Deep Learning - MAI

Feed-forward and convolutional neural networks

THEORY

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A Bit of History

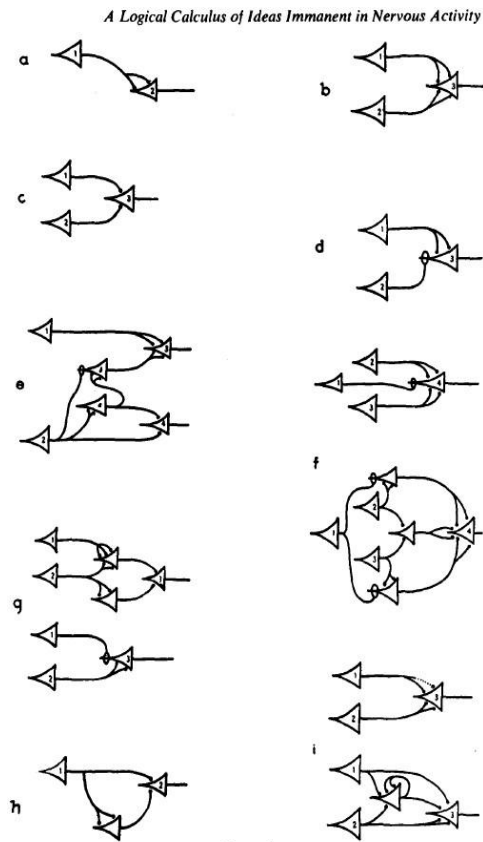The not so distant origin story

Connectionism & Hebbian Learning

Warren McCulloch & Walter Pitts (1943):

- From neurons to complex thought
- Binary threshold activations

Howard Hebb (1949):

- "Neurons that fire together wire together"
- Weights yield *learning* and *memory*

A Logical Calculus of Ideas Immanent in Nervous Activity

FIGURE 1

Ref: [1,31]

Rosenblatt's Perceptron

Rosenblatt (1948): Hebb's learning + McCulloch & Pitts design
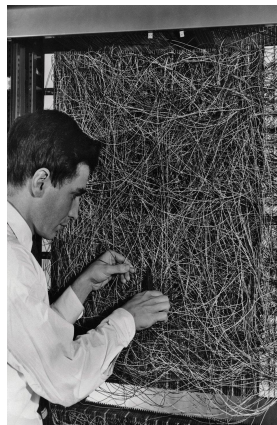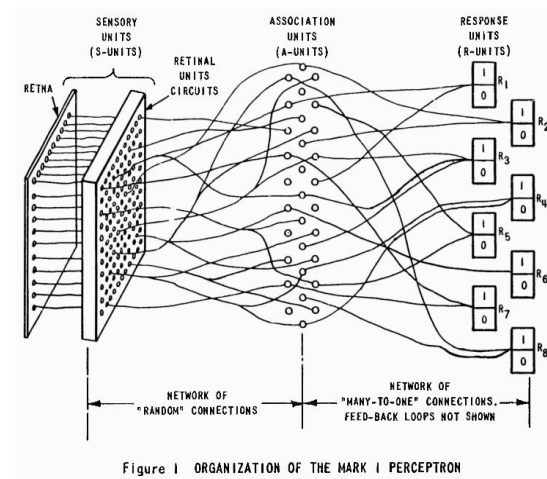
Mark I Perceptron

- 400 photosensitive receptors (sensory units)
- 512 stepping motors (association units, trainable)
- 8 output neurons (response units)

Figure 1 ORGANIZATION OF THE MARK I PERCEPTRON

Threshold function

$$f(x) = \begin{cases} 1 \text{ if } w \cdot x + b > 0 \\ 0 \text{ otherwise} \end{cases}$$

w real-valued weights
· dot product
b real scalar constant
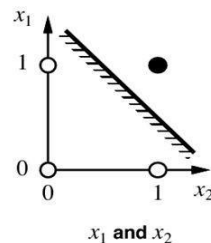

[2,3,4,5]

Minsky & Papert: The XOR affair

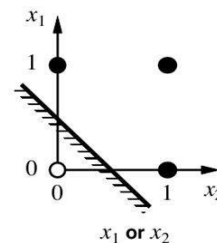The perceptron capabilities were limited (Rosenblatt)

Linear separability

"Perceptrons: an introduction to computational geometry"
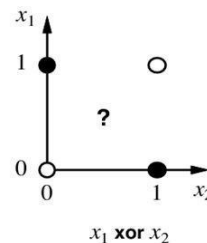
(Minsky & Papert, 1969):

- Perceptron cannot learn non-linearities
- Multi-Layer networks cannot be trained

NNs abandoned until the mid 80s: **1st AI WINTER**

Shift from connectionism to symbolism

Backpropagation Algorithm

How to optimize weights not directly connected to the error?

