Deep Learning for Image Analysis - Visualization of Neural Networks

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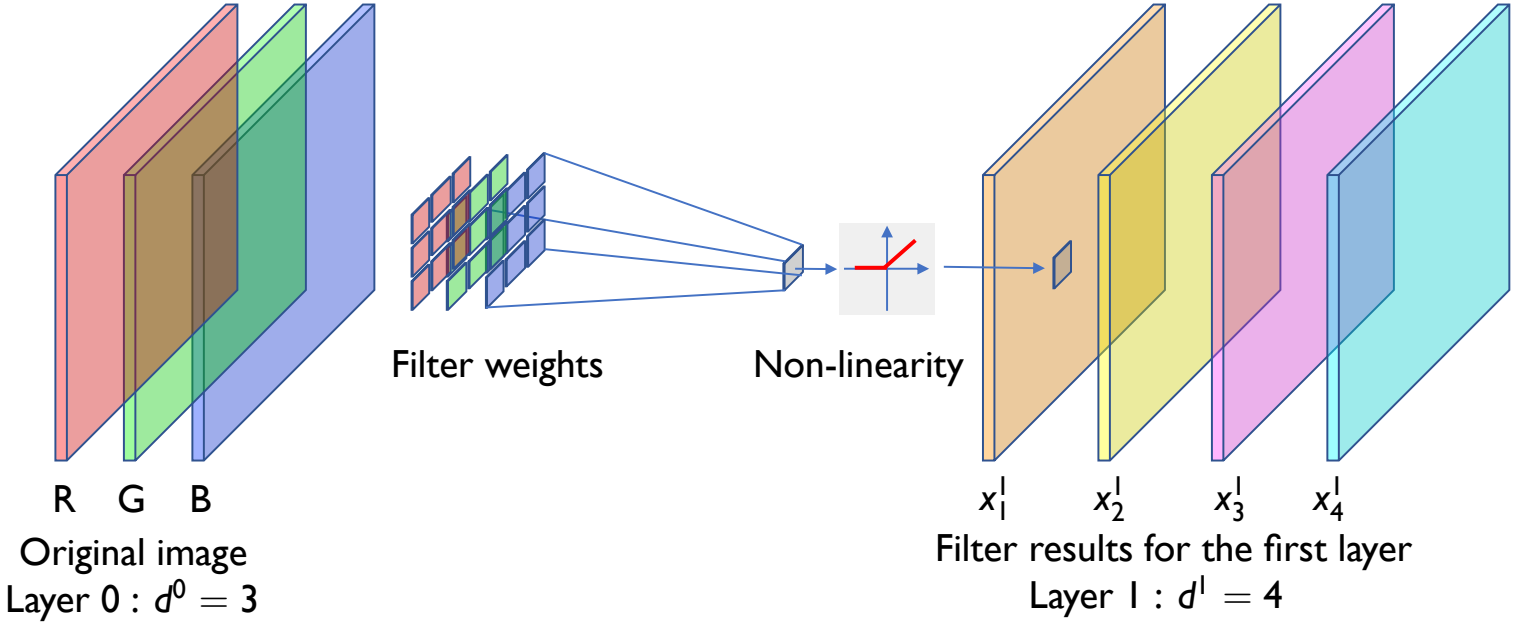
Overview

Motivation: visualization and understanding

- Convolutional Neural Networks have achieved stunning performance for many tasks, such as image classification, image segmentation and object detection.
- CNN can be difficult to train, and results can be very variable for different settings of hyperparameters.
- It is unclear, how design choices (network architecture, initialization, weight decay, ...) effect trainability and performance.
- It is not very well understood what Neural Networks actually learn.
- One idea to approach some of these issues relies on **visualization**.

