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- Previous assignments
- The Mini-Project
- Introduction
- Convolution
- Convolutional Neural Networks
  - The Convolution Layer
  - The Pooling Layer
  - Regularization
  - Examples
- Transfer learning
- Practical Methodology

# Machine learning – Block 4

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Department of Statistics, Uppsala University

Autumn 2022



- Previous assignments
  - The Mini-Project
  - Introduction
  - Convolution
  - Convolutional Neural Networks
    - The Convolution Layer
    - The Pooling Layer
    - Regularization
    - Examples
  - Transfer learning
  - Practical Methodology
- 
- Previous assignments
  - The Mini-Project and Master Thesis Projects
  - Convolutional Neural Networks
  - Transfer Learning



## Assignment 3: Evaluation

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  - Practical Methodology
- A little too simple? Too uneven workload.
  - Problems with computer labs
  - Problems with Tensorflow and R
  - Use python. Maybe as an VG assignment?





# On this weeks assignment

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- Previous assignments
  - The Mini-Project
  - Introduction
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    - Regularization
    - Examples
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- It takes long time to run the models this week. Start early!





# Mini-project

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- Time to start think about the project.



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## Mini-project

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- Time to start think about the project.
- **Supervised problem of choice on real data.**



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# Mini-project

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- Time to start think about the project.
- **Supervised problem of choice on real data.**
- 2-3 students.



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## Mini-project

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- Time to start think about the project.
- **Supervised problem of choice on real data.**
- 2-3 students.
- Supply a **project proposal** of data and problem at the end of *15th of December 23.59*.
- *Hint!* Submit page 1-1.5 of the project as project proposal.
- Deadline is after all lectures on supervised learning



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- Feel free to combine it with your master thesis project!



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- *Hint!* Submit page 1-1.5 of the project as project proposal.
- Deadline is after all lectures on supervised learning
- Feel free to combine it with your master thesis project!
- Check with me if you have questions.
- The project should result in a 4 page report (PDF) using the **ICML LaTeX template**.



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## Section 3

### Introduction



# Convolutional Neural Networks

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- Acknowledgements: Anders Eklund, Linköping University.

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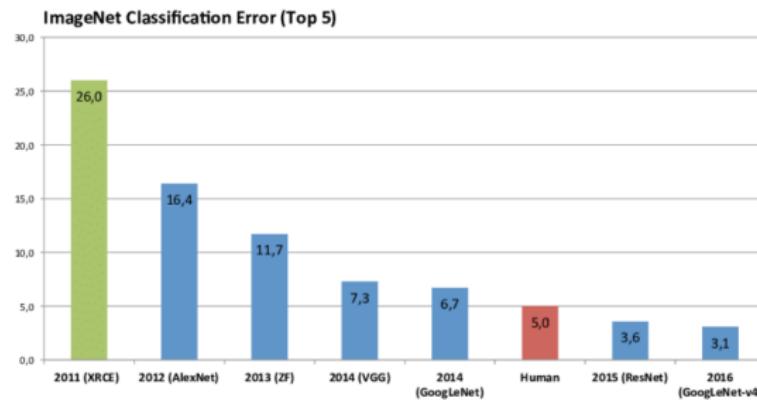


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# Convolutional Neural Networks

- **Acknowledgements:** Anders Eklund, Linköping University.
- **Convolutional** Neural Networks are behind great progress in the 2010s.
- It has revolutionized **Computer Vision**.
- Also called: ConvNets, Convolutional nets, Convolutional networks

Figure: ImageNet performance (Roessler, 2019)



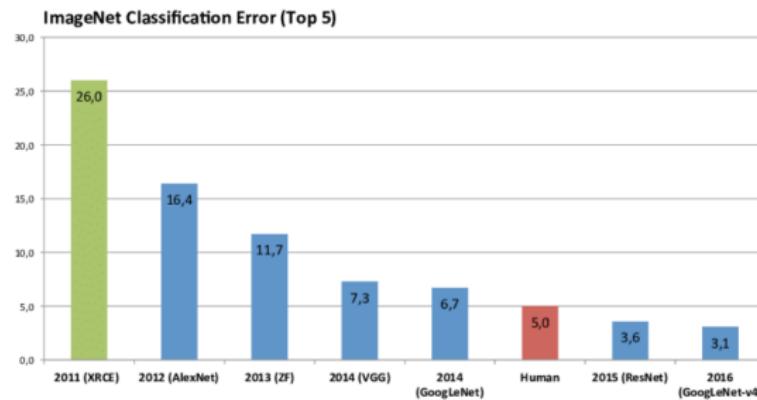


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- Special architecture that works well for data with a **grid structure**
    1. 1D-grids: Time series



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- Special architecture that works well for data with a **grid structure**
    1. 1D-grids: Time series
    2. 2D-grids: Gray-scale Images (pixels)



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- Special architecture that works well for data with a **grid structure**
    1. 1D-grids: Time series
    2. 2D-grids: Gray-scale Images (pixels)
    3. 3D-grids: Color Images (pixels and channels)



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- Special architecture that works well for data with a **grid structure**
    1. 1D-grids: Time series
    2. 2D-grids: Gray-scale Images (pixels)
    3. 3D-grids: Color Images (pixels and channels)
    4. 4D-grids: Color Video (pixels, channels, frames)



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- Problems
  - Image Classification



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- Problems
  - Image Classification
  - Image Segmentation



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# Computer Vision

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- Problems
  - Image Classification
  - Image Segmentation
  - Object Detection



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# Computer Vision

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## ● Problems

- Image Classification
- Image Segmentation
- Object Detection
- Object Localization



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- Problems
  - Image Classification
  - Image Segmentation
  - Object Detection
  - Object Localization
- **Focus:** 2D and 3D data



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# Computer Vision

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- **Problems**
  - Image Classification
  - Image Segmentation
  - Object Detection
  - Object Localization
- **Focus:** 2D and 3D data
- **Very Large Datasets:**
  - ImageNet: 14M Images, 20k classes, 1M bounding boxes



