# Deep Learning

Lessons: **Kevin Scaman** TPs: Paul Lerner



### Class overview

### Lessons

1. Introduction, simple architectures (MLPs) and autodiff	09/02
2. Training pipeline, optimization and image analysis (CNNs)	16/02
3. Sequence regression (RNNs), stability and robustness	08/03
4. Generative models in vision and text (Transformers, GANs)	15/03
Practicals	
Tacticals	
TP1: MLPs and CNNs in Pytorch	01/03
TP2: RNNs and generative models	22/03

# Projects

### Overview

- Teams of up to 4 students
- DL task with Pytorch implementation
- You can chose your topics from: https://kscaman.github.io/teaching/2023\_ENSAE\_DL.html
- Can also propose one, but better to start with an existing library

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# Deadlines

- (01/03) Team formation and topics: Send email (kevin.scaman@inria.fr) with team and topic (link to repo + short description)
- (29/03) Deliverables: Report (pdf) + code (link to a colab/git repo)

# Projects

# Guidelines and tips

- Usually better to start with an existing library.
- Re-obtaining the results and implementing one alternative method / adaptation to another setting / use on an application is sufficient.
- Usually, the first try doesn't work... Investigate why!
- ▶ We're not looking for SOTA performance... hard work is more valued. :)
- Don't start too late... debugging takes time.

# Pytorch tensors The building blocks of DL implementations

### Pytorch tensors

- A tensor is a d-dimensional array in Pytorch.
- Can store real values, vectors, matrices...
- Made to mimic Numpy arrays.

1	2	5	1	
0	4	0	0	
-4	5	3	-1	
3	0	2	6	
1	0	1	4	
0	0	3	0	
6	1	1	4	
2d tensor shape: (7,4)				

			-
2	5	1	╟
4	0	0	╟
5	3	-1	╟
0	2	6	╟
0	1	4	╟
0	3	0	╟
1	1	4	╟
	2 4 5 0 0 0 0 1	2         5           4         0           5         3           0         2           0         1           0         3           1         1	2         5         1           4         0         0           5         3         -1           0         2         6           0         1         4           0         3         0           1         1         4

3d tensor shape: (7,4,3)

10		6
411		

shape: (7)

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- 4. **Reshaping:** "x.view(1,3,-1)" or "x.unsqueeze(0)" to add a dimension of size 1.
- 5. Other operations: See doc ③. "torch.sum(x)", "torch.mean(x)"...

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- Many errors can be unnoticed due to wrong tensor sizes and Python's dynamic typing...
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A tensor of shape (5,1) is not the same a tensor of shape (5)!

# Deep learning training pipeline Training and testing neural networks (in Pytorch)

# Back to cats and dogs

Typical binary classification task. Objective is to distinguish cat images from dog images.



DL training pipeline

# Pytorch training pipeline

#### Data loader $\rightarrow$ model creation $\rightarrow$ loss function $\rightarrow$ optimization loop

# Dataloading

Dataset class

torch.utils.data.Dataset is an abstract class representing a dataset. Your custom dataset should inherit Dataset and override the following methods:

- > \_\_len\_\_ so that len(dataset) returns the size of the dataset.
- > \_\_getitem\_\_ to support the indexing such that dataset[i] gives the ith sample.

### Iterating through the dataset with Dataloader

By using a simple for loop to iterate over the data, we are missing out on:

- Batching the data,
- Shuffling the data,
- Load the data in parallel using multiprocessing workers.

torch.utils.data.DataLoader is an iterator which provides all these features.

# Dataloading (advanced)

Transformations

- torchvision.transforms allows to easily compose data transformations to the data.
- img\_transform = transforms.Compose([transforms.CenterCrop(224),

transforms.ToTensor(),
transforms.Normalize(mean, std)])

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# Dataloader

- To create a dataloader for the training set, use torch.utils.data.DataLoader: loader = DataLoader(dataset, batch size=64, shuffle=True, num workers=6)
- Includes a random mini-batch selection mechanism and parallelization.
- Used as an iterator: for inputs, targets in train\_loader: ...

