation: learning a discriminative classifier when training data does not follow the same distribution as the test data.
- Let $\mathcal{X}$ be an input space and $\mathcal{Y} = \{1, \ldots, L\}$ the set of L possible labels. We call a domain the distribution over $\mathcal{X} \times \mathcal{Y}$.
- Here we consider two domains: the source domain $\mathcal{D}_S$ and the target domain $\mathcal{D}_T$.
- The source samples are then drawn from $\mathcal{D}_S$, the test samples from $\mathcal{D}_T^X$:

$$\begin{aligned} S &= \{(x_i, y_i)\}_{i=1}^{n} \sim \mathcal{D}_S^n \\ T &= \{(x_i, y_i)\}_{i=n+1}^{N} \sim (\mathcal{D}_T^X)^{N-n} \end{aligned}$$

The divergence of domains



(a) Low divergence (b) High divergence

Figure: Illustration of h-divergence between domains.

- The divergence of domains can be quantified by trying to classify samples according to their source label.
- Hence, we train a classifier from a training set $T = \{(x_i, d_i)\}$:

$$d_i = \begin{cases} 0, & \text{if } x_i \sim \mathcal{D}_S^X \\ 1, & \text{if } x_i \sim \mathcal{D}_T^X \end{cases} \tag{5}$$

- In this case, the h-divergence can be written as $2(1 - 2\epsilon)$, where ϵ is the error of the classifier.

Domain adaptation by adversarial training

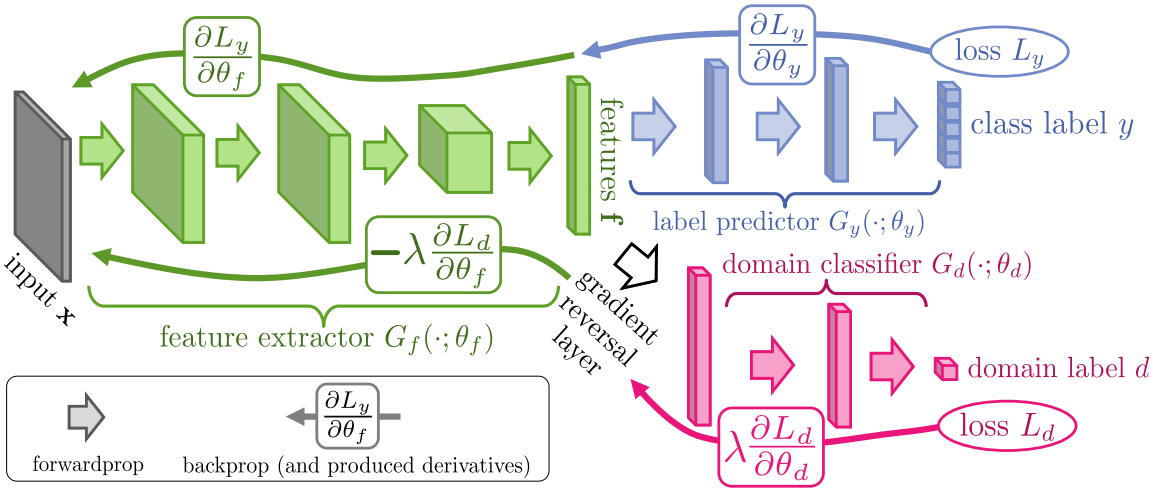


Figure: Domain adaptation by adversarial training. Image taken from [Ganin et al., 2016]

- We seek a representation that provides good prediction results, but low h-divergence.
- This means that this representation (f in the figure) should not allow us to distinguish between source domain and target domain.