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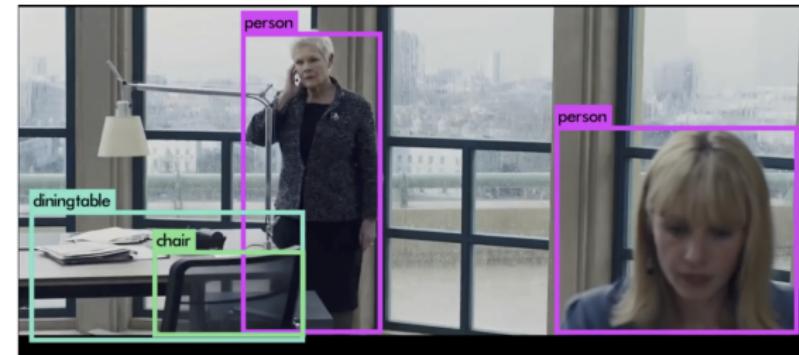
# Computer Vision

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- **Problems**
  - Image Classification
  - Image Segmentation
  - Object Detection
  - Object Localization
- **Focus:** 2D and 3D data
- **Very Large Datasets:**
  - ImageNet: 14M Images, 20k classes, 1M bounding boxes
  - Many different pre-trained models (e.g. VGG16)



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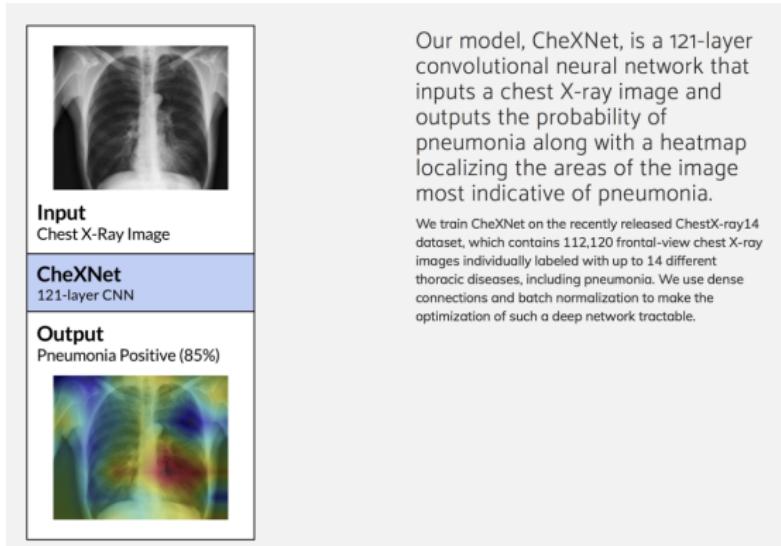
**Figure:** Object detection (see  
<https://www.youtube.com/watch?v=VOC3huqHrss>)



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## Example: Pneumonia detection



Our model, CheXNet, is a 121-layer convolutional neural network that inputs a chest X-ray image and outputs the probability of pneumonia along with a heatmap localizing the areas of the image most indicative of pneumonia.

We train CheXNet on the recently released ChestX-ray14 dataset, which contains 112,120 frontal-view chest X-ray images individually labeled with up to 14 different thoracic diseases, including pneumonia. We use dense connections and batch normalization to make the optimization of such a deep network tractable.

**Figure:** Rajpurkar et al. (2017). Chexnet: Radiologist-level pneumonia detection on chest x-rays with deep learning. arXiv preprint arXiv:1711.05225.



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## Example: Fracture detection



Figure 1. 2 images from the dataset. The area within the red box is the section presented to the network in order to classify the image. The left image is of a wrist fracture while the right image is without any apparent fracture.

**Figure:** Olczak et al, (2017) Artificial intelligence for analyzing orthopedic trauma radiographs, Acta Orthopaedica, 88:6, 581-586



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# What is an Image?

---

- 2-dimensional object
- Each pixel has:
  1. a coordinate
  2. a value (light intensity)



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- **Grayscale:** single channel
- **Color:** three channel (RGB)



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# What is an Image?

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- Each pixel has:
  1. a coordinate
  2. a value (light intensity)
- **Grayscale:** single channel
- **Color:** three channel (RGB)
- Spatial and hierarchical correlation structures



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## MNIST example

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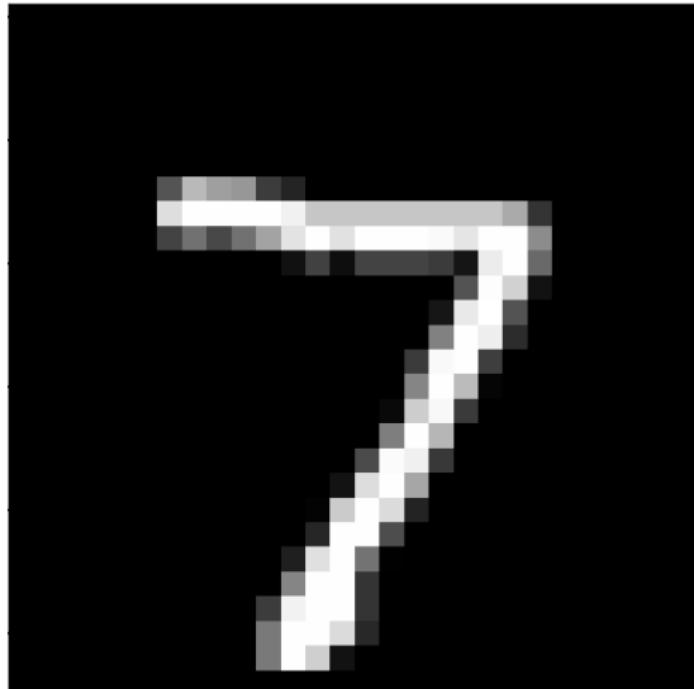


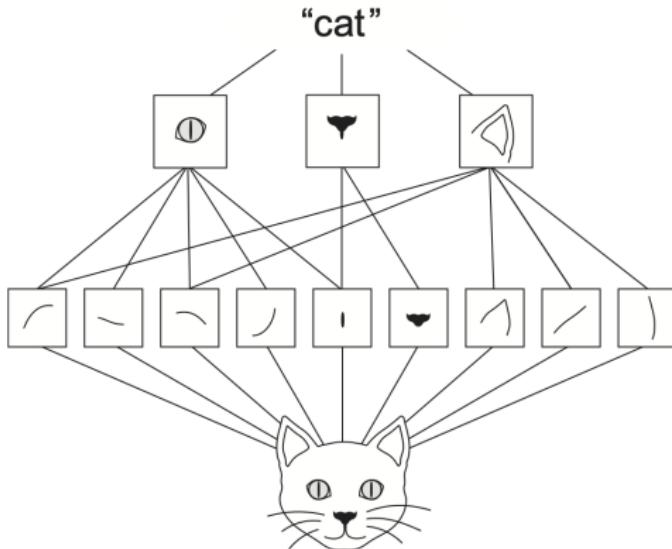
Figure: Example from the MNIST dataset (28 by 28 pixels)



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# How to train models for images?