## Model creation

### Sequential neural networks and MLPs

- One liner for MLPs: model = nn.Sequential(nn.Linear(2,4), nn.ReLU(),...)
- More generally any sequence of already existing layers.
- How to create new layers or entirely new architectures?

### The Module class

- ▶ All models are exentions of the nn.Module class.
- Need to implement a model.forward(x) function.
- Can be called as a function model(x).

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```
Example (function of two variables)
class YourModel(nn.Module):
    def __init__(self):
        super().__init__()
        self.lin = nn.Linear(10, 100)
    def forward(self, x, y)
        x = self.lin(x)
```

```
return y + torch.exp(torch.mean(x, dim=1))
```

DL training pipeline

# Neural networks in Pytorch (2)

A function backward is automatically implemented to perform **backpropagation**.

DL training pipeline

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- A function backward is automatically implemented to perform **backpropagation**.
- By default, the parameters model.parameters() are randomly initialized.
- Hierarchical structure: All layers also extend nn.Module, and any module can be used in another module. All modules used by a model are accessible via model.children().

# Loss functions (recap)

### Empirical risk minimization

Let  $(x_i, y_i)_{i \in [\![1,n]\!]}$  be a collection of n observations drawn independently according to  $\mathcal{D}$ . Then, the objective of *empirical risk minimization* (ERM) is to find a minimizer  $\hat{\theta}_n \in \mathbb{R}^p$  of

$$\min_{\theta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n \ell(g_\theta(x_i), y_i)$$

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### Losses used for training

- Regression: Mean sqaure error (MSE)  $\ell(y,y') = \|y-y'\|_2^2 = \sum_i (y_i y'_i)^2$
- Classification: Cross entropy (CE)  $\ell(y, y') = -\sum_i y'_i \ln\left(\exp(y_i) / \sum_j \exp(y_j)\right)$

# Cross entropy

▶ Intuition: The model outputs a score for each class  $y_i = g_{\theta}(x)$ . We create a probability on the classes  $p_i = \frac{\exp(y_i)}{\sum_j \exp(y_j)}$ . We then take the negative logarithm of the true class's probability  $\ell(y, y') = -\log(p_k)$ , where  $k \in [\![1, C]\!]$  s.t.  $y'_i = \mathbb{1}\{i = k\}$ .

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$$\mathbb{P}_{\theta}((X_i, Y_i)) = \prod_i \mathbb{P}(X_i) \mathbb{P}_{\theta}(Y_i \mid X_i) \propto \prod_i \frac{\exp(g_{\theta}(X_i)_{Y_i})}{\sum_k \exp(g_{\theta}(X_i)_k)}$$

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▶ Interpretation #2: Difference between the scores of the predicted and true classes.

$$\ell(y, y') = \log\left(\sum_{i} \exp(y_i)\right) - y_k \approx \max_{i} y_i - y_k$$

# Cross entropy: in practice

- **Definition:**  $\ell(x, y) = -\log\left(\frac{\exp(x_y)}{\sum_i \exp(x_i)}\right).$
- PyTorch: criterion = nn.CrossEntropyLoss()
- Several parameters (reduction='sum' or reduction='mean', see the doc)
- criterion takes as input the scores (a tensor of shape [b, d]), and either a class index per sample, or class probabilities for each sample.
- Composition of nn.LogSoftmax() and nn.NLLLoss().



Gradient through a softmax can explode due to numerical errors (taken care of by the Pytorch implementation of nn.CrossEntropyLoss() and nn.LogSoftmax()).

# First-order optimization Gradient descent and co.
Find a **minimizer**  $\theta^{\star} \in \mathbb{R}^d$  of a given objective function  $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ ,