Overview

Filters in Neural Networks

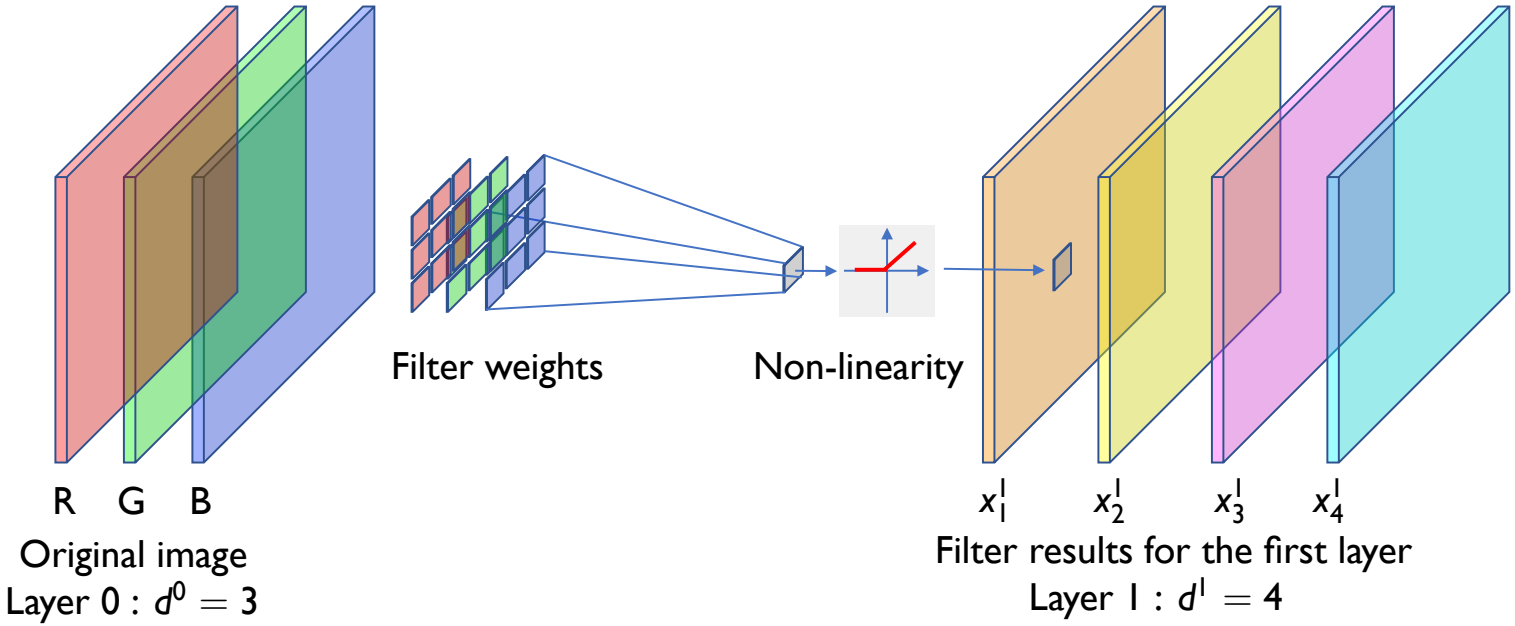


In Convolutional Neural Networks (CNN), a pixel value in activation map r in layer l depends on the pixel values in layer $l-1$ within the receptive field of the filter W_r^l across all channels. The pixel value $x_r^l(n,m)$ at position n,m in the activation map r in layer l is[1]:

$$x_r^l(n,m) = g\Big(\sum_k \sum_{i,j} W_r^l(i,j,k) x_k^{l-1}(n+i, m+j) + b_r^l\Big) \qquad (1)$$

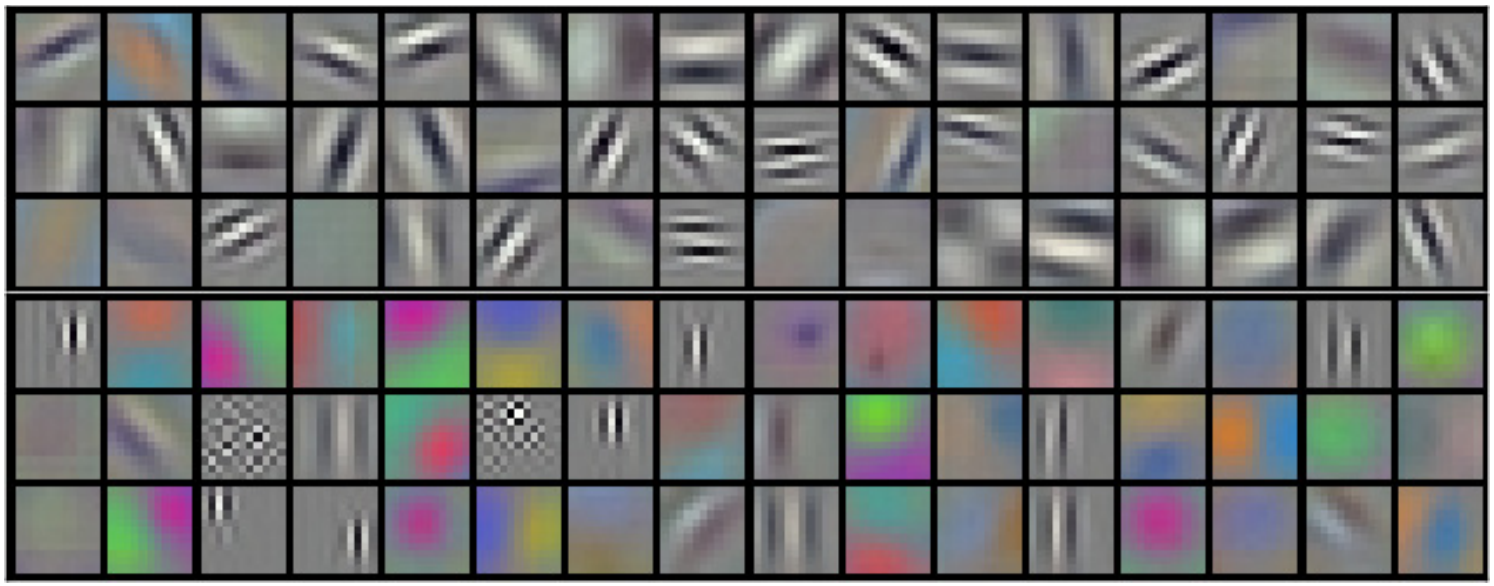
[1]For simplicity, we do not consider downsampling operations and to not

