Deep learning

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- Deep neural networks
- Challenges and tricks

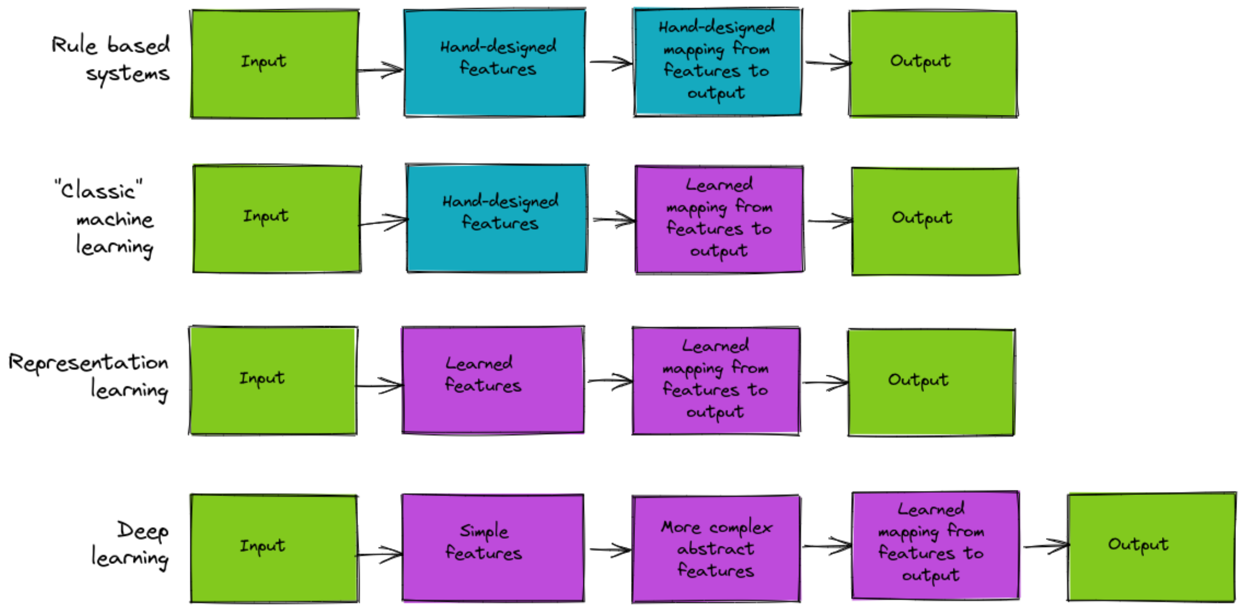
Math prerequisites for this lesson: None.

Recap

Last week: neural networks with one hidden layer

- Hidden layer learns feature representation
- Output layer learns classification/regression tasks

With the neural network, the "transformed" feature representation is *learned* instead of specified by the designer.



Rule based systems
Input
Hand-designed features
Hand-designed mapping from features to output
Output
"Classic" machine learning
Input
Hand-designed features
Learned mapping from features to output
Output
Representation learning
Input
Learned features
Learned mapping from features to output
Output
Deep learning
Input
Simple features
More complex abstract features
Learned mapping from features to output
Output

Figure 1: Image is based on a figure in Deep learning, by Goodfellow, Bengio, Courville.

A neural network with non-linear activation, with one hidden layer and many units in it *can* approximate virtually any continuous real-valued function, with the right weights. (Refer to the *Universal Approximation Theorem*.) But (1) it may need a very large number of units to represent the function, and (2) those weights might not be learned by gradient descent - the loss surface is very unfriendly.

Instead of a single hidden layer, if we use multiple hidden layers they can "compose" functions learned by the previous layers into more complex functions - use fewer units, and tends to learn better weights .

Deep neural networks

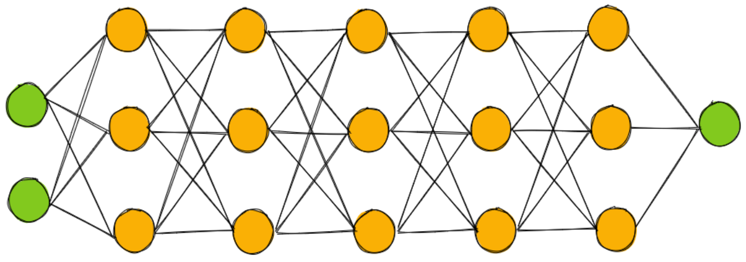


Figure 2: Illustration of a deep network, with multiple hidden layers.