- We want to learn **representations** of parts of images



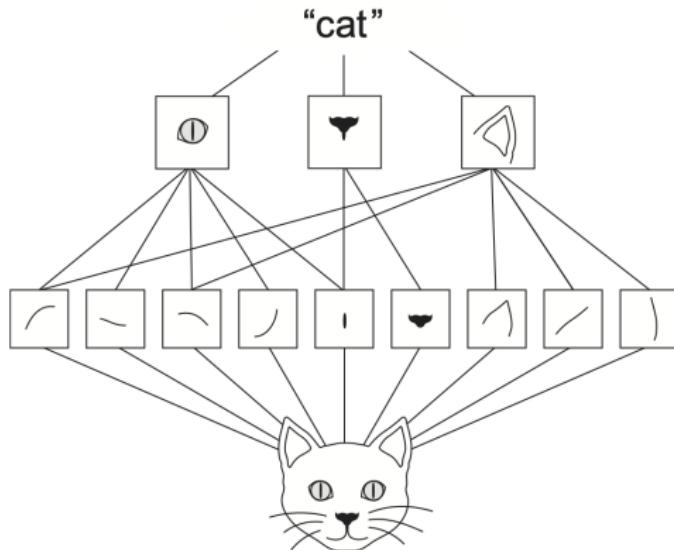
**Figure:** The representations of a cat (Chollet and Allair, 2018, Fig 5.2)



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# How to train models for images?

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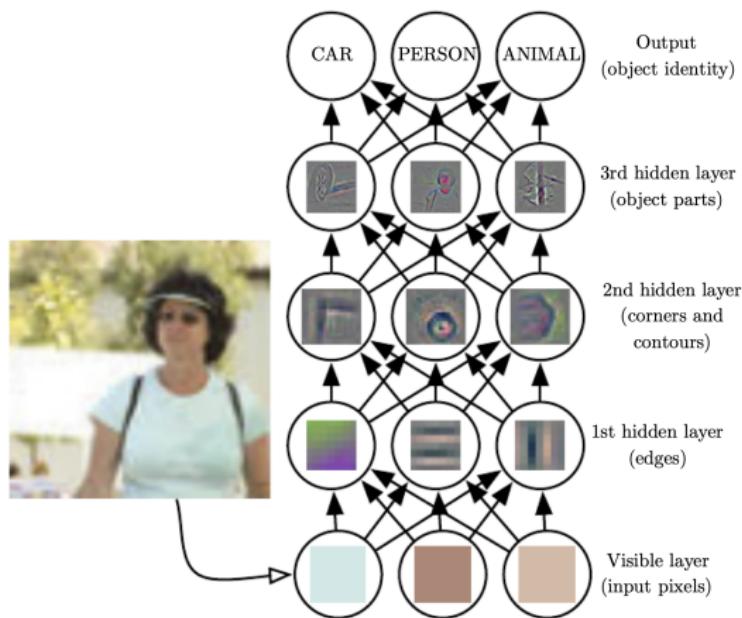
**Figure:** The representations of a cat (Chollet and Allair, 2018, Fig 5.2)

- CNN uses **Convolutional Layers** to learn **parameter efficient** representations



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# Learning Representations for Images (again)



**Figure:** Learning representations for images (Goodfellow et al, 2017, Fig. 1.2)



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## Section 4

### Convolution



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# Convolution

---

- Different definitions are common, one example:

$$y(t) = \int x(\tau)k(t - \tau)d\tau = (x * k)(t)$$

- Intuition: "Weighting together two functions"
- In a convolutional layer:

1.  $x(t)$ : Input
2.  $k(t)$ : Kernel, filter, "feature"
3.  $y(t)$ : Output, feature map



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# Discrete Convolution

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- If  $t$  is discrete (as in a grid):

$$y(t) = (x * k)(t) = \sum_{\tau=-\infty}^{\infty} x(\tau)k(t - \tau)$$

- In the case of images we have 2 discrete dimensions

$$Y(i, j) = (X * K) \sum_m \sum_n X(m, n)K(i - m, j - n)$$

- Sometimes the cross-correlation is called convolution:

$$Y(i, j) = (X * K) \sum_m \sum_n X(m, n)K(i + m, j + n)$$

1.  $X(i, j)$ : Input (2D)
2.  $K(i, j)$ : Kernel, filter, "feature" (2D)
3.  $Y(i, j)$ : Output, feature map (2D)



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# Convolution of Images: 2D

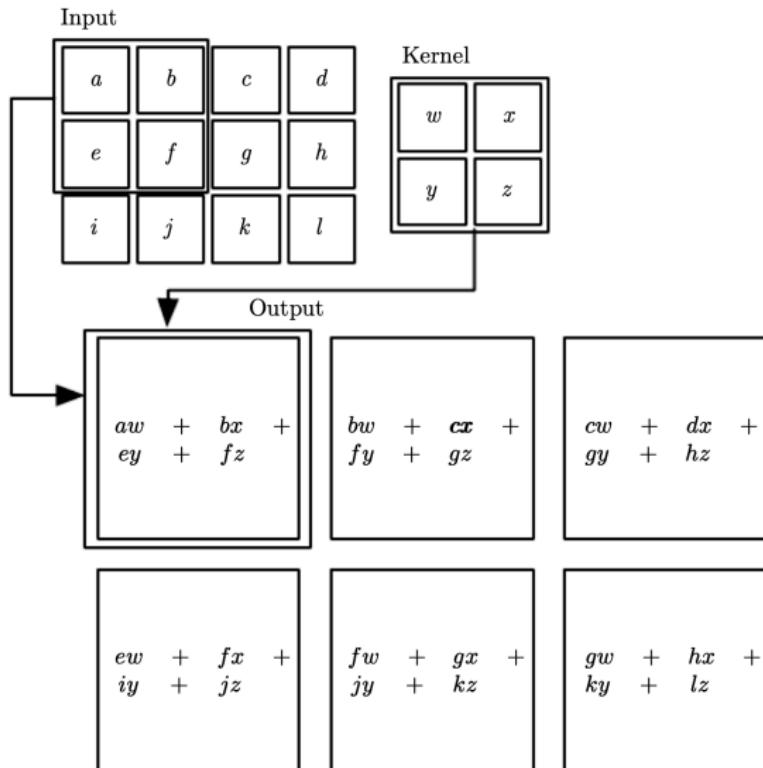


Figure: Convolution for an Image (Goodfellow et al, 2017, Fig. 9.1)