Filters in Neural Networks



- Each filter W_r^l (filter r in layer l) is thus a 3D tensor of values with dimension $d^{l-1} \times s^l \times s^l$.
- For the first layer, the number of input channels is typically 3, i.e. for each pixel, there are 3 values available (R, G and B).
- For this reason, all filters of layer 1 have the dimension $3 \times s^1 \times s^1$.
- This means that each filter corresponds itself to an RGB image of size $s^1 \times s^1$.

Visualization of the first layer filters



- First layer filters obtained by the Alexnet in the Imagenet competition [Krizhevsky et al., 2012].
- Observation: they contain oriented contours (top row) and color blobs (bottom row).
- How can we interpret this?

Visualization of first layer filters

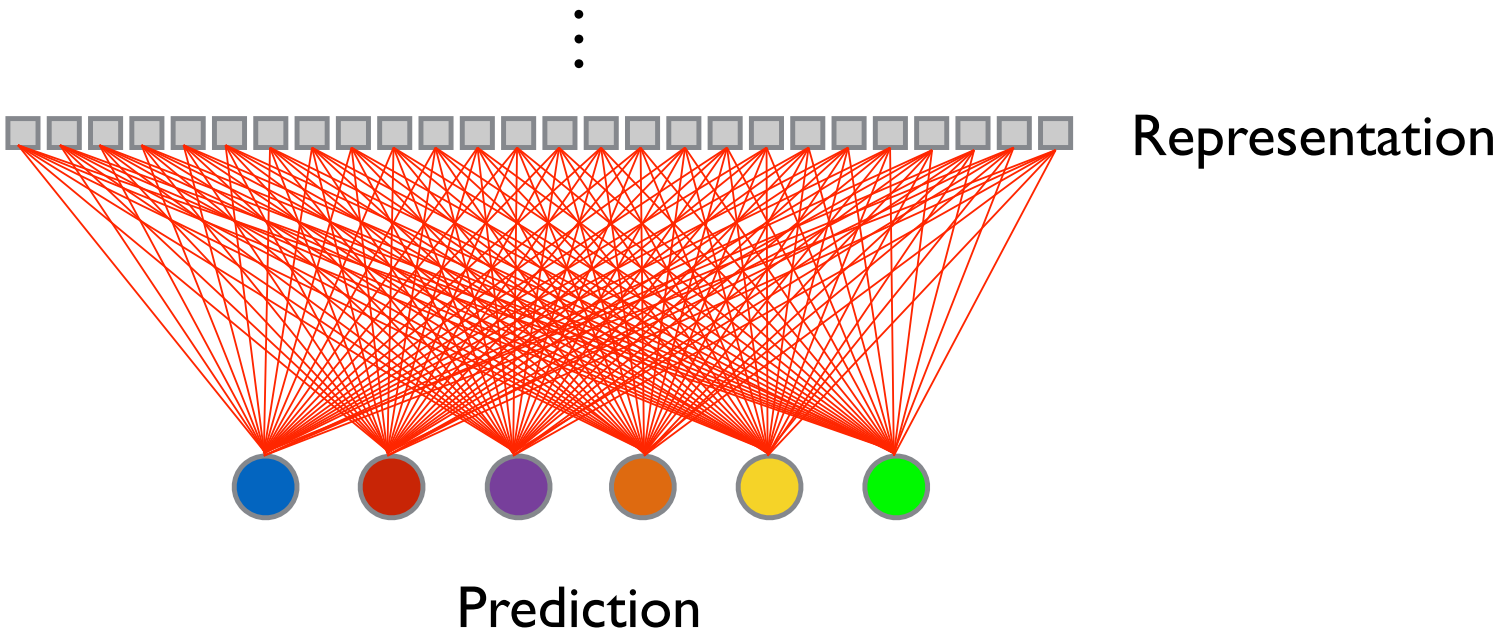
- The scalar product $w^T x$ is maximal if x points into the same direction as w:

$$w^T x = \|w\|\|x\| \cos \alpha_{x,w}$$

- Consequently the activation maps have high values, if the patterns in the image coincide with the filters.
- We therefore see, that the first layer of a trained convolutional neural network extracts low-level visual information, such as corners, edges, colors.
- The filter visualization strategy is not really applicable to deeper layers: as the filters in deeper layers act on the outputs of the first layer activation maps, it is unclear how to interpret the patterns they might show.