Some comments:

- each layer is fully connected to the next layer
- each unit still works the same way: take the weighted sum of inputs, apply an activation function, and that's the unit output
- still trained by backpropagation

We call the number of layers the "depth" of the network and the number of hidden units in a layer its "width."

Challenges with deep neural networks

- Efficient learning
- Generalization

Loss landscape

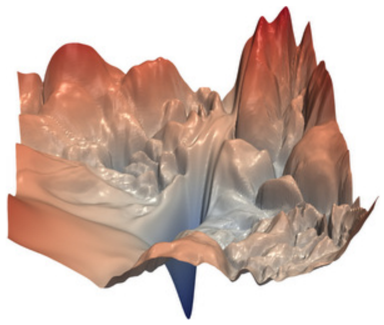


Figure 3: "Loss landscape" of a deep neural network in a "slice" of the high-dimensional feature space.

Image source: Hao Li, Zheng Xu, Gavin Taylor, Christoph Studer and Tom Goldstein. Visualizing the Loss Landscape of Neural Nets. NIPS, 2018.

Neural networks are optimized using backpropagation over the computational graph, where the loss is a very challenging function of *all* the weights. (Not convex!)

Double descent curve

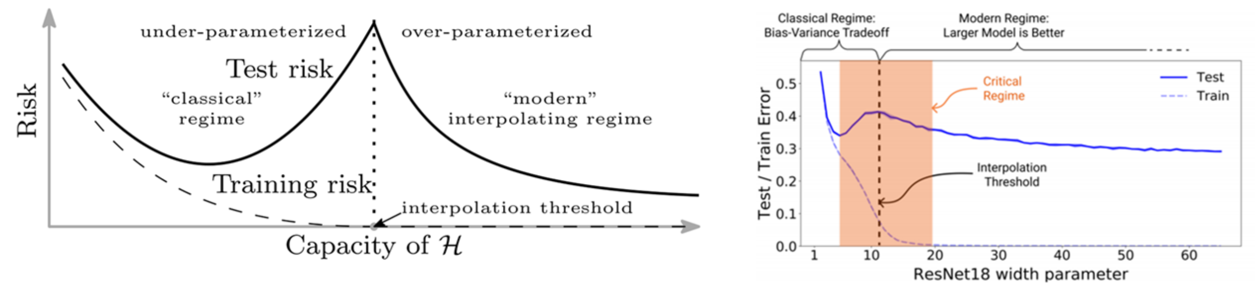


Figure 4: Double descent curve (left) and realization in a real neural network (right).

Interpolation threshold: where the model is just big enough to fit the training data exactly.

- too-small models: can't represent the "true" function well
- too-big models (before interpolation threshold): memorizes the input, doesn't generalize well to unseen data (very sensitive to noise)
- REALLY big models: many possible weights that memorize the input, but SGD finds weight combination that memorizes the input *and* does well on unseen data

Double descent: animation

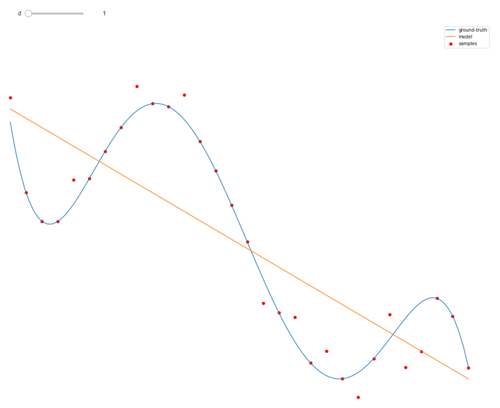


Figure 5: Polynomial model before and after the interpolation threshold. Image source: Boaz Barak, click link to see animation.

Explanation (via Boaz Barak):

> When d of the model is less than d_t of the polynomial, we are "under-fitting" and will not get good performance. As d increases between d_t and n, we fit more and more of the noise, until for $d = n$ we have a perfect interpolating polynomial that will have perfect training but very poor test performance. When d grows beyond n, more than one polynomial can fit the data, and (under certain conditions) SGD will select the minimal norm one, which will make the interpolation smoother and smoother and actually result in better performance.

What this means: in practice, we let the network get big (have capacity to learn complicated data representations!) and use other methods to help select a "good" set of weights from all these candidates.