Backpropagation algorithm:

- Use the chain rule to find the derivative of cost with respect to any variable

Optimization through Gradient Descent

Used for training MLPs in (Werbos in 1974, Rumelhart et al. in 1985)

End of NNs Winter (Begining of 2nd AI Winter)

[7,8]

Feedforward Neural Networks

Optimization & Learning

Training through backprop (1) + gradient descent (2)

- **Forward pass**
  - Compute output for a given input
  - Error measurement (loss function)

- **Backward pass**
  - Find gradients minimizing error layer by layer (1)
  - Apply gradients (2)

The Gradient Descent Family

Batch GD: Compute gradients of *all training samples* before descending
- Deterministic outcome
- Large memory cost

Stochastic GD: Apply gradient of *one random training sample* at a time
- Very stochastic
- Does not guarantee learning
- Poor parallelization

Mini-batch GD: Combine gradients of a *random subset of train samples*
- Mildly Stochastic
- Good parallelization
- Subset size aka *"Batch size"*

WARNING: This naming is not universally respected!

Mini-batch Training Nomenclature

Num. samples computed together: **The batch size**

One feedforward/backward cycle (one batch): **A step**

N steps (all training samples once): **An epoch**

$$N = \frac{dataset\_size}{batch\_size}$$

Factors for defining the batch size (rarely)

- Instance size ⬇
- Computational efficiency ⬆
- Stochasticity ⬇
- Powers of 2

Factors for defining the number of epochs (constantly)

- Convergence ⬆
- Reliability ⬆
- Footprint ⬇

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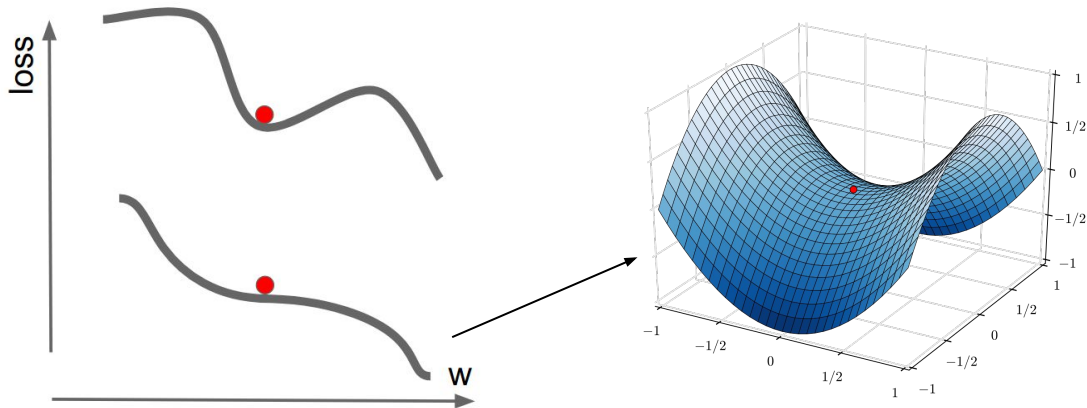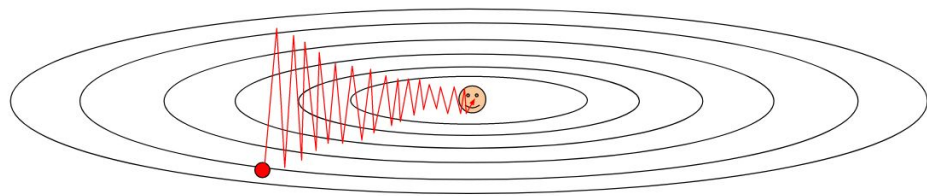# The Art of Descending