Overview

Visualization of image representation



- CNNs learn representations of the images. Here, we call the representation the last layer prior to classification.
- We can now collect these representations $x^{l_{max}}$ for all images in the training set.
- In order to visualize these representations, we seek low dimensional representations of these high dimensional vectors.

t-SNE (sketch) 1/2

- Many low dimensional representations: PCA, ICA, ...
- A recent technique that is widely used in this field is called *t-Distributed Stochastic Neighbor Embedding (t-SNE)* [**?**].
- Let $\{x_i\}_{0 \leq i < N}$ be the set of representations for all images in the training set.
- We define the pairwise probabilities p_{ij} that x_i and x_j are neighbors (which depends on $\|x_i - x_j\|$).
- We now seek a low-dimensional space for which these neighborhood probabilities q_{ij} are conserved.
- This is achieved by minimizing for each point x_i the Kulback-Leibler divergence between the distributions P_i (distribution of p_{ij}) and Q_i (distribution of q_{ij})

t-SNE (sketch) 2/2

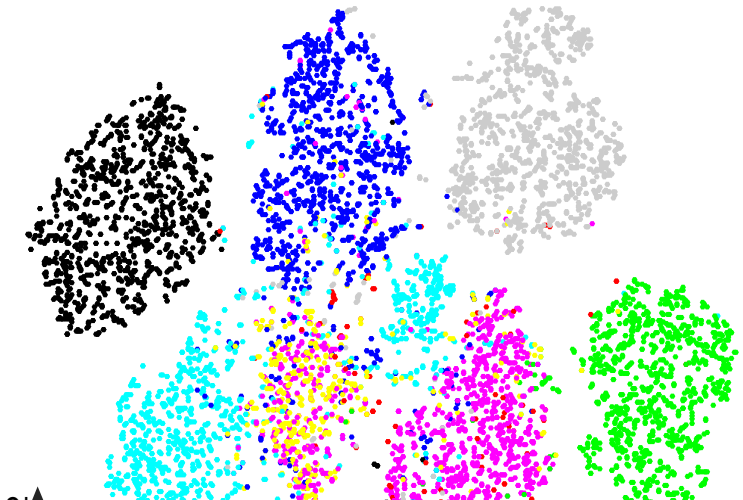
- The cost C that is minimized:

$$C = \sum_i KL(P_i \| Q_i) = \sum_i \sum_j -p_{ij} \log \frac{p_{ij}}{q_{ij}} \tag{2}$$

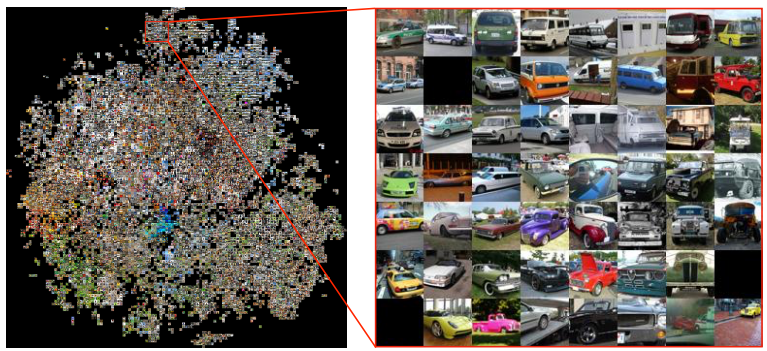
- If x_i and x_j are close in the original space, the algorithm will try to push q_{ij} to become close to x_{ij}.
- If x_i and x_j are far in the original space, only a small contribution is to be expected in any case.
- For this reason, t-SNE is known to respect local structure.

t-SNE map: example (cell images)