Domain adaptation by adversarial training

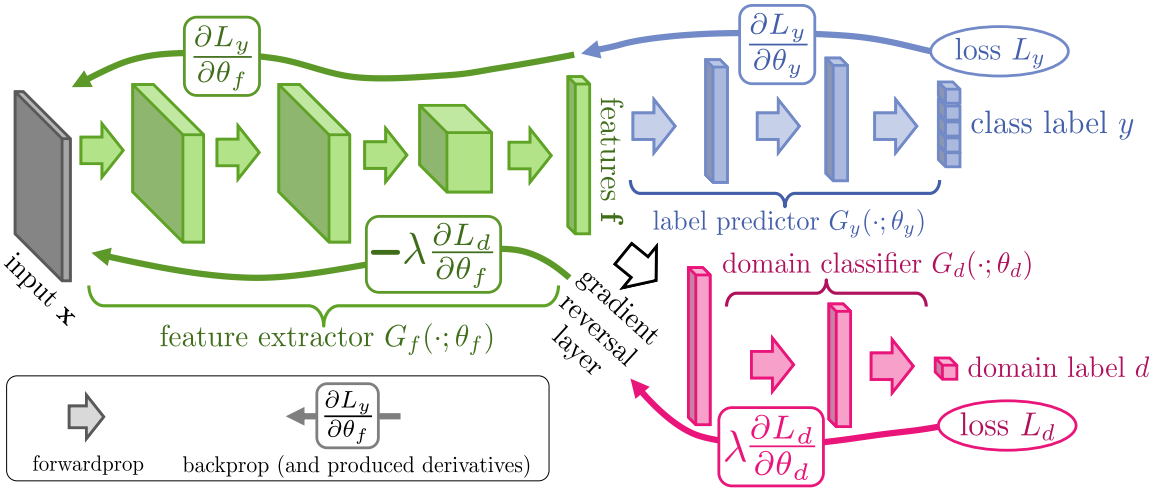


Figure: Domain adaptation by adversarial training. Image taken from [Ganin et al., 2016]

For this we consider the following architecture [Ganin et al., 2016]:

- $G_f(;,\theta_f)$: feature extractor
- $G_y(;,\theta_y)$: label predictor
- $G_d(;,\theta_d)$: domain classifier

Domain adaptation by adversarial training

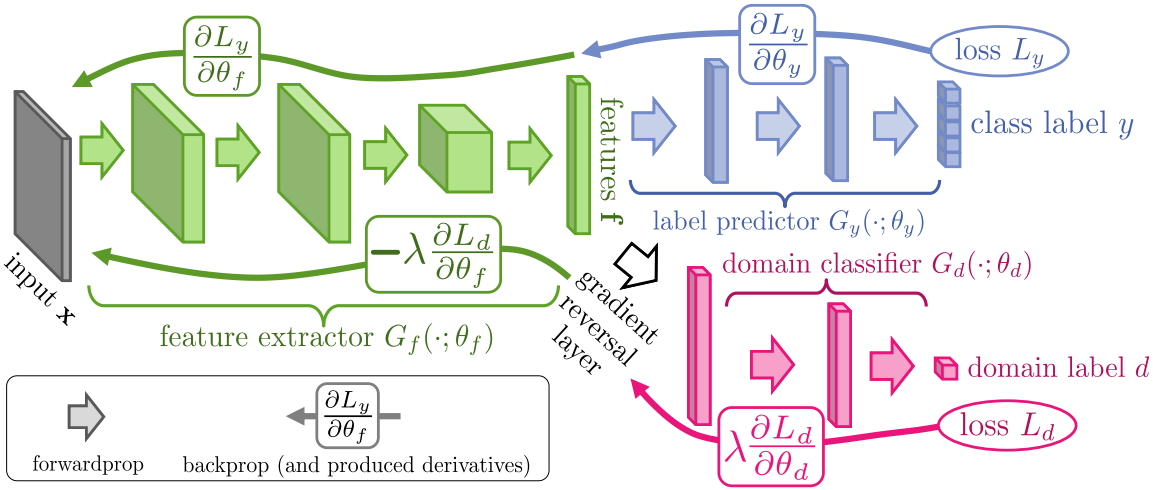


Figure: Domain adaptation by adversarial training. Image taken from [Ganin et al., 2016]

The forward propagation produces then the following loss:

$$L(\theta_f, \theta_y, \theta_d) = L_y(\theta_f, \theta_y) - \lambda L_d(\theta_f, \theta_d) \tag{6}$$

where $L_y(\theta_f, \theta_y)$ is the standard prediction loss for samples from the training set (and thus the source domain), while $L_d(\theta_f, \theta_d)$ is the domain loss, calculated on all samples (labeled samples from the source domain and the unlabeled samples from the target domain).

