#### **Machine Learning Tricks**

Philipp Koehn

13 October 2020



#### **Machine Learning**



- Myth of machine learning
  - given: real world examples
  - automatically build model
  - make predictions

### **Machine Learning**



- Myth of machine learning
  - given: real world examples
  - automatically build model
  - make predictions
- Promise of deep learning
  - do not worry about specific properties of problem
  - deep learning automatically discovers the feature

# **Machine Learning**



- Myth of machine learning
  - given: real world examples
  - automatically build model
  - make predictions
- Promise of deep learning
  - do not worry about specific properties of problem
  - deep learning automatically discovers the feature
- Reality: bag of tricks

# Today's Agenda



- No new translation model
- Discussion of failures in machine learning
- Various tricks to address them

# Fair Warning



# Fair Warning



• At some point, you will think:

Why are you telling us all this madness?

# Fair Warning



• At some point, you will think:

Why are you telling us all this madness?

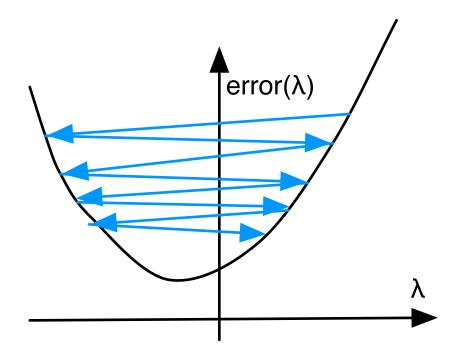
• Because pretty much all of it is commonly used



# failures in machine learning

### Failures in Machine Learning



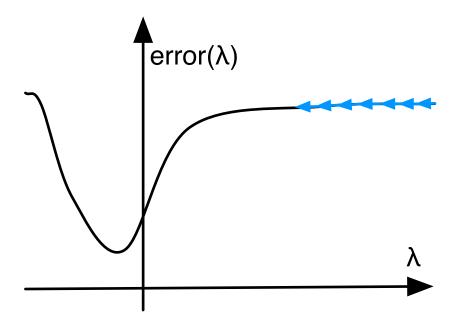


Too high learning rate may lead to too drastic parameter updates

→ overshooting the optimum

### Failures in Machine Learning

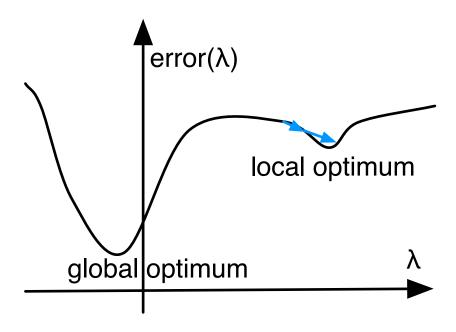




Bad initialization may require many updates to escape a plateau

## Failures in Machine Learning





Local optima trap training

# **Learning Rate**



- Gradient computation gives direction of change
- Scaled by learning rate
- Weight updates

# **Learning Rate**



- Gradient computation gives direction of change
- Scaled by learning rate
- Weight updates

• Simplest form: fixed value

# **Learning Rate**

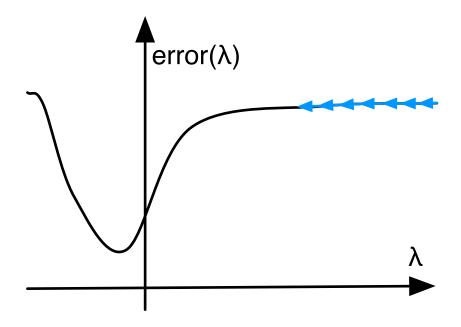


- Gradient computation gives direction of change
- Scaled by learning rate
- Weight updates
- Simplest form: fixed value
- Annealing
  - start with larger value (big changes at beginning)
  - reduce over time (minor adjustments to refine model)