../graphics/Vis_tsne.pdf

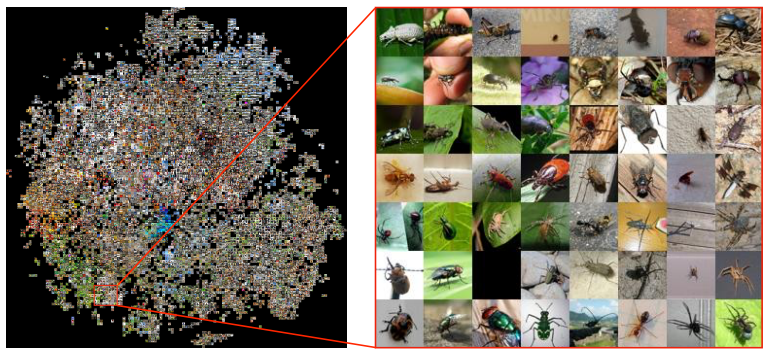


t-SNE map: ImageNet



Credits: adapted from
https://cs.stanford.edu/people/karpathy/cnnembed/

t-SNE map: ImageNet



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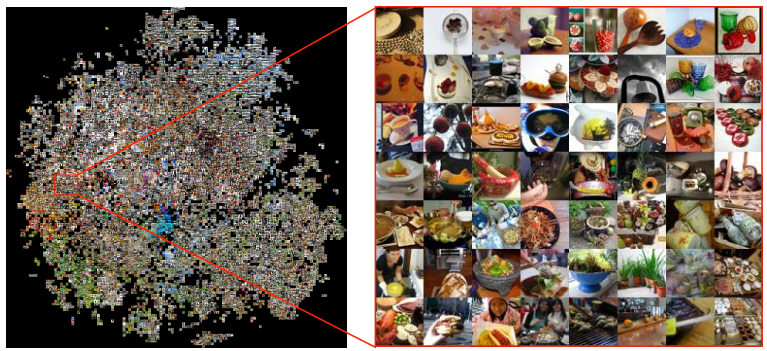
t-SNE map: ImageNet



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Overview

Motivation: visualization of the loss function

- We have seen that training a Neural Networks corresponds to solving a minimization problem:

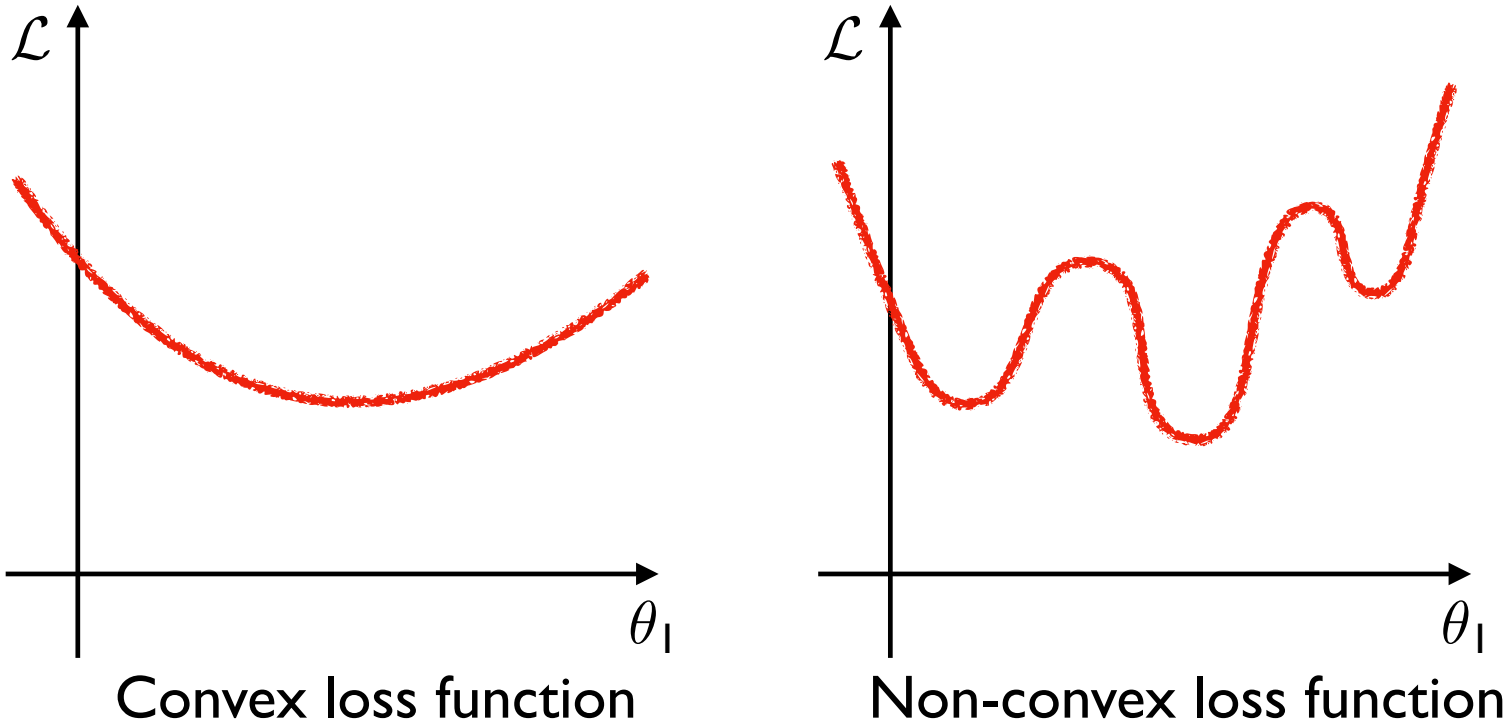
$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) + \mathcal{R}(\boldsymbol{\theta})$$

  where $\boldsymbol{\theta}$ is the vector of all parameters, $\mathcal{R}(\boldsymbol{\theta})$ a regularization term and $L(\boldsymbol{\theta})$ the loss term calculated on the training data:

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{N} L_i(\boldsymbol{\theta})$$

- Visualization of the loss can give us a hint on how complicated this task really is.
- Visualization can also allow us to compare different architectures or initialization schemes.