Hard to go down in a high dimensional space

❖ Different loss speed among dimensions

■ Slow and jitter

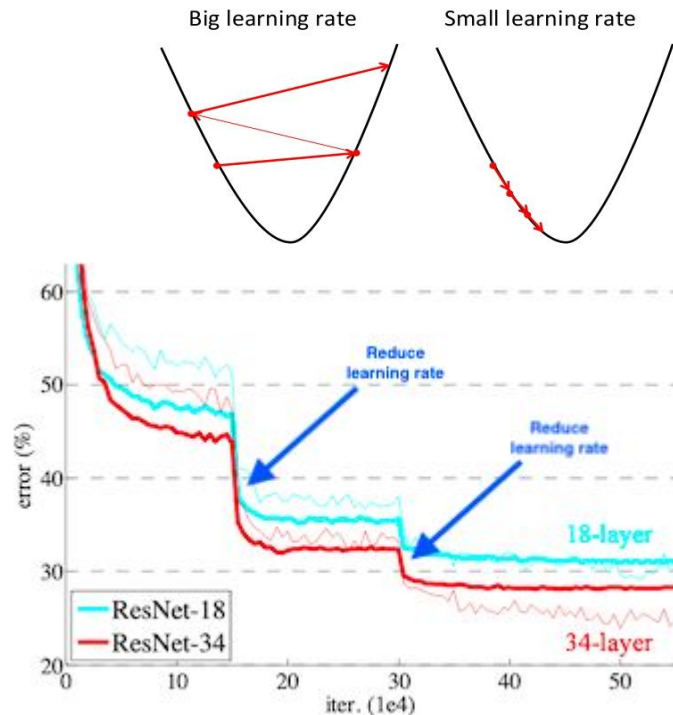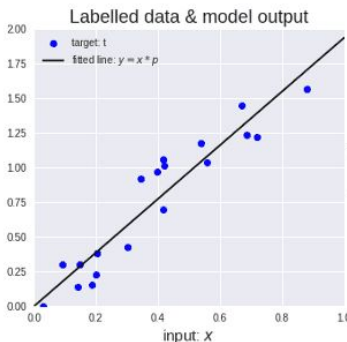❖ Local minima & saddle points

■ Stuck gradient

❖ Mini-batches are noisy

[32]

The Art of Descending

Learning rate: How much you move in the direction of the gradient

Direct effect on convergence and speed

The same LR may not always be the right one

Practical Tips II
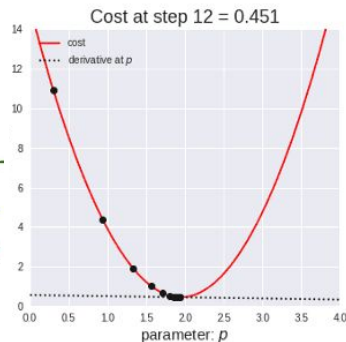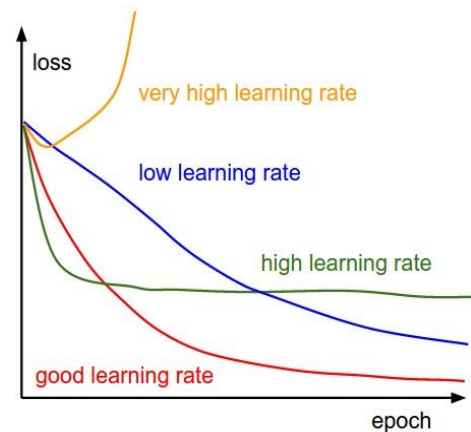
Tuning the Learning Rate

- Fix the batch size (or viceversa)
    - Theory: Double one, double the other
- Always smaller than 1
- Search by orders of magnitude
- Grid search < Random search
- In case of doubt, go small
- When stuck, reduce it

Inertia in Optimizers

Momentum:
- ❖ Add a fraction of the previous gradient. *Inertia.*
- ❖ Decaying weight parameter. *Friction.*
- ❖ Faster, smoother convergence
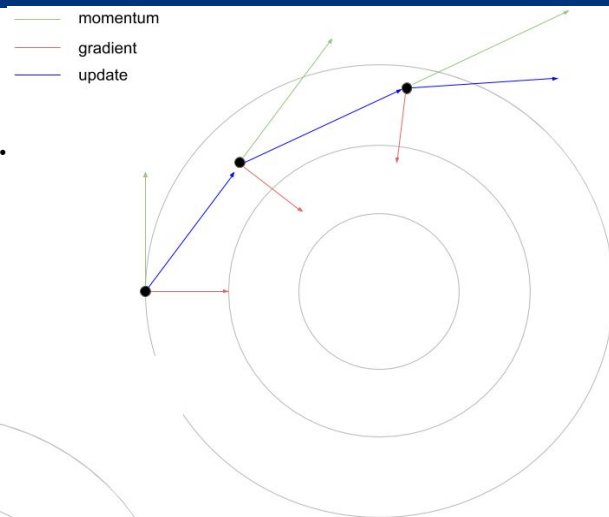
Nesterov:
- ❖ Gradient computed after inertia
- ❖ See the slope ahead
- ❖ Faster convergence

[33]

Adaptative LR Optimizers

Adagrad:
- ❖ Parameter-wise LR considering past updates.
- ❖ High LR for infrequent ones. Low LR for frequent ones.
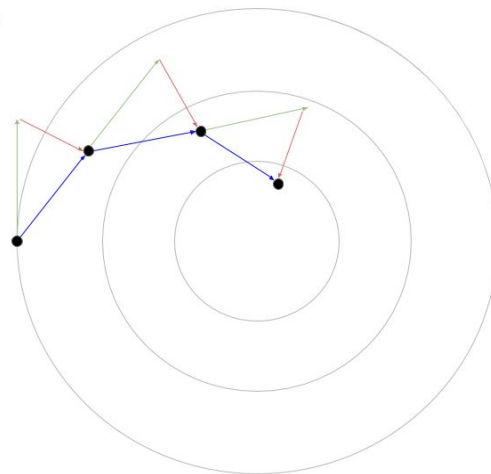- ❖ Good for sparse data. Vanishing step size due to growing history.