Addressing the challenges

- Efficient learning
- Generalization

In deep learning, we don't want to use "smaller" (simpler) models, which won't be as capable of learning good feature representations. Instead, lots of work around (1) finding good weights quickly, and (2) finding weights that will generalize.

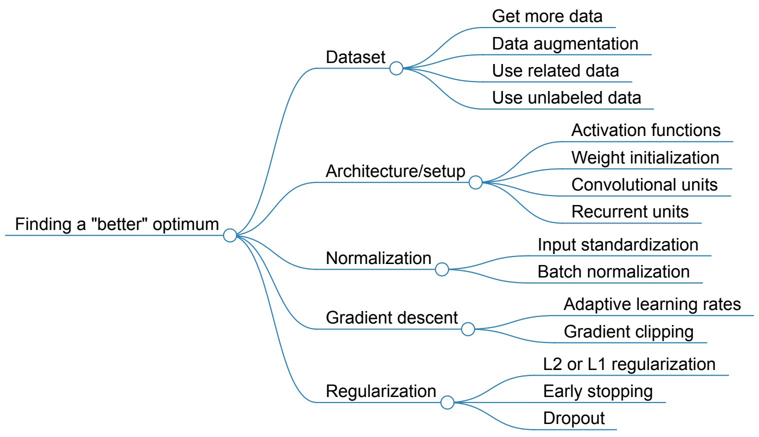


Figure 6: Image credit: Sebastian Raschka

Dataset

- Get more data
- **Data augmentation**
- **Use related data (transfer learning)**
- Use unlabeled data (self-supervised, semi-supervised)

We won't talk much about getting more data, but if it's possible to get more labeled data, it is almost always the most helpful thing you can do!

- Example: JFT-300M, a Google internal dataset for training image models, has 300M images
- Example: GTP-3 trained on 45TB of compressed plaintext, about 570GB after filtering

Reference: Revisiting Unreasonable Effectiveness of Data in Deep Learning Era. Chen Sun, Abhinav Shrivastava, Saurabh Singh, Abhinav Gupta; Proceedings of the IEEE International Conference on Computer Vision (ICCV), 2017, pp. 843-852.

It's not always possible to get a lot of *labeled* data for training a supervised learning model. But sometimes we can use *unlabeled* data, which is much easier to get. For example:

- In self-supervised learning, the label can be inferred automatically from the unlabeled data. e.g. GPT is trained to predict "next word".
- In semi-supervised/weakly-supervised learning learining, we generate labels (probably imperfectly) for unlabeled data (maybe using a smaller volume of labeled data to train a model!)

These are mostly out of scope of this course. But we *will* talk about data augmentation and transfer learning...

Data augmentation

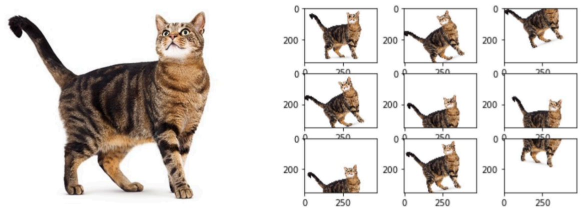


Figure 7: Data augmentation on a cat image.

It doesn't restrict network capacity - but it helps generalization by increasing the size of your training set!

- For image data: apply rotation, crops, scales, change contrast, brightness, color.
- For text you can replace words with synonyms, simulate typos.
- For audio you can adjust pitch or speed, add background noise etc.

Transfer learning

Idea: leverage model trained on *related* data.

Using pre-trained networks

- State-of-the-art networks involve millions of parameters, huge datasets, and days of training on GPU clusters
- Idea: share pre-trained networks (network architecture and weights)
- Some famous networks for image classification: Inception, ResNet, and more
- Can be loaded directly in Keras

Transfer learning from pre-trained networks

Use pre-trained network for a different task

- Use early layers from pre-trained network, freeze their parameters
- Only train small number of parameters at the end

Base model is a powerful feature extractor (learns transformation into a more useful feature space), then you just have to train for the mapping from this feature space to the target variable.

In practice: when applying deep learning, we almost always use a pre-trained base model! It saves time, energy, and cost.

Example: To pre-train the 7B parameter (smallest) Llama 2, Meta's open source language model, takes 184,320 GPU hours (21 GPU YEARS!) and anywhere from $100,000-800,000 (depending on cost of GPU instance).