Domain adaptation by adversarial training - Optimization

- More formally, we write:

$$
\begin{aligned}
L_y(\theta_f, \theta_y) &= \frac{1}{n} \sum_{i=1}^{n} L_y(G_y(G_f(x_i, \theta_f), \theta_y), y_i) \\
L_d(\theta_f, \theta_d) &= \frac{1}{n} \sum_{i=1}^{n} L_d(G_d(G_f(x_i, \theta_f), \theta_d), d_i) \\
&+ \frac{1}{N-n} \sum_{i=n}^{N} L_d(G_d(G_f(x_i, \theta_f), \theta_d), d_i) \\
L(\theta_f, \theta_y, \theta_d) &= L_y(\theta_f, \theta_y) - \lambda L_d(\theta_f, \theta_d)
\end{aligned}
$$

- This loss has to be minimized with respect to some parameters and maximized with respect to other parameters:

$$
\begin{aligned}
(\hat{\theta}_f, \hat{\theta}_y) &= \arg\min_{\theta_f, \theta_y} L(\theta_f, \theta_y, \hat{\theta}_d) \\
\hat{\theta}_d &= \arg\max_{\theta_d} L(\hat{\theta}_f, \hat{\theta}_y, \theta_d)
\end{aligned}
$$

Domain adaptation by adversarial training - gradient reversal

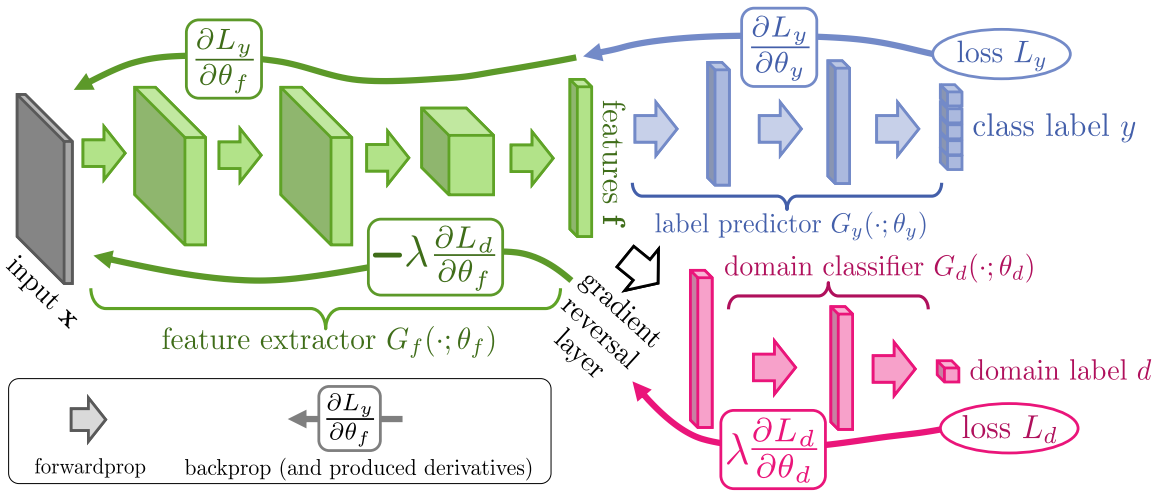


Figure: Domain adaptation by adversarial training. Image taken from [Ganin et al., 2016]

The solution of simultaneous minimization and maximization can be elegantly solved by reversing a gradient layer during back-propagation, as indicated in the figure.