Adadelta:
- ❖ Adagrad with a decaying average over history (typically around 0.9)

RMSprop:
- ❖ Similar to Adadelta

Adam:
- ❖ Adadelta + Momentum

Nadam:
- ❖ Adadelta + Nesterov

[33]

Optimizers

- Adam: Current popular default. Competitive with minimal tuning.

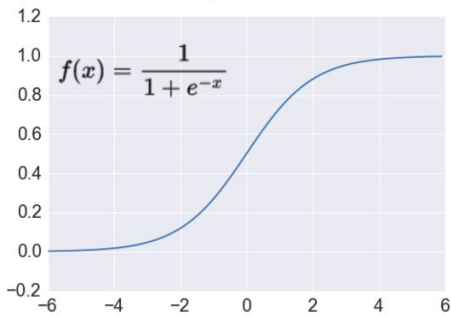- SGD + Momentum: Great if LR is decayed properly

Hyperparameters incomplete list #1 (training)

1. Batch size

2. Number of epochs

3. Learning rate

4. Weight decay

Activation Functions

Transform the output of a layer to a given range.

Sigmoid

$$f(x) = \frac{1}{1 + e^{-x}}$$

TanH

$$\tanh(x) = \frac{2}{1 + e^{-2x}} - 1$$
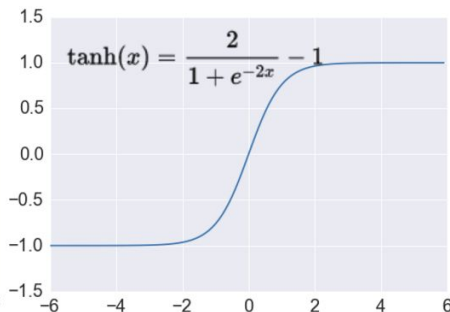
❖ Zero gradient most of f(x): Saturates!
❖ Gradient is 0.25 or 1 max. Vanishes!

ReLU

$$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$$
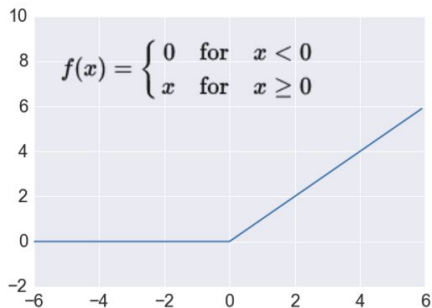
❖ Does not saturate
❖ Does not vanish
❖ Faster computation
❖ May die with high LR

ReLU is a safe choice in most cases

Undying alternatives: Leaky ReLU, PReLU, ELU, SELU, …

ReLU: The linear non-linearity

ReLU(-4-2x+y) +
ReLU(4+2x+y) +
ReLU(5-x-2y)