Transfer learning illustration (1)

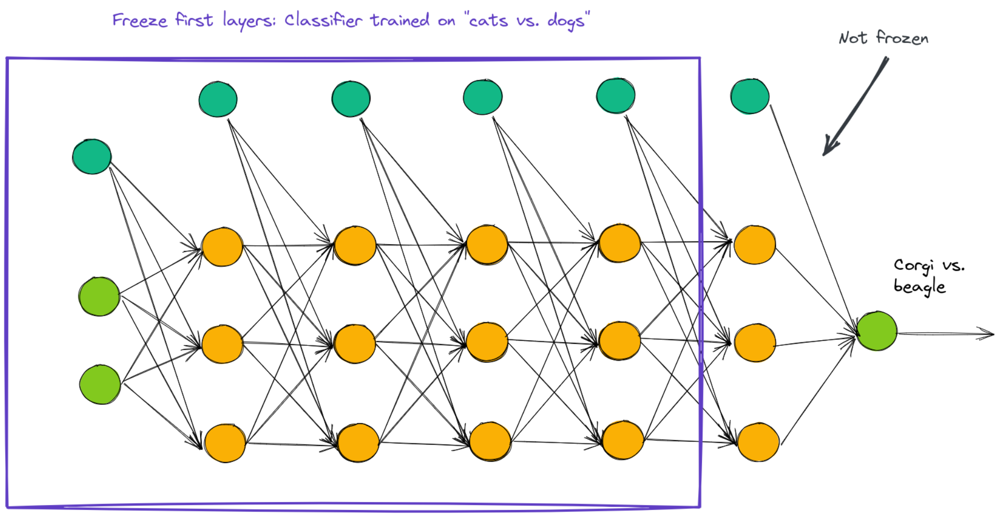


Figure 8: When the network is trained on a very similar task, even the abstract high-level features are probably very relevant, so you might tune just the classification head.

Transfer learning illustration (2)

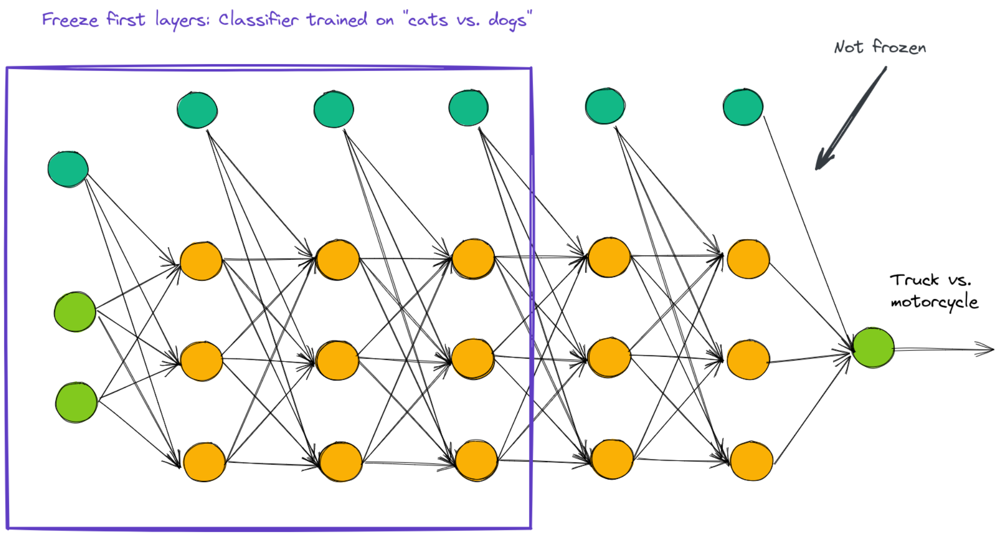


Figure 9: If the original network is not as relevant, may fine-tune more layers.

Architecture/setup

- **Activation functions**
- **Weight initialization**
- **Convolutional units**
- Recurrent units
- ... many more ideas

Again, this is mostly out of scope of this course, but we'll talk about the first three items very briefly.

Recall: activation functions

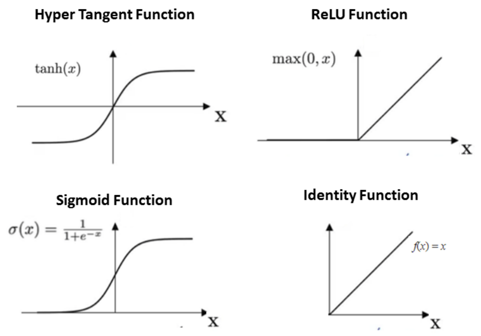


Figure 10: Candidate activation functions for a neural network.