Application example: character classification

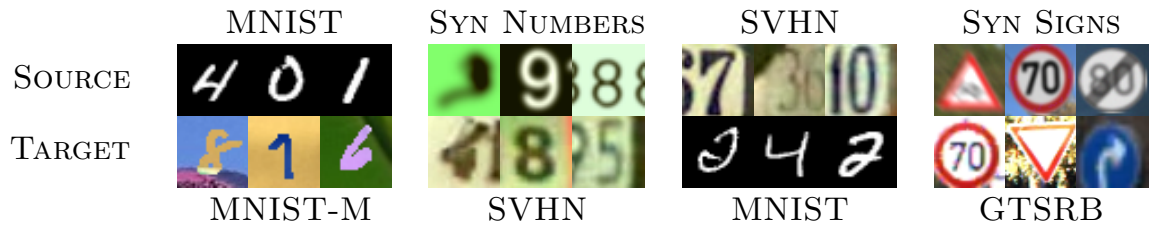
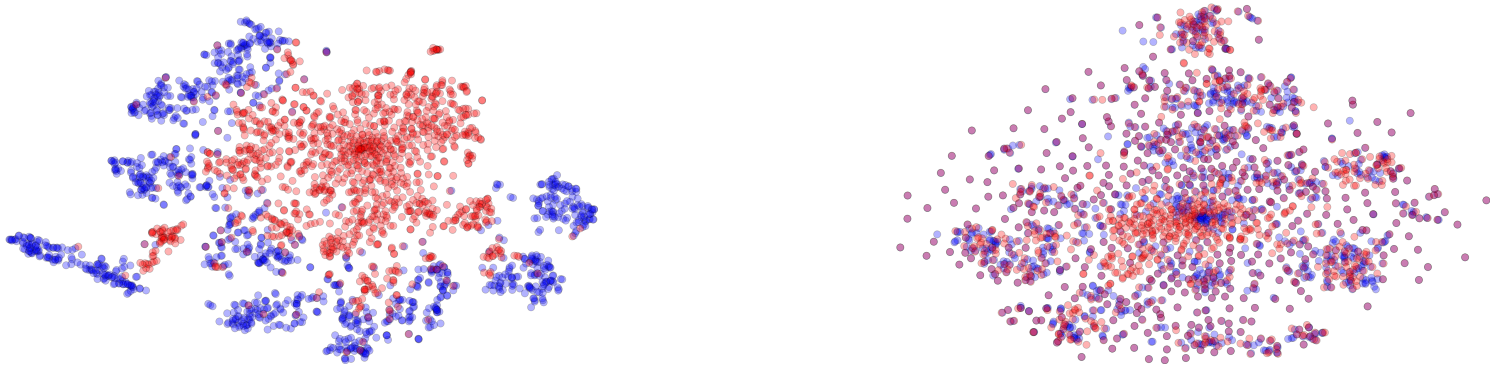


Figure: Domain adaptation between simulated and real data. MNIST: hand-written digits, MNIST-M: MNIST on top of random image patches, SYN Numbers: simulation created by varying Windows fonts, SVHN: street view house numbers, Image taken from [Ganin et al., 2016]

Results indicate that the achievable improvements can reach up to 20% in cases where the simulations are relatively far from the real-world examples.

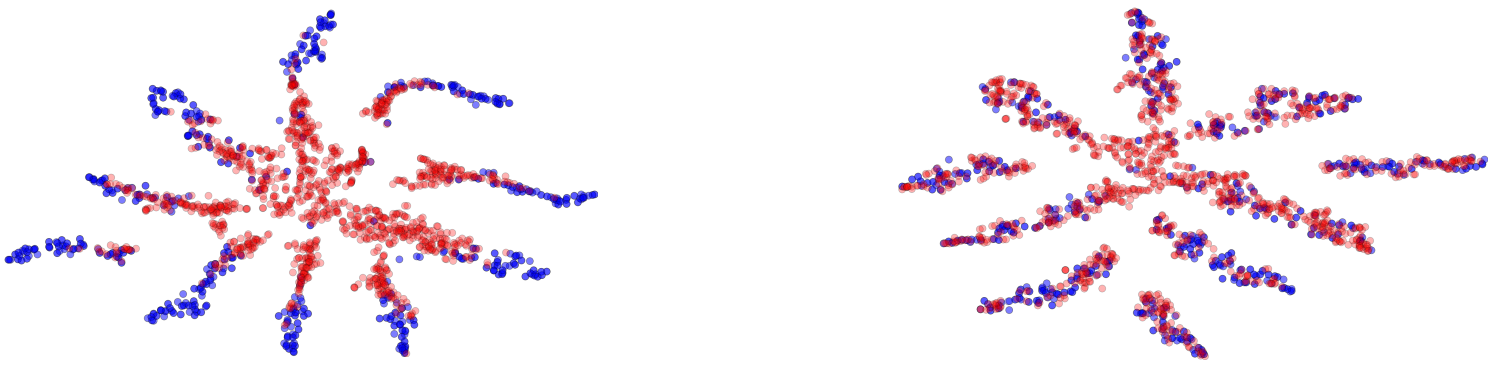
Application example: character classification

MNIST → MNIST-M: top feature extractor layer



(a) Non-adapted (b) Adapted

SYN NUMBERS → SVHN: last hidden layer of the label predictor



(a) Non-adapted (b) Adapted

Figure: Learned representations with and without domain adaptation. Domains are colored in red and blue. Image taken from [Ganin et al., 2016].