[30]
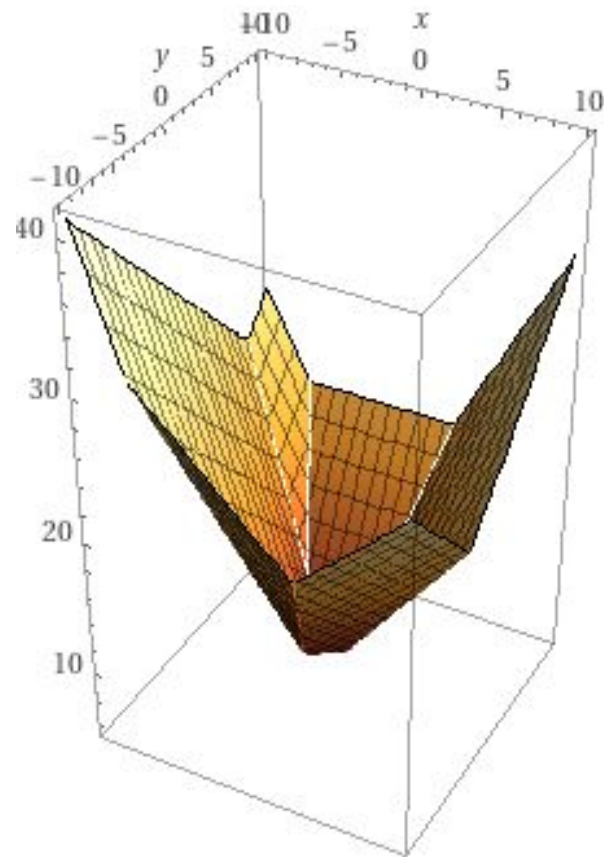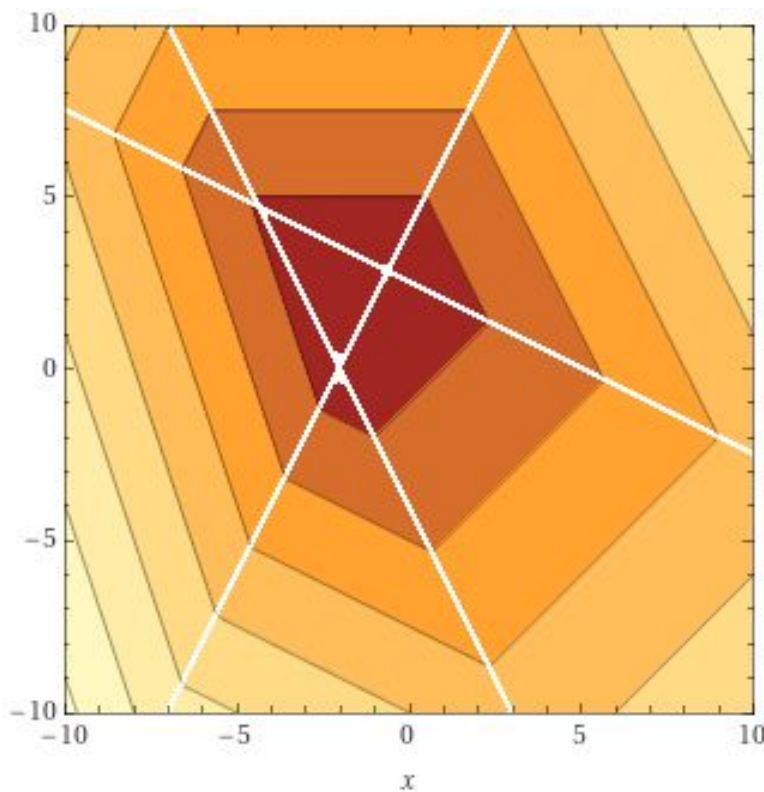
Input Pre-processing

Make your model's life easier. She would do it for you.

Unnormalized:
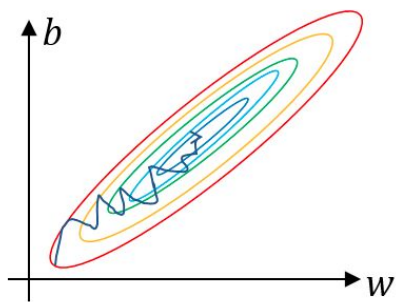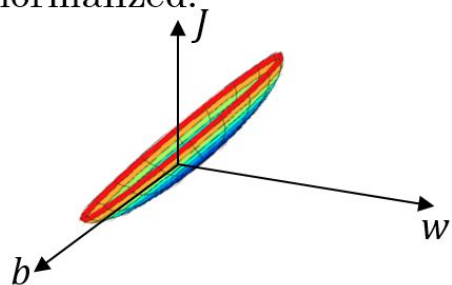
Normalized:
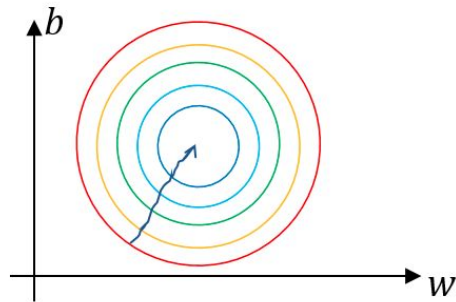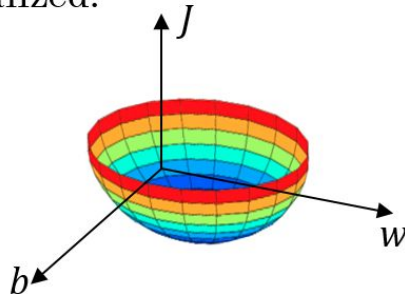
Options

❖ Mean substraction
❖ Normalization
  ▪ - mean / std
  ▪ Image-wise?
  ▪ Channel-wise?

Also, beware of the *imbalance*!!