Sigmoid: vanishing gradient (1)

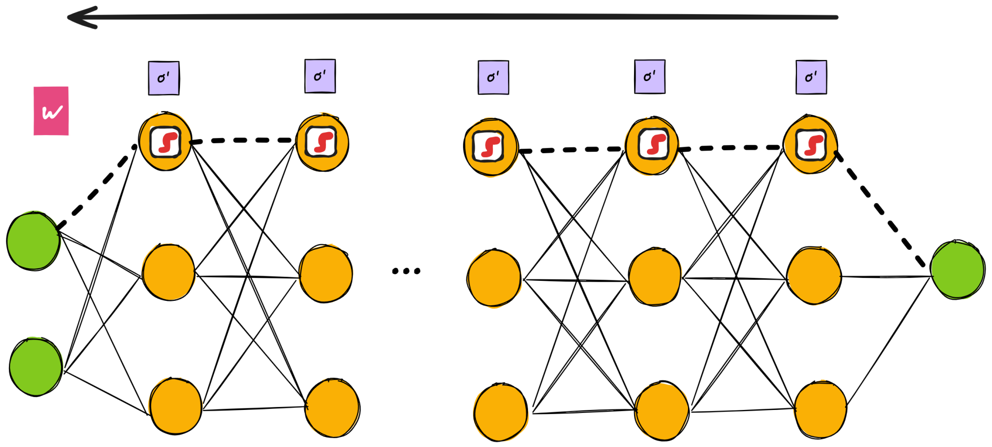


Figure 11: Computing gradients by backpropagation. At a hidden unit, $\delta_j = g'(z_j) \sum_k w_{k,j} \delta_k$.

Suppose we want to compute the gradient of the loss with respect to the weight shown in pink.

- We will *multiply* local gradients (pink) all along each path between weight and loss function, starting from the end and moving toward the input.
- Then we *add* up the products of all the paths.
- With σ activation, gradient along each path includes the product of a LOT of σ' terms.

Sigmoid: vanishing gradient (2)

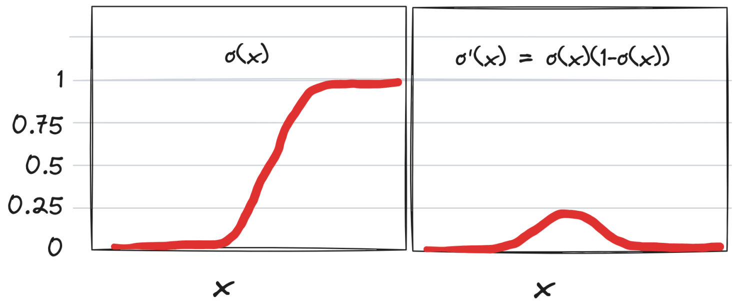


Figure 12: Sigmoid function and its derivative.

What happens when you are in the far left or far right part of the sigmoid?

- Gradient is close to zero
- Weight updates are also close to zero
- The "downstream" gradients will also be values close to zero! (Because of backpropagation.)
- And, when you multiply quantities close to zero - they get even smaller.

The network "learns fastest" when the gradient is large. When the sigmoid "saturates", it "kills" the neuron!

Even the maximum value of the gradient is only 0.25 - so the gradient is always less than 1, and we know what happens if you multiply many quantities less than 1...

(tanh is slightly better - gradient has a larger max + some other advantages - still has vanishing gradient.)

ReLU: Dead ReLU

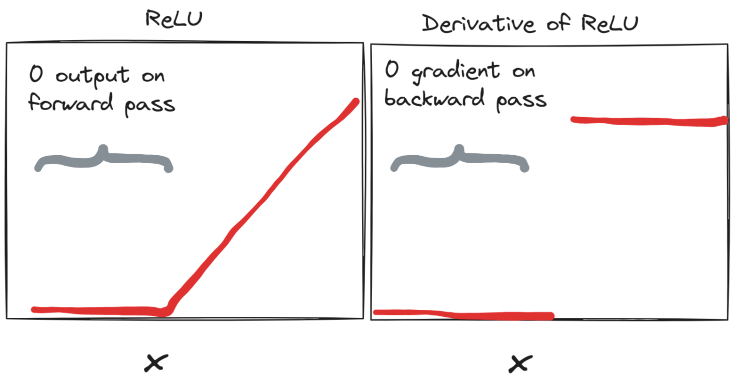


Figure 13: ReLU function and its derivative.