```
\theta^{\star} \in \operatorname*{argmin}_{\theta \in \mathbb{R}^d} \mathcal{L}(\theta)
```

• Using an iterative algorithm relying on the **gradient**  $\nabla \mathcal{L}(\theta_t)$  at each iteration  $t \ge 0$ .



source: https://distill.pub/2017/momentum/



#### Iterative optimization algorithms

- ▶ Initialization:  $\theta_0 \in \mathbb{R}^d$  (important in practice!).
- **Iteration:** Usually  $\theta_{t+1} = \varphi_t(\theta_t, \nabla \mathcal{L}(\theta_t), s_t)$  where  $s_t$  is a hidden variable that is also updated at each iteration.
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▶ **Non-convexity:** If  $\mathcal{L}$  is **convex**, i.e.  $\forall \theta, \theta', \mathcal{L}(\frac{\theta+\theta'}{2}) \leq \frac{\mathcal{L}(\theta)+\mathcal{L}(\theta')}{2}$ , the optimization problem is **simple**. Most theoretical results use this assumption to prove convergence.

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- High dimensionality: number of parameters  $d \gg 1000$ .
- Access to the gradient: the gradient of  $\mathcal{L}$  is too expensive to compute! In practice,  $\nabla \mathcal{L}(\theta_t)$  is replaced by a stochastic or mini-batch approximation  $\widetilde{\nabla}_t$ .

▶ Let  $\mathcal{L}_i(\theta) = \ell(g_\theta(x_i), y_i)$ . Recall empirical risk minimization, aka training error:

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$$\theta_{t+1} = \theta_t - \eta \nabla \mathcal{L}_{i_t}(\theta)$$

Mini-batch gradient descent: gradient approximated with multiple random samples.

$$\theta_{t+1} = \theta_t - \frac{\eta}{b} \sum_{i=1}^{b} \nabla \mathcal{L}_{i_{b,t}}(\theta)$$

### Some warnings about optimization in deep learning



#### Our final goal is to reduce the **population risk**, i.e. $\mathbb{E}(\ell(g_{\theta}(X), Y))!$

- We need to pay attention to overfitting in addition to using the optimization algorithm to reduce the training error.
- In this class, we focus specifically on the **performance** of the optimization algorithm in minimizing the objective function, rather than the model's generalization error.
- In the next lessons, we will see techniques to avoid overfitting.

# Challenges

- Mini-batch gradient descent is the algorithm of choice when training a neural network. The term SGD is usually employed also when mini-batches are used!
  - Choosing a learning rate can be difficult. How to **adapt the learning rate** during training?
  - Why applying the same learning rate to all parameter updates?
  - How to escape saddle points where the gradient is close to zero in all dimension?
- > In the rest of the lecture, we will introduce modifications to (S)GD.
- Nice survey by Sebastian Ruder: http://ruder.io/optimizing-gradient-descent/





source: Visualizing the Loss Landscape of Neural Nets, Li et.al., 2018

#### Momentum

Accelerating SGD by dampening oscillations, i.e. by averaging the last values of the latest gradients.

$$v_{t+1} = \gamma v_t + \eta \nabla \mathcal{L}(\theta_t)$$
  
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• Why does it work? With  $g_t = \nabla \mathcal{L}(\theta_t)$ , we have for any  $k \ge 0$ :

$$v_{t+1} = \gamma^k v_{t-k} + \eta \qquad \sum_{i=0}^k \gamma^i g_{t-i}$$

average of last gradients

• Typical value for  $\gamma = 0.9$ .

### Adagrad

We would like to adapt our updates to each individual parameter, i.e. have a different decreasing learning rate for each parameter.

$$s_{t+1,i} = s_{t,i} + \nabla \mathcal{L}(\theta_t)_i^2$$
  
$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{s_{t+1,i} + \epsilon}} \nabla \mathcal{L}(\theta_t)_i$$

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- No manual tuning of the learning rate.
- Typical default values:  $\eta = 0.01$  and  $\epsilon = 10^{-8}$ .

source: Duchi et al., Adaptive Subgradient Methods for Online Learning and Stochastic Optimization, JMLR 2011

## RMSProp

- > Problem with Adagrad, learning rate goes to zero and never forgets about the past.
- ▶ Idea proposed by G. Hinton in his Coursera class: use exponential average.

$$s_{t+1,i} = \gamma s_{t,i} + (1-\gamma)\nabla \mathcal{L}(\theta_t)_i^2$$
$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{s_{t+1,i} + \epsilon}}\nabla \mathcal{L}(\theta_t)_i$$

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▶ With a slight abuse of notation, we re-write the update as follows:

$$s_{t+1} = \gamma s_t + (1 - \gamma) \nabla \mathcal{L}(\theta_t)^2$$
  
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{s_{t+1} + \epsilon}} \nabla \mathcal{L}(\theta_t)$$

• Typical values:  $\gamma = 0.9$  and  $\eta = 0.001$ .

source: Hinton Coursera lecture 6

ENSAE

#### Adam

Mixing RMSProp and momentum, we get Adam = Adaptive moment Estimation.

$$m_{t+1} = \beta_1 m_t + (1 - \beta_1) \nabla \mathcal{L}(\theta_t)$$

$$v_{t+1} = \beta_2 v_t + (1 - \beta_2) \nabla \mathcal{L}(\theta_t)^2$$

$$\hat{m}_{t+1} = \frac{m_{t+1}}{1 - \beta_1^{t+1}}$$

$$\hat{v}_{t+1} = \frac{v_{t+1}}{1 - \beta_2^{t+1}}$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_{t+1}} + \epsilon} \hat{m}_{t+1}$$

- $\hat{m}_t$  and  $\hat{v}_t$  are estimates for the first and second moments of the gradients. Because  $m_0 = v_0 = 0$ , these estimates are biased towards 0, the factors  $(1 \beta^{t+1})^{-1}$  are here to counteract these biases.
- Typical values:  $\beta_1 = 0.9$ ,  $\beta_2 = 0.999$  and  $\epsilon = 10^{-8}$ .

source: Kingma et al., Adam: a Method for Stochastic Optimization, ICLR 2015

ENSA

## PyTorch optimizers

- All have similar constructor torch.optim.\*(params, lr=..., momentum=...). Default values are different for all optimizers, check the doc.
- params should be an iterable (like a list) containing the parameters to optimize over. It can be obtained from any module with module.parameters().
- The step method updates the internal state of the optimizer according to the grad attributes of the params, and updates the latter according to the internal state.

## Pytorch training loop

#### Training over one epoch becomes:

```
model = YourModel()
train_loader = DataLoader(train_dataset, batch_size=64, shuffle=True)
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.SGD(model.parameters(), lr=1e-3)
```

```
for inputs, targets in train_loader:
    outputs = model(inputs)
    loss = criterion(outputs, targets)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

#### Last details

#### Faster parallel computations with GPUs

To know if you have access to GPUs:

device = torch.device("cuda:0" if torch.cuda.is\_available() else "cpu")
print('Using gpu: %s ' % torch.cuda.is\_available())

Tensors are allocated on a device using: x.to(device).

#### Testing, metrics and more

- We need to create a **test set** separate from the training set to **evaluate** the model.
- We need to store all loss values and accuracies after each epoch.
- Set the model to model.train() or model.eval().
- Perform multiple epochs.

## Updated Pytorch training loop

```
The training pipeline becomes: (dataloader \rightarrow model \rightarrow loss \rightarrow optimizer \rightarrow visualization)
model.to(device)
model.train()
for epoch in range(num_epochs):
    running_loss = 0.
    for inputs, targets in train_loader:
         inputs, targets = inputs.to(device), targets.to(device)
         outputs = model(inputs)
         loss = criterion(outputs, targets)
         optimizer.zero_grad()
         loss.backward()
         optimizer.step()
         running_loss += loss.item()
    print(f"Epoch {epoch}: Loss: {running_loss/n_data:.2f}")
```