Weight Initialization

We want:

❖ Small numbers

❖ Half positive, half negative

Options:

❖ ~~Constant values~~: No symmetry breaking

❖ Normal distribution sample: Ok for shallow, but deviation grows with size

❖ Glorot/Xavier: Normalize variance by number of inputs

❖ He/Kaming/MSRA: Specific for ReLUs.

What about bias?

● If weights are properly initialized, bias can be zero-init.

- Start with ReLUs. Explore variants as a long shot.

- Always zero-mean the data. Or normalize (init depends on it)

- If using ReLUs, *He* init. Otherwise *Glorot*.

Hyperparameters incomplete list #2 (initialization & preprocessing)

5. Activation function

6. Input normalization

7. Weight Initialization

Regularization

Why do we need regularization?

❖ **Generalization:** Difference between *Machine Learning* and *Optimization*

 ■ We want to learn the "good" patterns

 ■ Neural nets are lazy. They will always go for the "easy" patterns

 ■ Generalization is a sweet spot that may be unreachable

From underfit to overfit

Underfit: Insufficient learning of training data patterns

Overfit: "Excessive" learning of training data patterns

Key players:
❖ Model capacity
❖ Data input
❖ Regularizers

Train, Test and Val

Doing a good train/val/test split is not easy! Take your time & do it right.

Training set
- ❖ Data used by _the model_ for learning parameters
- ❖ Keep an eye for variance (spurious patterns)
- ❖ As large and varied as possible
- ❖ Use mostly as a sanity check
- ❖ Overfitting is inevitable
  - ■ Sometimes it's desirable!

Validation set
- ❖ Data used by _you_ for tuning hyperparameters
- ❖ Size entails reliability
- ❖ Overfitting is possible

Test set
- ❖ Hide under a rock
- ❖ Must be 100% independent
- ❖ Run once. Cite forever.

Never, ever, ever

- Mix correlated data in train/val/test
- Process data in an order
  - Do shuffle with seed!
  - Reproducibility for your own sake
- Believe train results generalize
- The dataset is free of bias
- Assume balanced dataset

Training milestones

1. Learn, **anything**! (Train set)
   - Little capacity makes it easier
   - Rough hyperparameter estimation
   - *Goal*: Underfit
     i. Better than random

2. Learn, **everything**! (Train set)
   - Growing capacity
   - Hyperparameter refinement
   - *Goal*: Overfit

3. Learn **the right thing** (Val set)
   - Regularization
   - *Goal*: Fit

Back to Regularization

Takes us from overfit to fit

The must do ones (if overfitting):

❖ **Early Stopping**
- ■ Overfitting is the end of the road
- ■ The guide: Validation loss/accuracy
- ■ Enough to understand the model (mind the footprint!)
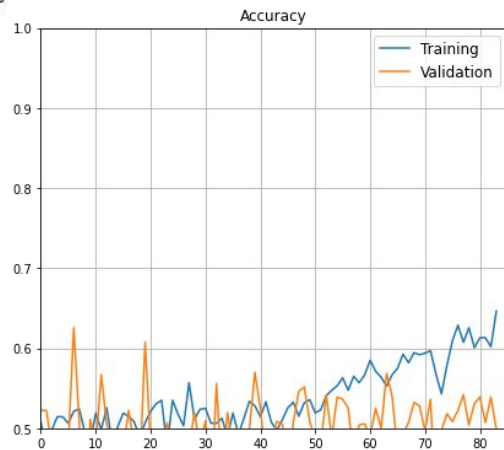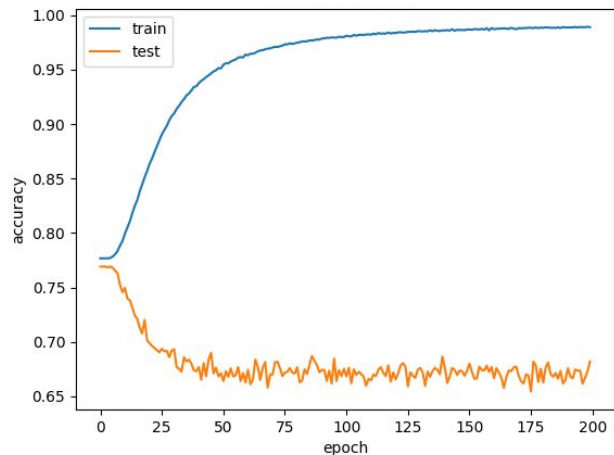
❖ **Data Augmentation**
- ■ More data for free
- ■ Huge impact
- ■ As any data preprocessing, think thoroughly!

Diagnosing the curves (loss & acc.*)

- Random performance?