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# Convolution of images: Example

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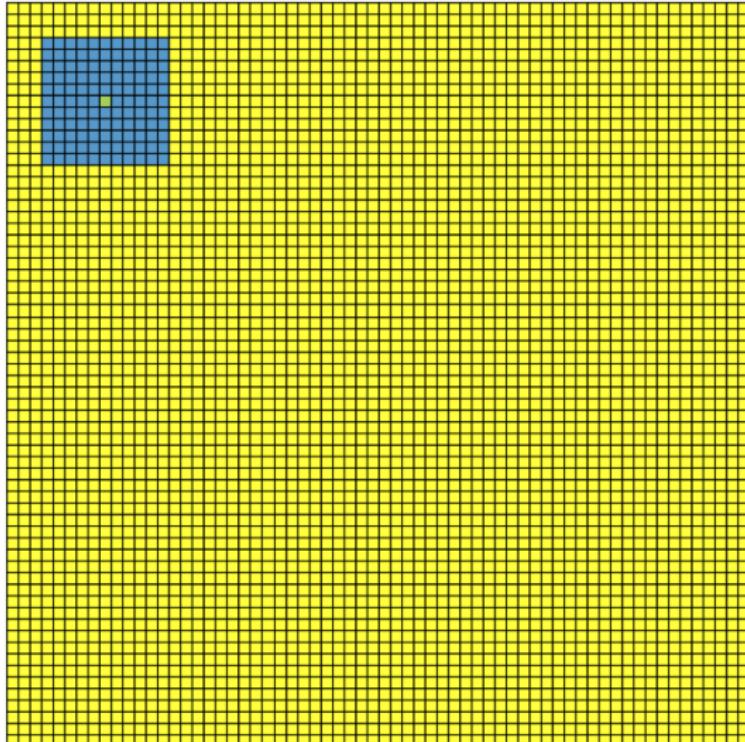


Figure: Convolution example.



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# Convolution of images: Examples

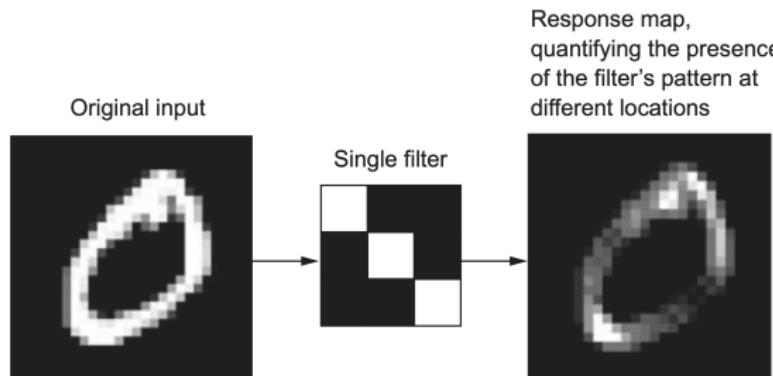


Figure: Convolution for an Image (Chollet and Allaire, 2018, Fig. 5.3)



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$$X = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}, K = \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$



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## Convolution of images: Example

---

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$$Y = \begin{bmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 1 & 2 & 0 \end{bmatrix},$$



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## Section 5

# Convolutional Neural Networks



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# Convolutional Neural Networks

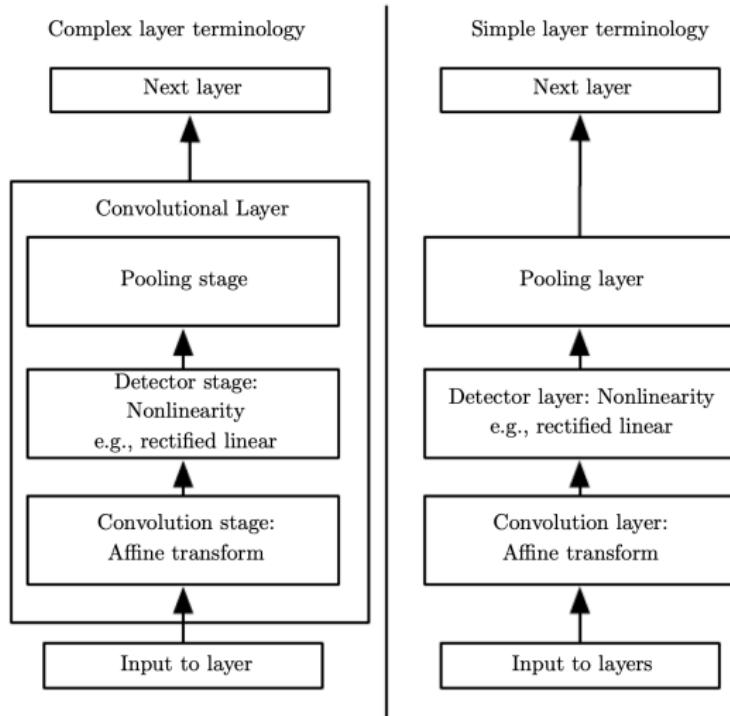


Figure: Convolution layer (Goodfellow et al, 2018, Fig. 9.7)



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# Convolutional Neural Networks

---

- Most convolutional neural networks have:
  1. Many convolutional layers
  2. More kernels higher up in the network
  3. A classification head (usually a feed-forward neural network)



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- Benefits:
  1. Few(er) parameters (filters)
  2. Captures **local structures**
  3. Efficient computations



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- How to choose filters?
  1. Before: **manually handcrafted**



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- Benefits:
  1. Few(er) parameters (filters)
  2. Captures **local structures**
  3. Efficient computations
- How to choose filters?
  1. Before: **manually handcrafted**
  2. Now: **learn the filters**



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# Convolution layer

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- **Input:** Data or Feature Maps



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# Convolution layer

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- **Input:** Data or Feature Maps
- **Parameters:**
  - $N$  filters/kernels of size  $m \times m$
  - $N$  bias terms (one per filter)



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# Convolution layer

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- **Input:** Data or Feature Maps
- **Parameters:**
  - $N$  filters/kernels of size  $m \times m$
  - $N$  bias terms (one per filter)
- **Activation functions:** Applied element wise on feature maps



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- **Parameters:**
  - $N$  filters/kernels of size  $m \times m$
  - $N$  bias terms (one per filter)
- **Activation functions:** Applied element wise on feature maps
- **Output:** Feature Maps