Convexity



- Convex optimization functions: only one local minimum (which is also the global minimum).
- In neural networks, the loss is often not convex.
- The shape of the loss is very important for the success of the optimization.
- How can we visualize the loss w.r.t $\sim 10^6$ parameters?

Visualization of the loss function

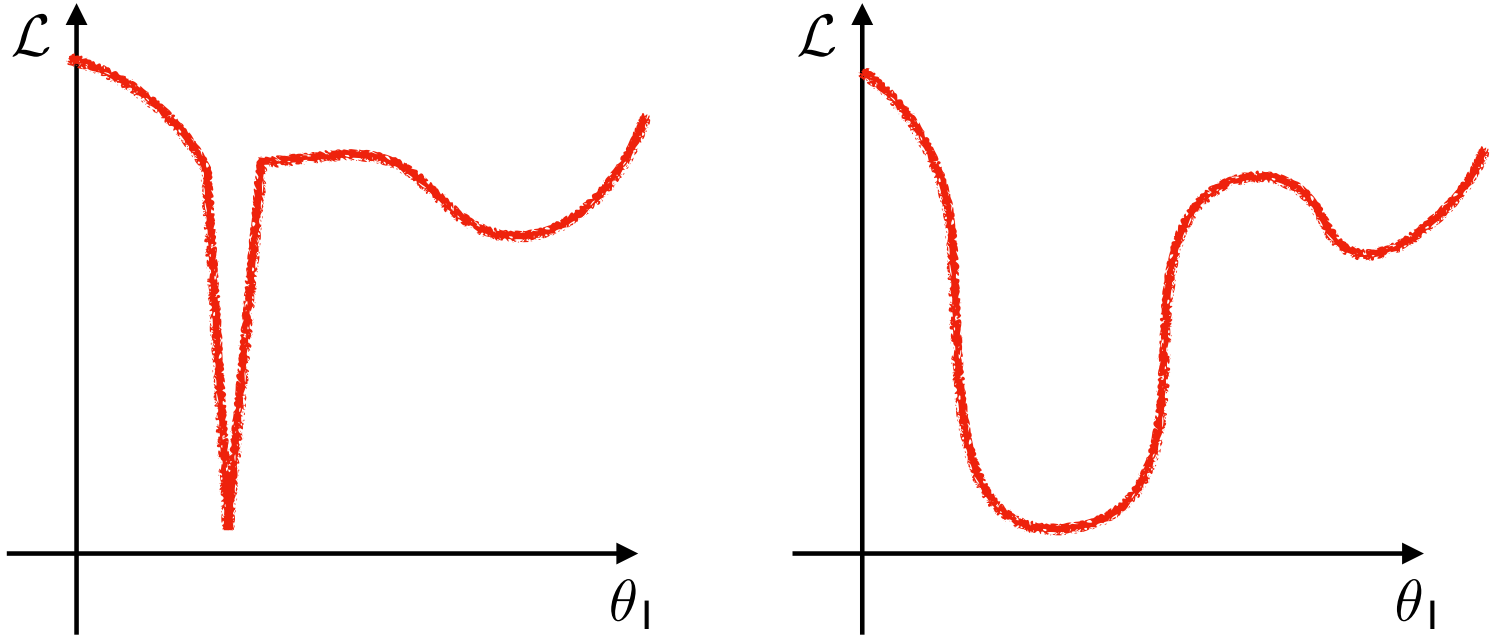
- Visualizations are limited to 2D or 3D plots.
- We can only plot the loss as a function of one or two parameters.
- Idea: to draw two random directions δ, η in parameter space and plot the loss function in these directions:

$$L(\alpha, \beta) = L(\theta^* + \alpha\delta + \beta\eta) \tag{3}$$

  with L^* our solution which is supposed to be optimal.
- Alternative: if we wish to compare two networks $\boldsymbol{\theta}^A$ and $\boldsymbol{\theta}^B$, we can also visualize the loss in the direction of the difference between these two points in parameter space [Goodfellow and Vinyals, 2014]:

$$\boldsymbol{\theta}(\alpha) = (1 - \alpha)\boldsymbol{\theta}^A + \alpha\boldsymbol{\theta}^B \tag{4}$$