- General trend?
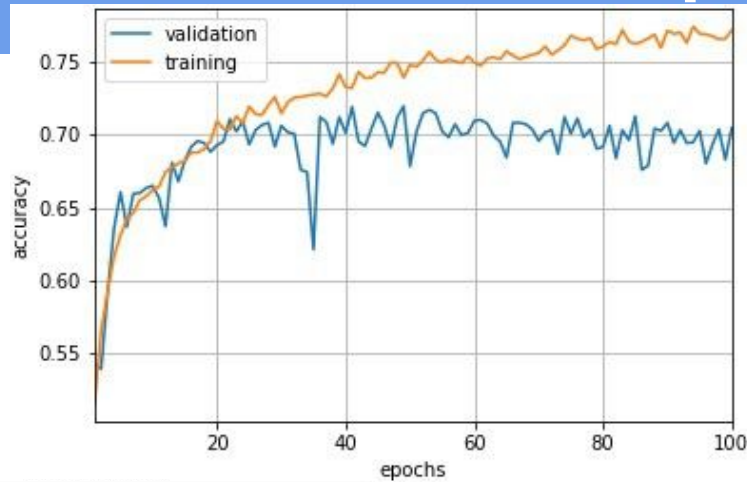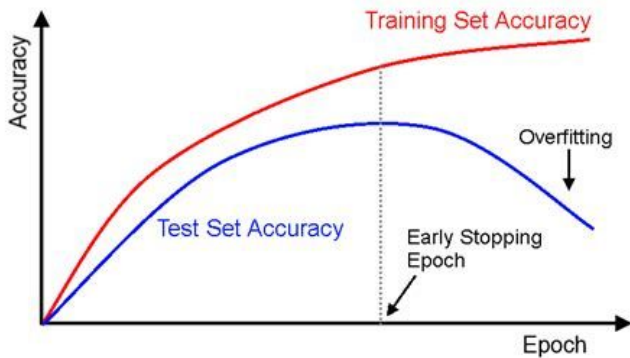
- Fails to converge? No trend?
    - Simplify problem/model. Decrease LR.
    - Data corrupted? Pre-processing? Weight init?

**Weird curves
are the worst!**

- Loss explosion? Sudden spike?
    - Problematic data instances.
    - Exploding gradients ⟹ weights.

- Loss goes down and accuracy goes down (what??)
    - Raw outcome improves, but threshold metric is not met
    - Imbalance?

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Parameter Norm Penalty methods

Add a regularizing term to the loss function

❖ **L2/L1 norm** on weights by factor (another hyperparam!)

❖ Makes gradients and weights smaller (L1 sparsifies inputs)

❖ Safe for SGD, not so for adaptive learning optimizers (e.g., Adam)

■ Uneven normalization :S

Weight decay is similar to L2-norm (often confused)

❖ Scaling factor on the update rule (another hyperparam!)

❖ Analogous to L2-norm for SGD, not for adaptative optimizers

❖ Theoretically safe for all (if implemented!)

[10,11,12]

Max-Norm

Limits the magnitude of the weights vector

- ❖ Constant c (another hyperparam!)
- ❖ Typically around 3 or 4
- ❖ Goes well with dropout
- ❖ May be redundant with L2-norm/weight decay

[10,11,12]

Batch Normalization

Force the *activations* within a normal distribution

❖ Applied between neurons and activation functions

❖ Statistics computed per mini-batch (practical reasons)

❖ On inference, use population of mini-batch statistics

❖ Helps with initialization and regularization (avoid the radicals)

❖ Allows higher LR

❖ Faster convergence

❖ Requires minimum & fixed batch size
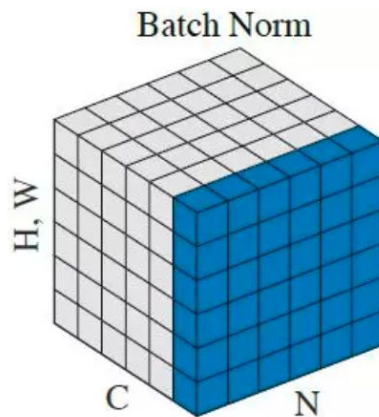
Batch Norm