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# Convolution layer

---

- **Input:** Data or Feature Maps
- **Parameters:**
  - $N$  filters/kernels of size  $m \times m$
  - $N$  bias terms (one per filter)
- **Activation functions:** Applied element wise on feature maps
- **Output:** Feature Maps
- In Keras:  
`layer_conv_2d(filters = 32, kernel_size = c(3,3), activation = "relu", input_shape = c(32,32,3))`



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# Padding

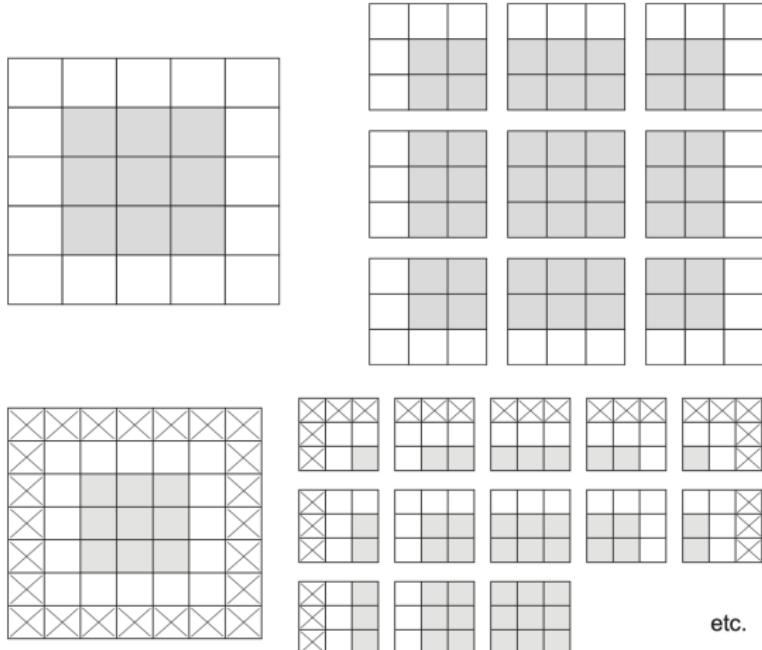
---

- Handling edges
- *Padding*: add 0 around the image
- Necessary to **keep size** of feature maps



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# Padding



**Figure:** Padding and valid edge handling (Chollet and Allair (2018), Fig. 5.5, 5.6)



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# Stride

---

- Skip every  $n$ th pixel
- Reduces the computations

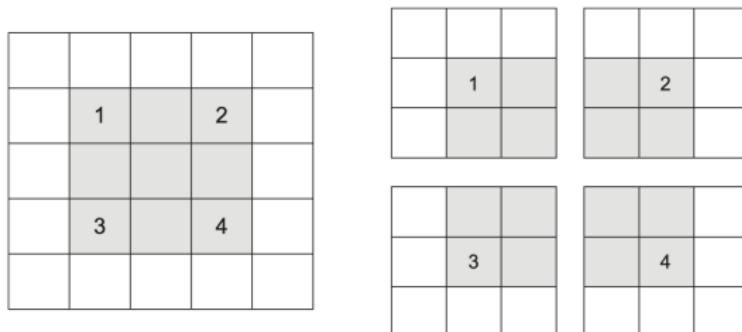


Figure: Strides (Chollet and Allair (2018), Fig. 5.5, 5.6)



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# Why Convolution Layers?

---

- Captures local spatial structure
- Reduces the number of parameters (parameter sharing)
  1. The number and size of filters
  2. We use the same filters everywhere



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# Why Convolution Layers?

---

- Captures local spatial structure
- Reduces the number of parameters (parameter sharing)
  1. The number and size of filters
  2. We use the same filters everywhere
- Example: a 1 megapixel image ( $1000 \times 1000$  pixels)
  1. Dense network with 100 nodes: **100M** parameters
  2. CNN network with 100  $3 \times 3$  filters: **1000** parameters  
(900 from filters, 100 bias terms)



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# Convolution Neural Nets

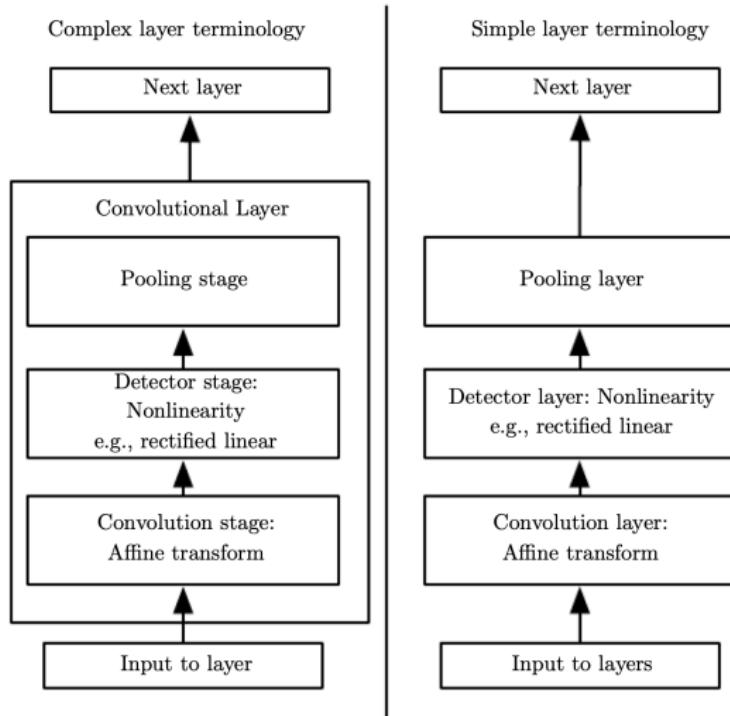


Figure: Convolution layer (Goodfellow et al, 2018, Fig. 9.7)



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## Detector stage

---

- Remember, in feed-forward networks:  $\mathbf{h} = \sigma(\mathbf{XW} + b)$
- In CNN:
  1.  $\mathbf{W}$  is the filter



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## Detector stage

---

- Remember, in feed-forward networks:  $\mathbf{h} = \sigma(\mathbf{XW} + b)$
- In CNN:
  1.  $\mathbf{W}$  is the filter
  2.  $\mathbf{X}$  is the input feature map



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## Detector stage

---

- Remember, in feed-forward networks:  $\mathbf{h} = \sigma(\mathbf{XW} + b)$
- In CNN:
  1.  $\mathbf{W}$  is the filter
  2.  $\mathbf{X}$  is the input feature map
  3.  $\mathbf{XW}$  is the convolutional feature map