Overview

1 Motivation

2 Strategies

3 Contrastive Learning

4 Weak supervision

5 Learning from simulated data

6 Conclusion

7 References

Conclusion

- The need for large annotated data sets is currently a bottleneck in many real-world applications of deep learning.
- There is a number of strategies to overcome massive manual image annotation.
- Here, we have seen three strategies:
  1. Contrastive Learning.
  2. Learning from weakly supervised data
  3. Learning from simulations
- Usually, the way in which we setup the annotation strategy usually also influences the methodological developments.

References I

[Chen et al., 2020] Chen, T., Kornblith, S., Norouzi, M., and Hinton, G. (2020). A Simple Framework for Contrastive Learning of Visual Representations. *arXiv:2002.05709 [cs, stat]*. arXiv: 2002.05709.

[Christiansen et al., 2018] Christiansen, E. M., Yang, S. J., Ando, D. M., Javaherian, A., Skibinski, G., Lipnick, S., Mount, E., O'Neil, A., Shah, K., Lee, A. K., Goyal, P., Fedus, W., Poplin, R., Esteva, A., Berndl, M., Rubin, L. L., Nelson, P., and Finkbeiner, S. (2018). In Silico Labeling: Predicting Fluorescent Labels in Unlabeled Images. *Cell*, 173(3):792–803.e19.

[Courtiol et al., 2017] Courtiol, P., Tramel, E. W., Sanselme, M., and Wainrib, G. (2017). Classification and disease localization in histopathology using only global labels: A weakly supervised approach. *CoRR*, pages 1–13.

References II

[Durand et al., 2016] Durand, T., Thome, N., and Cord, M. (2016). WELDON: Weakly Supervised Learning of Deep Convolutional Neural Networks. In *2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 4743–4752, Las Vegas, NV, USA. IEEE.

[Ganin et al., 2016] Ganin, Y., Ustinova, E., Ajakan, H., Germain, P., Larochelle, H., Laviolette, F., Marchand, M., and Lempitsky, V. (2016). Domain-Adversarial Training of Neural Networks. *Journal of Machine Learning Research*, 17(17):1–35.

[Iandola et al., 2017] Iandola, F. N., Han, S., Moskewicz, M. W., Ashraf, K., Dally, W. J., and Keutzer, K. (2017). SqueezeNet: AlexNet-level accuracy with 50x fewer parameters and <0.5MB model size. In *ICLR*, pages 1–13.

References III

[J. Boyd et al., 2020] J. Boyd, Z. Gouveia, F. Perez, and T. Walter (2020). Experimentally-Generated Ground Truth for Detecting Cell Types in an Image-Based Immunotherapy Screen. In *2020 IEEE 17th International Symposium on Biomedical Imaging (ISBI)*, pages 886–890.

[Oquab et al., 2015] Oquab, M., Bottou, L., Laptev, I., and Sivic, J. (2015). Is object localization for free? - Weakly-supervised learning with convolutional neural networks. In *2015 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 685–694, Boston, MA, USA. IEEE.

[Ouyang et al., 2018] Ouyang, W., Aristov, A., Lelek, M., Hao, X., and Zimmer, C. (2018). Deep learning massively accelerates super-resolution localization microscopy. *Nature Biotechnology*, 36:460.

References IV

[Russakovsky et al., 2015] Russakovsky, O., Deng, J., Su, H., Krause, J., Satheesh, S., Ma, S., Huang, Z., Karpathy, A., Khosla, A., Bernstein, M., Berg, A. C., and Fei-Fei, L. (2015). ImageNet Large Scale Visual Recognition Challenge. *International Journal of Computer Vision (IJCV)*, 115(3):211–252.

[Sullivan et al., 2018] Sullivan, D. P., Winsnes, C. F., Åkesson, L., Hjelmare, M., Wiking, M., Schutten, R., Campbell, L., Leifsson, H., Rhodes, S., Nordgren, A., Smith, K., Revaz, B., Finnbogason, B., Szantner, A., and Lundberg, E. (2018). Deep learning is combined with massive-scale citizen science to improve large-scale image classification. *Nature Biotechnology*, 36(9):820–828.

[Zhou, 2018] Zhou, Z.-H. (2018). A brief introduction to weakly supervised learning. *National Science Review*, 5(1):44–53.