The problem of scale invariance



- Sharpness of a minimum: the intuition is that sharp minima are hard to find and less robust.
- Scale invariance: two neural networks with ReLu as non-linearities are equivalent, if we multiply the weights of one layer with a factor and divide the weights of the next layer by the same factor.
- 1D and 2D plots of the loss can therefore be misleading: the

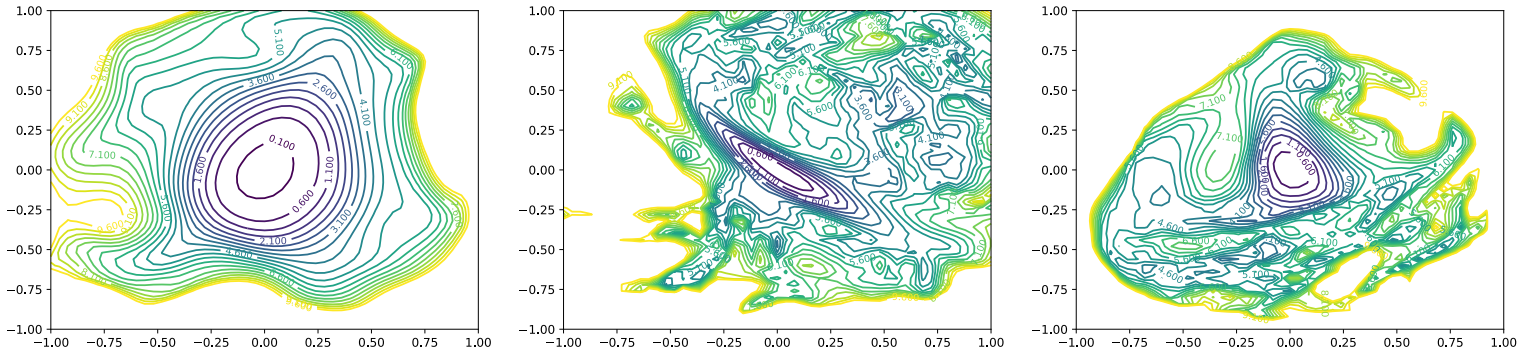
Scale invariance and filter-wise normalization

- One idea to cope with scale invariance is to normalize the directions with respect to the filter weights [Li et al., 2017].
- First we draw a random direction d.
- We then require that the parameters belonging to the same filter r in layer l are normalized such that their norm is that of the filter:

$$d_r^l \leftarrow \frac{d_r^l}{\|d_r^l\|}\boldsymbol{\theta}_r^l \tag{5}$$

where $\|\cdot\|$ is the Frobenius norm.

Example: effect of deeper networks



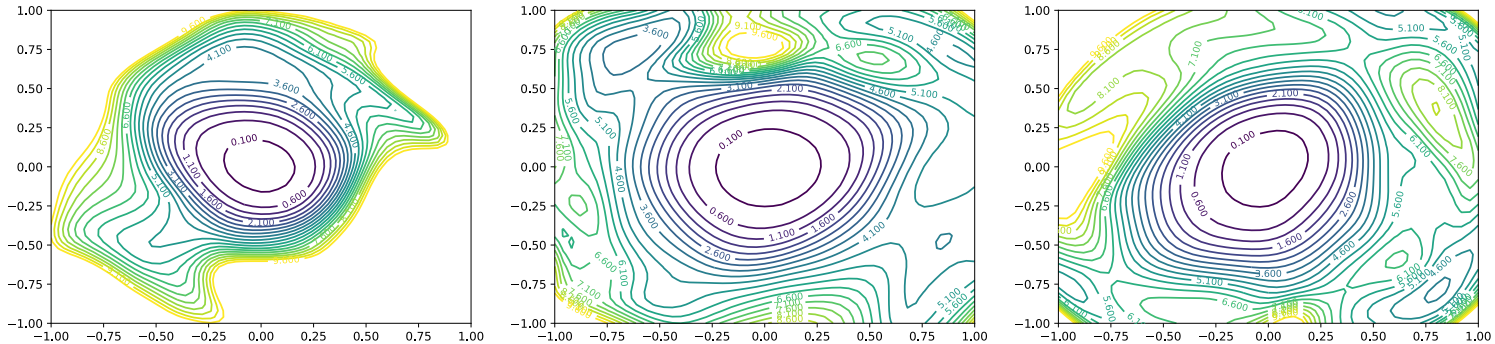
(d) ResNet-20-noshort, 8.18% (e) ResNet-56-noshort, 13.31% (f) ResNet-110-noshort, 16.44%

Figure: Resnet architecture without skip connections (varying depth)

- With 20 layers, we observe a fairly convex loss function.
- With more layers, the loss function becomes chaotic and the gradient does not point to the global minimum.
- In addition, the minima are steep and sometimes ill-conditioned (anisotropy).