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## Detector stage

---

- Remember, in feed-forward networks:  $\mathbf{h} = \sigma(\mathbf{XW} + b)$
- In CNN:
  1.  $\mathbf{W}$  is the filter
  2.  $\mathbf{X}$  is the input feature map
  3.  $\mathbf{XW}$  is the convolutional feature map
  4.  $b$  is a bias (one per filter)



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## Detector stage

---

- Remember, in feed-forward networks:  $\mathbf{h} = \sigma(\mathbf{XW} + b)$
- In CNN:
  1.  $\mathbf{W}$  is the filter
  2.  $\mathbf{X}$  is the input feature map
  3.  $\mathbf{XW}$  is the convolutional feature map
  4.  $b$  is a bias (one per filter)
  5.  $\sigma$  is the activation function (usually a ReLU)



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- We take a function  $f$  that return one value per pooling kernel



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# Pooling layer

---

- We take a function  $f$  that return one value per pooling kernel
- Most commonly  $f = \max$
- Commonly a  $2 \times 2$  pooling kernel with stride 2
- **Why?** Reduce the size of feature map, but keep the activation



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# Pooling layer

---

- We take a function  $f$  that return one value per pooling kernel
- Most commonly  $f = \max$
- Commonly a  $2 \times 2$  pooling kernel with stride 2
- **Why?** Reduce the size of feature map, but keep the activation
- In Keras:  
`layer_max_pooling_2d(pool_size = c(2, 2))(`



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# Max Pooling

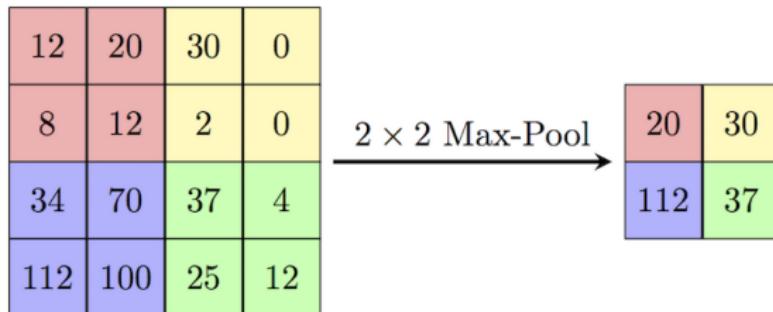


Figure: Strides (Computer Science Wikipedia)



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## Using pooling to learn invariances

- pooling over spatial positions: invariant to translation
- pooling over different filters: invariant to transformations

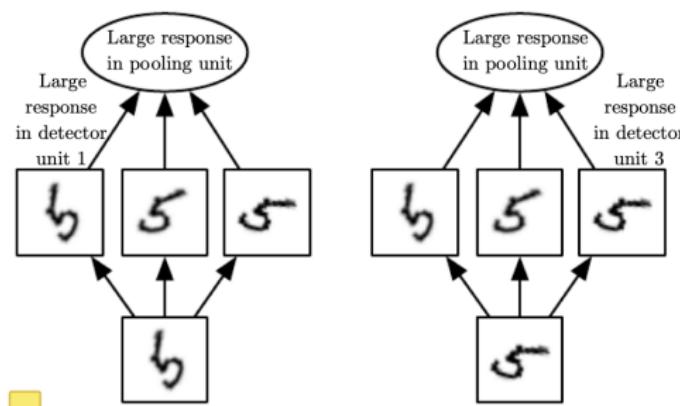


Figure: Learning invariances (Goodfellow et al., 2017, Fig. 9.9)



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# Data Augmentation

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Figure: Data Augmentation (Chollet and Allair, 2018, Fig 5.10)



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# Data Augmentation

---



Figure: Data Augmentation (Chollet and Allair, 2018, Fig 5.10)

- Can be done directly in Keras (data generator)

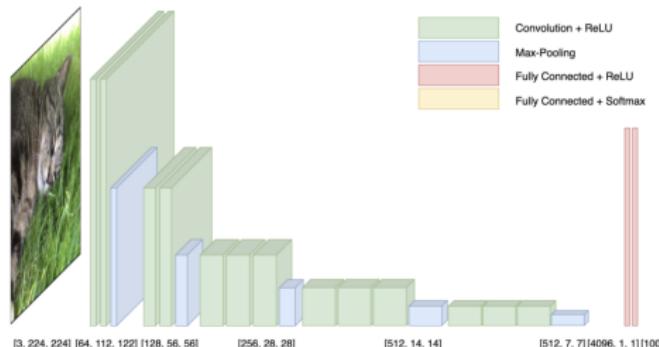


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- 
- AlexNet (2012), 5 convolutional layers
  - VGG16 (2014), 16 convolutional layers
  - ResNet (2015), 152 convolutional layers



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# VGG16



**Figure 2.4:** Illustration of the data flow through the network VGG16. Data size, of the format  $[c, h, w]$ , is shown for the input image, output of each max-pooling layer, output after the first two fully connected layers, and the final network output.

Jesper Westell, Multi-Task Learning using Road Surface Condition Classification and Road Scene Semantic Segmentation, LIU-IMT-TFK-A-19/570-SE



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## Section 6

### Transfer learning



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# Transfer learning

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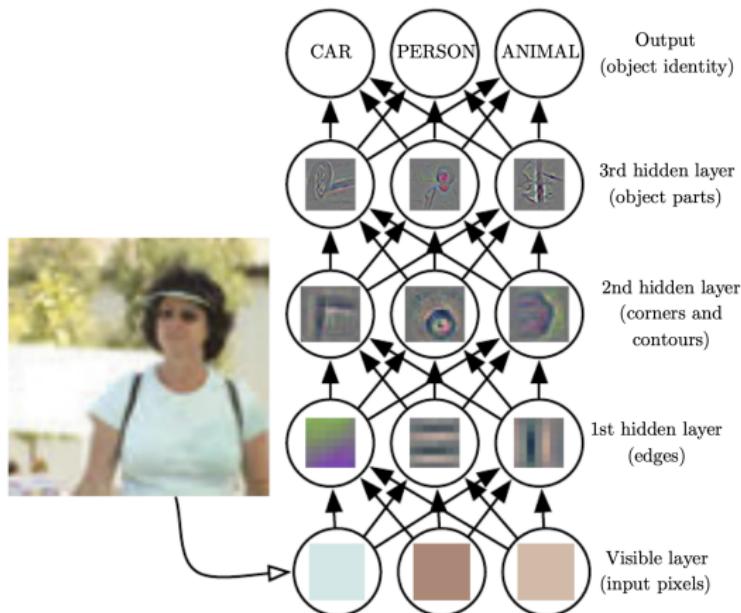
- "Transfer knowledge between problems"
- Learning representations in  $P_1$  will aid generalization in  $P_2$