## Pytorch test function

Test should not compute gradients, hence torch.no\_grad().

```
model.to(device)
model.eval()
running_loss, running_acc = 0., 0
with torch.no_grad():
    for inputs, targets in train_loader:
        inputs, targets = inputs.to(device), targets.to(device)
        output = model(inputs)
        loss = criterion(outputs, targets)
        preds = torch.argmax(outputs,1)
        running_loss += loss.item()
        running_acc += torch.sum(preds == targets)
    print(f"Loss: {running_loss/n_data:.2f} Acc: {running_acc/n_data:.2f}")
```

## Image analysis Introduction to convolutional neural networks

## ImageNet Large Scale Visual Recognition Challenge (ILSVRC)

- Object recognition challenge, from 2010 to 2017.
- ▶ 1.2 million images (avg. 469×387), 1000 object classes.



source: ImageNet Large Scale Visual Recognition Challenge. Russakovsky et.al., 2015.

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Performance of classification methods (top-5 accuracy)

- **Random strategy:** 0.5%.
- **Human performance:** Expert 1: 94.9%. Expert 2: 88%.

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- Winners of 2012: CNN (AlexNet) 84.7%.
- After 2012: Always DL architectures, current best  $\approx$  99%.

 ${\it Current \ leaderboard: \ https://paperswithcode.\ com/sota/image-classification-on-imagenet}$ 

### Encoding local information



- ▶ We want to find sharp edges, round eyes, fur-like textures...
- How can we encode these local characteristics?
- How can we ensure translation invariance?

#### Convolutional Neural Networks



source: ImageNet Classification with Deep Convolutional Neural Networks. Krizhevsky et.al., 2012.

- First idea introduced by **Fukushima in 1980**.
- Linear layers in MLPs are replaced by convolution and pooling layers.
- Higher-level structures are extracted via a hierarchical information processing.








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## Convolutions (1D)



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# Convolutions (1D)



• Continuous setting:  $(f * g)(u) = \int_{v=-\infty}^{+\infty} f(v) g(u-v) dv$ 

# Convolutions (1D)



▶ Continuous setting: (f \* g)(u) = ∫<sub>v=-∞</sub><sup>+∞</sup> f(v) g(u - v) dv
▶ Discrete version: (x \* y)<sub>i</sub> = ∑<sub>j=1</sub><sup>m</sup> x<sub>j</sub> y<sub>i-j[n]</sub>

# Convolutions (1D)



- Continuous setting:  $(f * g)(u) = \int_{v=-\infty}^{+\infty} f(v) g(u-v) dv$
- Discrete version:  $(x * y)_i = \sum_{j=1}^m x_j y_{i-j[n]}$
- Pytorch implementation:  $(x * y)_i = \sum_j x_j y_{i+j}$  (technically, a cross-correlation)
- Key properties: Local operation, limited receptive field, translation equivariant.

# Convolutions (2D)



source: https://github.com/vdumoulin/conv\_arithmetic/blob/master/README.md

### Technical details

- **Receptive field:** shape of the filter (typically 3x3).
- **Padding:** Adding a boundary of K > 0 layers of **zeros** (increases output image size).
- **Stride:** do the computation for one pixel every K > 0 (decreases output image size).
- See in action: https://setosa.io/ev/image-kernels/

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### Convolution channels



- Idea: Allows to store multiple local information (e.g. vertical/horizontal edges, corners,...)
- ▶ Definition: Dense connections between channels, i.e. for each output channel k, y<sub>k</sub> = ∑<sub>l</sub> W<sub>k,l</sub> \* x<sub>l</sub> + b<sub>k</sub> where W<sub>k,l</sub> is the filter for input channel l and output channel k.
  ▶ Rule of thumb: number of channels increases while image size decreases.

# Pooling



source: https://github.com/vdumoulin/conv\_arithmetic/blob/master/README.md

- Main idea: Aggregate local information to reduce complexity.
- **Example:** Is there an edge in this region of the image?
- **No parameters:** Applies a simple function to local image patches.
- **Two major variants: AvgPool** (mean over values) or **MaxPool** (max over values).