Credits: From [Li et al., 2017]

Example: importance of skip-layers



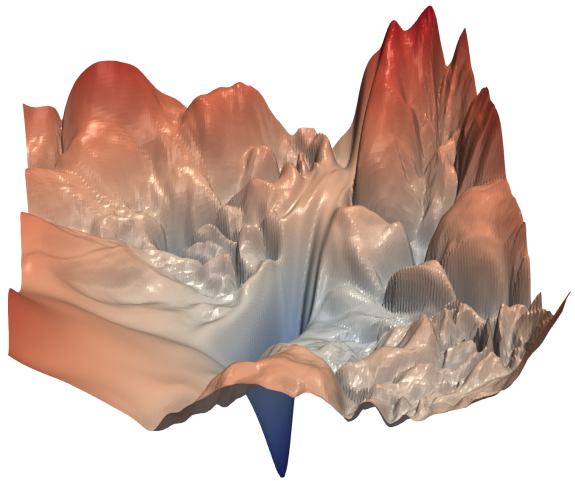
(a) ResNet-20, 7.37% (b) ResNet-56, 5.89% (c) ResNet-110, 5.79%

Figure: Resnet architecture with skip connections (varying depth)

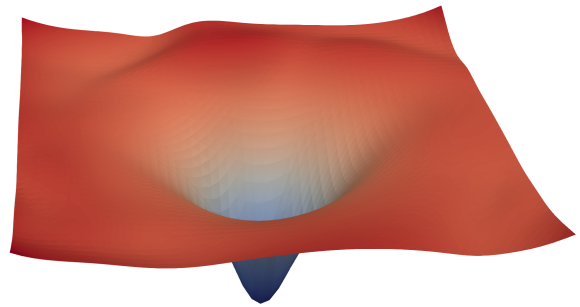
- Adding skip connections makes the objective function "more convex".
- This is particularly true for deeper networks (here: 56 and 110 layers).
- We therefore understand the impact of this architectural choice.

Credits: From [Li et al., 2017]

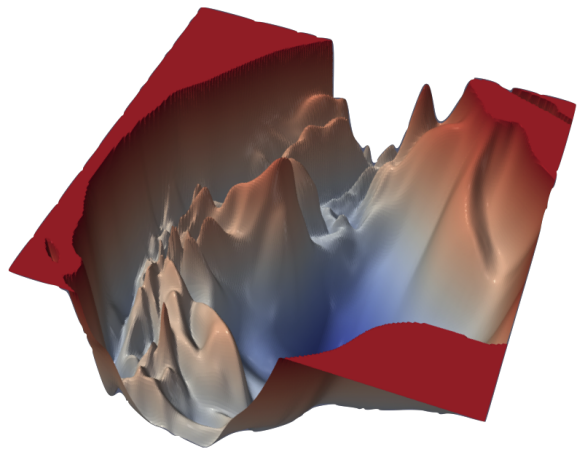
More examples for the importance of skip-layers



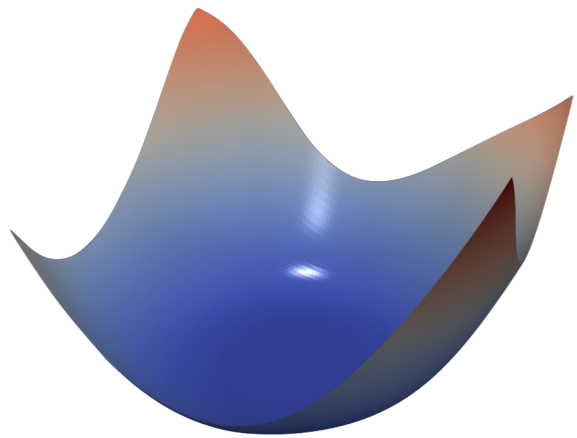
(a) without skip connections



(b) with skip connections



(a) 110 layers, no skip connections



(b) DenseNet, 121 layers

Credits: From [Li et al., 2017]

References I

[Goodfellow and Vinyals, 2014] Goodfellow, I. J. and Vinyals, O. (2014). Qualitatively characterizing neural network optimization problems. *CoRR*, abs/1412.6544.

[Krizhevsky et al., 2012] Krizhevsky, A., Sutskever, I., and Hinton, G. E. (2012). Imagenet classification with deep convolutional neural networks. In *Proceedings of the 25th International Conference on Neural Information Processing Systems - Volume 1*, NIPS'12, pages 1097–1105, USA. Curran Associates Inc.

[Li et al., 2017] Li, H., Xu, Z., Taylor, G., and Goldstein, T. (2017). Visualizing the loss landscape of neural nets. *CoRR*, abs/1712.09913.