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- 
- "Transfer knowledge between problems"
  - Learning representations in  $P_1$  will aid generalization in  $P_2$
  - A Bayesian perspective: A strong prior



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**Figure:** Learning representations can be crucial (Goodfellow et al, 2017, Fig. 1.2)



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- In practice: Transfer/reuse learned weights or rather some weights



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- In practice: Transfer/reuse learned weights or rather some weights
  - Use (large) pre-trained models for smaller problems
  - A reason for the success of CNN



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# Transfer learning

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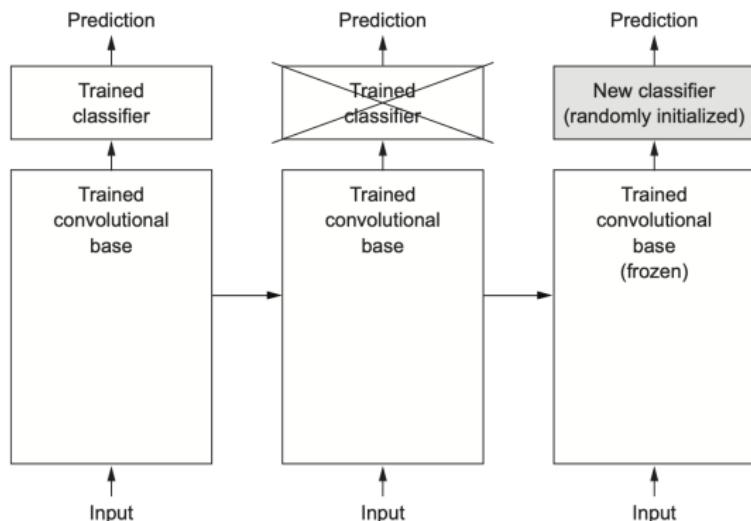
- In practice: Transfer/reuse **learned weights** or rather some weights
- Use (large) **pre-trained** models for smaller problems
- A reason for the success of CNN
- Two types of transfer learning in Neural Networks:
  - Feature extraction (use pre-trained networks for features)
  - Fine Tuning (adapt pre-trained features)



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## Feature Extraction



**Figure:** Using convnets as base for feature extraction (Chollet and Allair, 2018, Fig 5.12)



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## Fine-Tuning

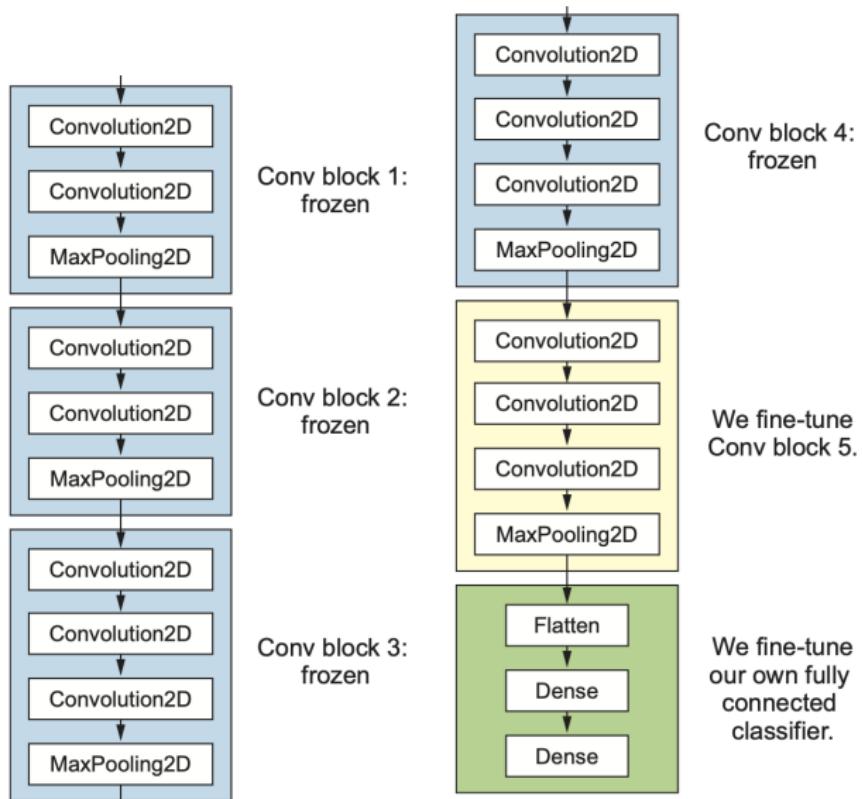


Figure: Finetuning a convolutional base (Chollet and Allair, 2018,  
Fig 5.15)



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# Transfer learning

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- Catastrophic forgetting



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- 
- Catastrophic forgetting
  - Domain adaptation: Same problem but at different input dataset
    - (e.g. language models for legal/medical/political data)



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# Transfer learning

---

- Catastrophic forgetting
- Domain adaptation: Same problem but at different input dataset  
(e.g. language models for legal/medical/political data)
- Concept drift: Similar problem



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# Transfer learning

---

- Catastrophic forgetting
- Domain adaptation: Same problem but at different input dataset  
(e.g. language models for legal/medical/political data)
- Concept drift: Similar problem
- Previously, popular with unsupervised pre-training.



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## Section 7

### Practical Methodology



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# Practical Methodology

---

## 1. Determine your goals



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# Practical Methodology

---

1. Determine your goals
2. Setup your baseline  
(establish a working end-to-end pipeline as soon as possible)



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# Practical Methodology

---

1. Determine your goals
2. Setup your baseline  
(establish a working end-to-end pipeline as soon as possible)
3. Diagnose your networks performance



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# Practical Methodology

---

1. Determine your goals
  2. Setup your baseline  
(establish a working end-to-end pipeline as soon as possible)
  3. Diagnose your networks performance
  4. Make incremental improvements
- 
- **General idea:** Increase data and model capacity until goal is reached





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# Practical Methodology

---

1. Determine your goals
  2. Setup your baseline  
(establish a working end-to-end pipeline as soon as possible)
  3. Diagnose your networks performance
  4. Make incremental improvements
- 
- General idea: Increase data and model capacity until goal is reached
  - End goal: Good enough performance on test set





# 1. Determine your goals

---

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- Why are you building a model?