ReLU is a much better non-linear function:

- does not saturate in positive region
- very very fast to compute

But, can "die" in the negative region. Once we end up there (e.g. by learning negative bias weight) we cannot recover - since gradient is also zero, gradient descent will not update the weights.

(ReLU is also more subject to "exploding" gradient than sigmoid/tanh.)

ReLU: Leaky ReLU

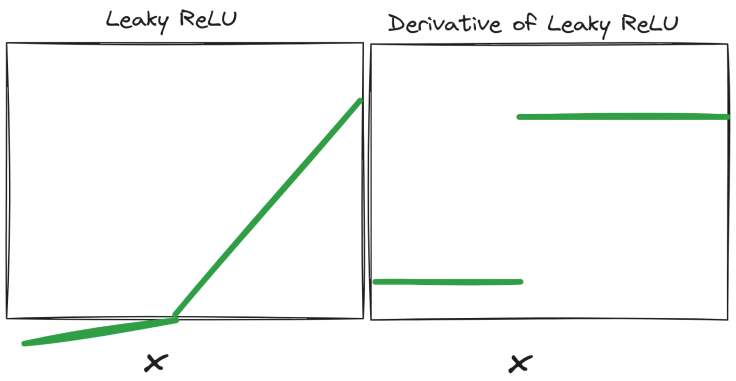


Figure 14: Leaky ReLU function and its derivative.

When input is less than 0, the ReLU (and downstream units) is *completely* dead (not only very small!) Alternative: **leaky ReLU** has small (non-zero) gradient in the negative region - can recover.

$$f(x) = \text{max}(\alpha x, x)$$

(α is a hyperparameter.)

Other activations

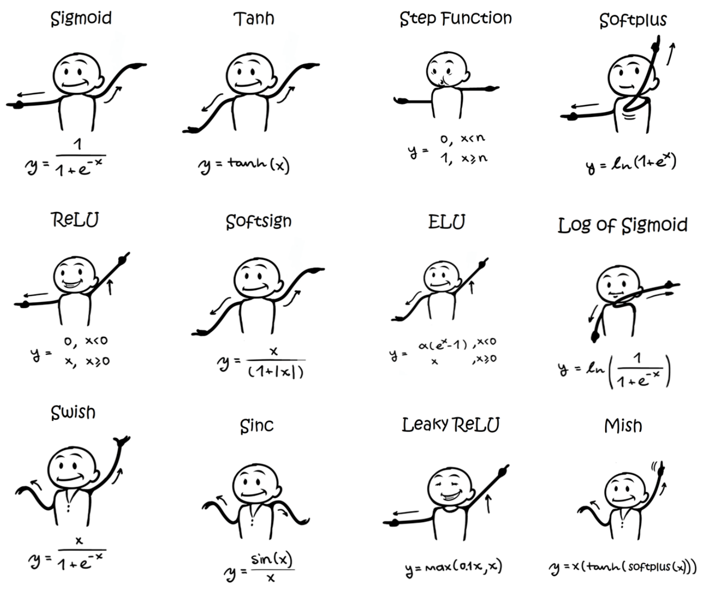


Figure 15: Other activations. Image via Sefik Ilkin Serengil.

Weight initialization

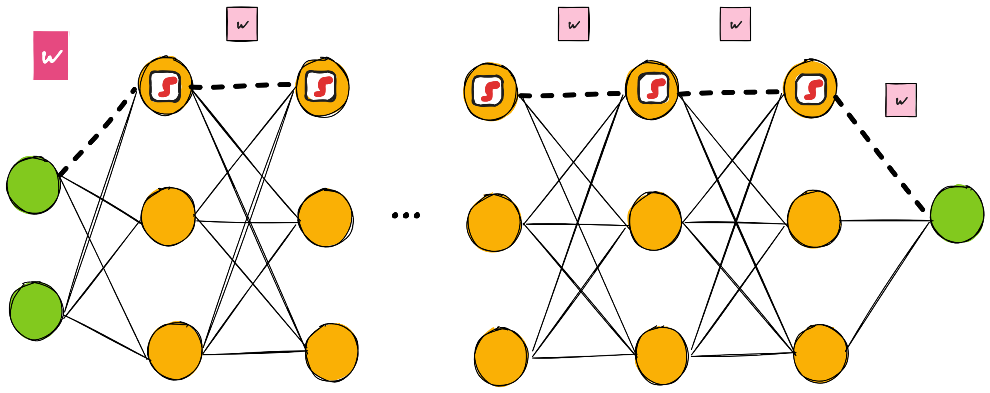


Figure 16: One path in forward pass on a neural network.