Norms, Norms, Norms
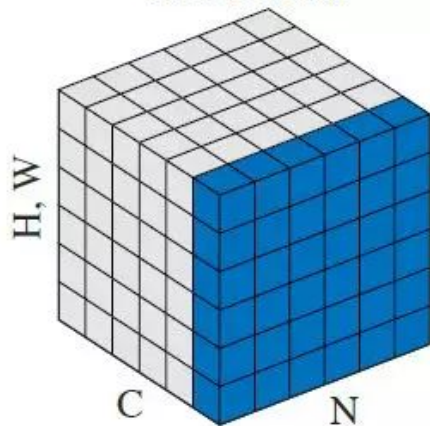
Batch Norm — All instances / One var
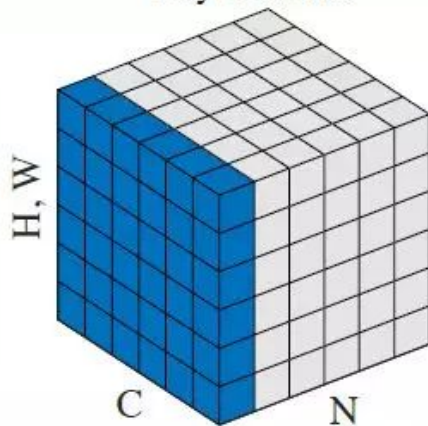
Layer Norm — One instance / All vars
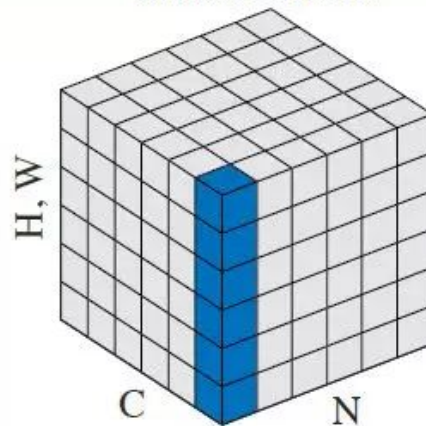
Instance Norm — One instance / One var
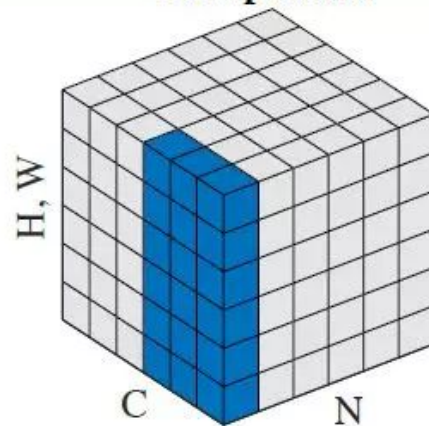
Group Norm — One instance / N vars

And more!!

Dropout

Cut-off neuron inputs with a given probability

- ❖ Dropout rate (typically between 0.2 and 0.5) applied on every step
- ❖ In practice trains an ensemble of networks with "shared" params
- ❖ Inference: Use all inputs, scaled by the same probability
- ❖ Reduces co-adaptation between neurons
- ❖ Slows down training (a lot)
- ❖ Affects many other hyperparameters
- ❖ Good on FC layers. Not on Convs.
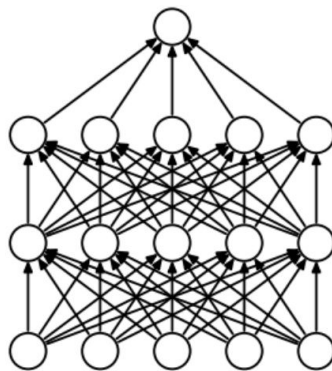
(a) Standard Neural Net
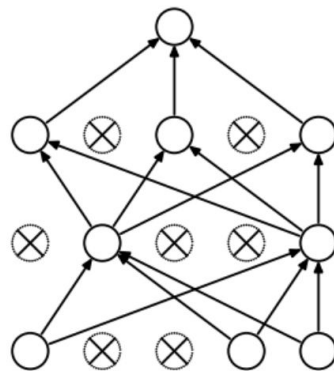
(b) After applying dropout.

One experiment at a time

1. Analysis
    - What is wrong/improvable?
    - How can it be solved/achieved?
2. Test
    - Which alternative works better?
    - Ablation study: Alone or combined?

Underfitting
- ❏ Initialization
- ❏ LR, batch size
- ❏ Complexity up

Overfitting
- ❏ Regularization
- ❏ Complexity down

Learning what?

Loss/Cost/Objective/Error function defines the optimization goal

❖ N-way Classification

  ■ Softmax (outs N probabilities) + Cross-Entropy (in N neurons)

❖ Regression

  ■ Mean Squared Error (in 1 neuron)

❖ And so many others!

Hyperparameters incomplete list #3 (capacity, regularization and loss)

8. Network *capacity* (layers, neurons)

9. Early stopping policy

10. Data Augmentations

11. Normalization layers + hyperparams

12. Loss function

Next class:
Convolutional Neural Networks

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[12] https://towardsdatascience.com/weight-decay-l2-regularization-90a9e17713cd

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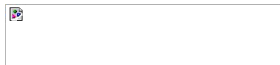[17] https://arxiv.org/pdf/1606.00915.pdf

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[21] https://arxiv.org/abs/1603.03417

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