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- 
- Why are you building a model?
  - Set up the metric based on the **overall goal** of the system!  
This may need multiple metrics.



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## 1. Determine your goals

---

- Why are you building a model?
- Set up the metric based on the **overall goal** of the system!  
This may need multiple metrics.
- What is good enough? Remember the **Bayes error**!



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## 1. Determine your goals

---

- Why are you building a model?
- Set up the metric based on the **overall goal** of the system!  
This may need multiple metrics.
- What is good enough? Remember the **Bayes error**!
- What performance can you expect?



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## 1. Determine your goals

---

- Why are you building a model?
- Set up the metric based on the **overall goal** of the system!  
This may need multiple metrics.
- What is good enough? Remember the **Bayes error**!
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- Some errors are worse than others, e.g. spam filters.



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## 1. Determine your goals

---

- Why are you building a model?
- Set up the metric based on the **overall goal** of the system!  
This may need multiple metrics.
- What is good enough? Remember the **Bayes error**!
- What performance can you expect?
- Some errors are worse than others, e.g. spam filters.
- Handling of uncertain predictions:
- **Coverage:** How large proportions can the system predict?



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## 1. Determine your goals

---

- Why are you building a model?
- Set up the metric based on the **overall goal** of the system!  
This may need multiple metrics.
- What is good enough? Remember the **Bayes error**!
- What performance can you expect?
- Some errors are worse than others, e.g. spam filters.
- Handling of uncertain predictions:
- **Coverage:** How large proportions can the system predict?
- Manual curation can be faster and easier.



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## 2. Setup your baseline

---

- Start with...
  - the most simple possible model (logistic regression)



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## 2. Setup your baseline

---

- Start with...
  - the most simple possible model (logistic regression)
  - previous approaches/baselines



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## 2. Setup your baseline

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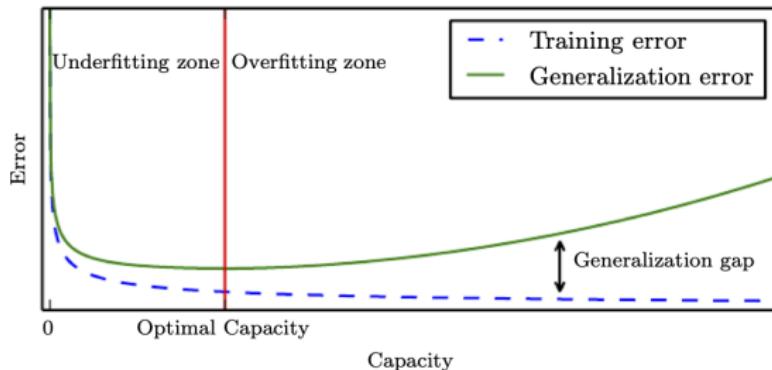
- Start with...
  - the most simple possible model (logistic regression)
  - previous approaches/baselines
  - a simple neural network that is common in the domain/defaults  
(CNN for images, Adam as optimizer)



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## Remember: Statistical Learning Theory

Figure: Test, training, and model complexity (Goodfellow et al, 2017, Figure 5.3)





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- High training loss: Training data not fully used  
Neural network generally performs best when training error is low



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### 3. Diagnose and improve

---

- High training loss: Training data not fully used  
Neural network generally performs best when training error is low
- High test loss: Low data quality, i.e. large Bayes error?



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### 3. Diagnose and improve

---

- High training loss: Training data not fully used  
Neural network generally performs best when training error is low
- High test loss: Low data quality, i.e. large Bayes error?
- Low training error and high test error: Common situation



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- High training loss: Training data not fully used  
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- High test loss: Low data quality, i.e. large Bayes error?
- Low training error and high test error: Common situation
  - You can always improve by gather more data, or
  - Regularize to optimal capacity



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  - You can always improve by gather more data, or
  - Regularize to optimal capacity
- How to know the improvements of additional data?



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# Learning curve

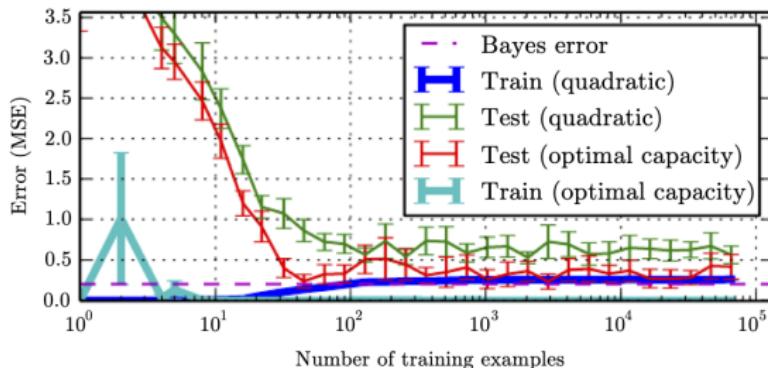


Figure: Learning curve to assess the need for more data (Goodfellow et al., 2017, Fig 5.4)



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### 3. Diagnosing and improving your model: Regularization

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- Best performance: Larger model that is regularized well.
- Warning: Avoid **the algorithm rabbit hole**



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  1. Get good training error. E.g. by tune learning rate and increasing capacity



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- Hyperparameter optimization
  1. Get good training error. E.g. by tune learning rate and increasing capacity
  2. Tune hyperparameters (regularization):  
Requires monitoring both training and test error



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# Hyper-parameter optimization

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- Neural networks has many hyperparameters
- What is a hyperparameter in a neural network?
- Grid search:
  - Setup a grid of potential values
  - For 1-4 hyperparameter: grid search can work well
  - Usually iterative/repeated grid search is best: start with three values, and work iteratively
  - Grows exponentially with the number of parameters
- Random search
  - Specify a marginal distribution for each hyperparameter (additional work)
  - Common: uniform on log scale
  - Can also be done iteratively
  - random search can be exponentially more efficient
  - reduce the error faster



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# Diagnosis and Debugging

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- Visualize the model predictions
- Analyze the worst errors: **why?**
- Use train and test error as a diagnostic: **Can you overfit the data?**
- Use test suites: Can you get known results on a toy data.  
Both training error and derivatives
- Monitor the gradients
- Monitor activation function statistics. Are some never activated?