What if we initialize weights to:

- **zero?** If weights are all initialized to zero, all the outputs are zero (for any input) - won't learn.
- **a constant (non-zero)?** If weights are all initialized to the same constant, we are more prone to "herding" - hidden units all move in the same direction at once, instead of "specializing".
- **a normal random value with small σ?** Small normal random values work well for "shallow" networks, but not for deep networks - it makes the outputs "collapse" toward zero at later layers.
- **a normal random value with large σ?** Large normal random values are bad - it makes the outputs "explode" at later layers.

Weight initialization - normal

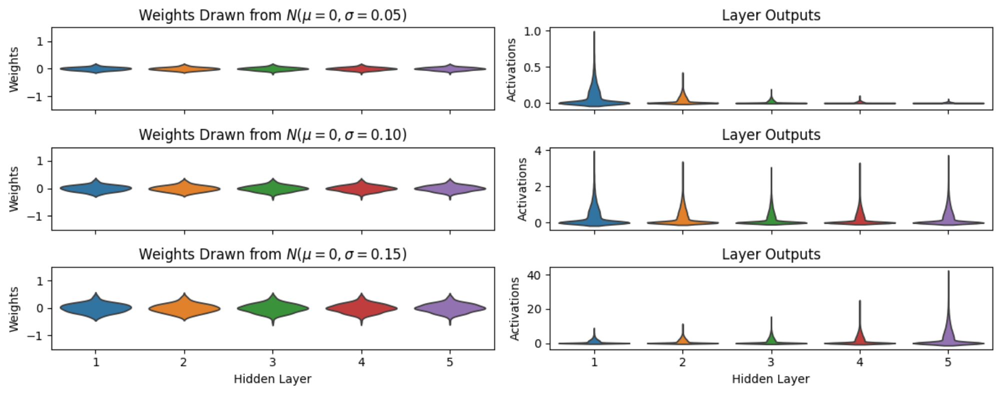


Figure 17: Initial weights and ReLU unit outputs for each layer in a network.

- top row: too-small initial weights, by the last layer the outputs "collapse" toward zero
- middle row: good initial weights, distribution is similar from input to output
- bottom row: too-large initial weights, by the last layer the outputs "explode"

Desirable properties for initial weights - principle

- The mean of the intial weights should be around 0
- The variance of the activations should stay the same across every layer

If you are interested, here's a derivation.

Desirable properties for initial weights - practice

- For tanh: Xavier scales by $\frac{1}{\sqrt{N_{in}}}$
- For ReLU: He by $\frac{2}{\sqrt{N_{in}}}$

N_{in} is the number of inputs to the layer ("fan-in").

Weight initialization - He

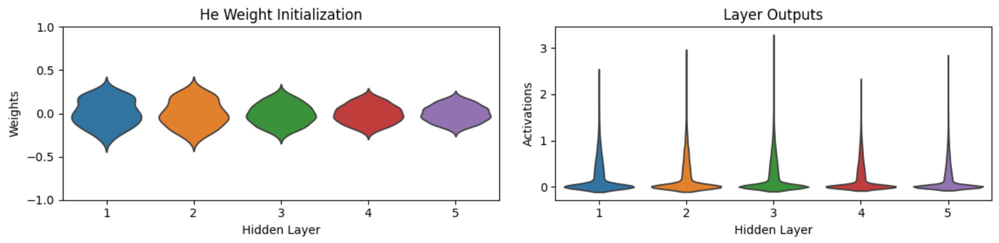


Figure 18: Initial weights and ReLU unit outpus for each layer in a network, He initialization. In this example, the size of the layers is: 100, 150, 200, 250, 300.

Normalization

- **Input standardization**
- **Batch normalization**

Data pre-processing

You can make the loss surface much "nicer" by pre-processing:

- Remove mean (zero center)
- Normalize (divide by standard deviation)
- OR decorrelation (whitening/rotation)

There are several reasons why this helps. We already discussed the "ravine" in the loss function that is created by correlated features.