Image analysis

#### Example of a real-world CNN: VGG-16



source: https://github.com/vdumoulin/conv\_arithmetic/blob/master/README.md

- Features: 13 layers of convolution and 5 layers of padding
- Classifier: Last layers are an MLP with 3 linear layers.
- First layers encode **low-level** information (e.g. edges or circles).
- Last layers encode high-level information. (e.g. "fluffiness" or "eye-shaped elements")
- See in action: https://distill.pub/2017/feature-visualization/

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### But... why convolutions?



Idea: why not take an MLP and make it translation invariant?



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- **Equivariance:** a function f is equivariant w.r.t. to a transformation  $\tau$  iff  $f \circ \tau = \tau \circ f$ .



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- Equivariance: a function f is equivariant w.r.t. to a transformation  $\tau$  iff  $f \circ \tau = \tau \circ f$ .
- ▶ Translations (circular): For any  $u \in \llbracket 1, N \rrbracket$  and input  $x \in \mathbb{R}^N$ , let  $\tau_u(x)_i = x_{i+u[N]}$ .



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#### Lemma (convolutions)

The only linear functions that are translation equivariant are the convolutions.



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### Lemma (convolutions)

The only linear functions that are translation equivariant are the convolutions.

Proof.

- By linearity, we have  $f(x)_i = \sum_j M_{i,j} x_j$ .
- ▶ Then, we have  $\sum_j M_{i,j} x_{j+u[N]} = \sum_j M_{i+u[N],j} x_j$  and  $\forall i, j, u$ ,  $M_{i,j} = M_{i+u[N],j+u[N]}$ .

# The ResNet architecture Creating deeper neural networks

### How deep can we go?



Some properties require a large number of simple operations.

Limitations of VGG: can't add too many layers (due to vanishing gradients).

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### Residuals



Idea: only encode the residual: x<sup>(l+1)</sup> = x<sup>(l)</sup> + g<sub>θ</sub>(x<sup>(l)</sup>) where g<sub>θ</sub> is a computation block.
Impact: Increases stability (gradients closer to 1, mapping closer to identity).

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source: K. He et al., Deep residual learning for image recognition, CVPR 2016.

### The ResNet architecture



source: K. He et al., Deep residual learning for image recognition, CVPR 2016.

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### The ResNet architecture

Even deeper ResNet models are possible: 34, 50, 101, and 152 layers!

## The ResNet architecture

Even deeper ResNet models are possible: 34, 50, 101, and 152 layers!

### ResNet50 compared to VGG

- ▶ Accuracy: Superior in all vision tasks: 5.25% top-5 error vs 7.1%
- Less parameters: 25M vs 138M
- Computational complexity: 3.8B Flops vs 15.3B Flops
- Fully Convolutional until the last layer

#### Performance of ResNet architectures



Figure 4. Training on **ImageNet**. Thin curves denote training error, and bold curves denote validation error of the center crops. Left: plain networks of 18 and 34 layers. Right: ResNets of 18 and 34 layers. In this plot, the residual networks have no extra parameter compared to their plain counterparts.

source: K. He et al., Deep residual learning for image recognition, CVPR 2016.

### Impact on the loss landscape



Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The vertical axis is logarithmic to show dynamic range. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

source: K. He et al., Deep residual learning for image recognition, CVPR 2016.

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### Performance of ResNet architectures

method	top-5 err. (test)
VGG [41] (ILSVRC'14)	7.32
GoogLeNet [44] (ILSVRC'14)	6.66
VGG [41] (v5)	6.8
PReLU-net [13]	4.94
BN-inception [16]	4.82
ResNet (ILSVRC'15)	3.57

Table 5. Error rates (%) of **ensembles**. The top-5 error is on the test set of ImageNet and reported by the test server.

source: K. He et al., Deep residual learning for image recognition, CVPR 2016.

#### Recap

- CNN = convolutions + pooling (+ activations + BatchNorm)
- Convolutions are (the only) local, translation equivariant linear mappings.
- First layers extract low-level **local** features of the image.
- Last layers extract high-level **global** features of the image.
- ▶ Receptive field of neurons increases as we move towards the output.
- Residuals improve stability and performance for very deep CNNs.