Data preprocessing (1)

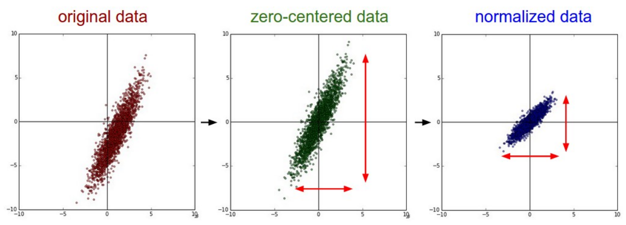


Figure 19: Image source: Stanford CS231n.

Data preprocessing (2)

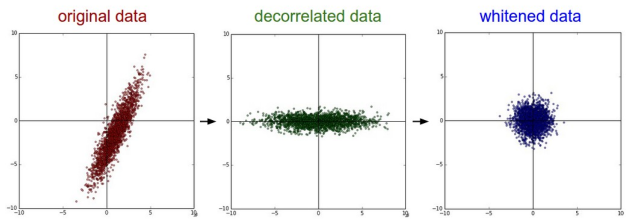


Figure 20: Image source: Stanford CS231n.

Input standardization helps with the first hidden layer, but what about the hidden layers?

Batch normalization

- Re-center and re-scale between layers
- Training: Mean and standard deviation per training mini-batch
- Test: Using fixed statistics

Gradient descent

Regularization

- **L2 or L1 regularization**
- **Early stopping**
- **Dropout**

L1 or L2 regularization

As with other models, we can add a penalty on the norm of the weights.

Normal gradient descent update rule:

$$w_{i,j}^{t+1} = w_{i,j}^{t} - \alpha \frac{\partial L}{\partial w_{i,j}^{t}}$$

With L2 regularization:

$$w_{i,j}^{t+1} = w_{i,j}^{t} - \alpha \left(\frac{\partial L}{\partial w_{i,j}^{t}} + \frac{2\lambda}{n} w_{i,j}^{t} \right)$$

Often called "weight decay" in the context of neural nets.

Early stopping

- Compute validation loss each performance
- Stop training when validation loss hasn't improved in a while
- Risk of stopping *too* early

Important: *must* divide data into training, validation, and test data - use validation data (not test data!) to decide when to stop training.

Dropout

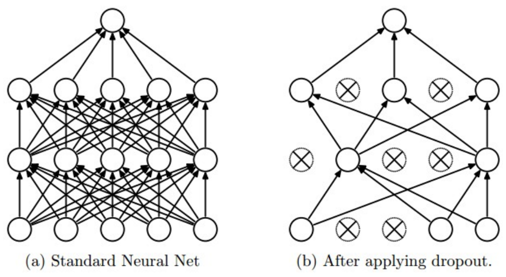


Figure 21: Dropout networks.

- During each training step: some portion of neurons are randomly "dropped".
- During each test step: don't "drop" any neurons, but we need to scale activations by dropout probability

Why does it work? Some ideas:

- Forces some redundancy, makes neurons learn robust representation
- Effectively training an ensemble of networks (with shared weights)

Note: when you use Dropout layers, you may notice that the validation/test loss seems better than the training loss! Why?

Example: Deep Neural Nets: 33 years ago and 33 years from now

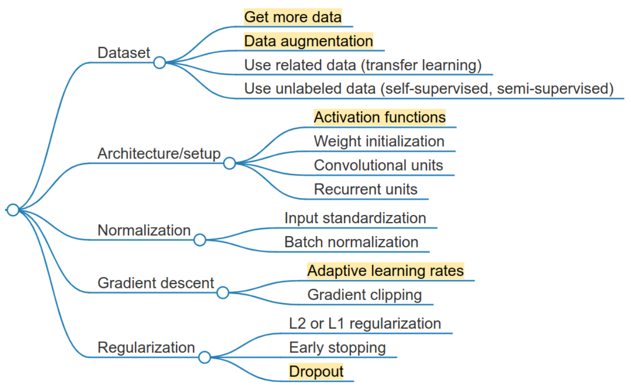


Figure 22: Techniques we will apply in this example.

In the Colab lesson, we will reproduce a 1989 paper about a neural network for handwritten digit classification, that was used in the late 90s to process 10-20% of all checks in the US.

- The original paper had 5% error
- Our realization has about 4.14%
- With a bunch of these changes (but keeping the basic network the same) we get to 2.09%
- The original model without any changes, but with more training data, gets to 3.05%
- With our changes + more data, we get to 1.31%

What does it mean that we can do this without changing the basic network? It means the network always had the *capacity* to do this well, but wasn't learning the best weights.