#### **Initialization of Weights**

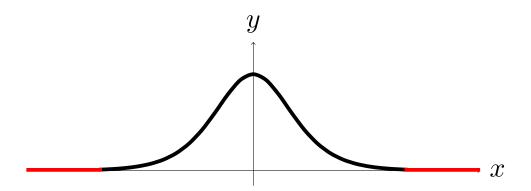


- Initialize weights to random values
- But: range of possible values matters



### **Sigmoid Activation Function**

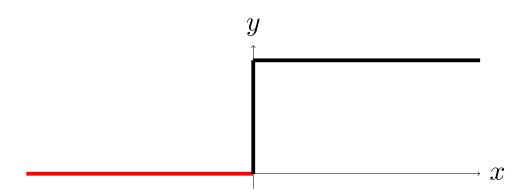




Near zero for large positive and negative values

#### **Rectified Linear Unit**





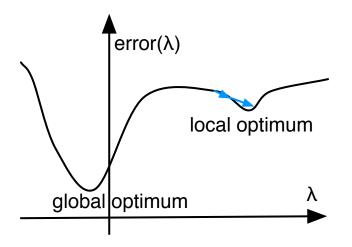
Flat and for large interval: Gradient is 0

"Dead cells" elements in output that are always 0, no matter the input

### **Local Optima**



• Cartoon depiction



- Reality
  - highly dimensional space
  - complex interaction between individual parameter changes
  - "bumpy"

# Vanishing and Exploding Gradients

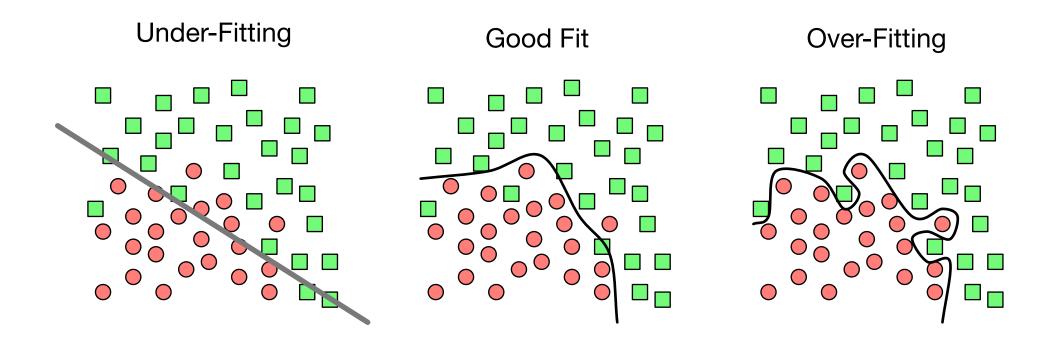




- Repeated multiplication with same values
- If gradients are too low  $\rightarrow 0$
- If gradients are too big  $\to \infty$

# **Overfitting and Underfitting**





- Complexity of the problem has too match the capacity of the model
- Capacity ≃ number of trainable parameters



# ensuring randomness

## **Ensuring Randomness**



• Typical theoretical assumption

independent and identically distributed

training examples

#### **Ensuring Randomness**



• Typical theoretical assumption

independent and identically distributed

training examples

- Approximate this ideal
  - avoid undue structure in the training data
  - avoid undue structure in initial weight setting

### **Ensuring Randomness**



• Typical theoretical assumption

independent and identically distributed

training examples

- Approximate this ideal
  - avoid undue structure in the training data
  - avoid undue structure in initial weight setting
- ML approach: Maximum entropy training
  - Fit properties of training data
  - Otherwise, model should be as random as possible (i.e., has maximum entropy)



- Typical training data in machine translation
  - different types of corpora
    - \* European Parliament Proceedings
    - \* collection of movie subtitles
  - temporal structure in each corpus
  - similar sentences next too each other (e.g., same story / debate)



- Typical training data in machine translation
  - different types of corpora
    - \* European Parliament Proceedings
    - \* collection of movie subtitles
  - temporal structure in each corpus
  - similar sentences next too each other (e.g., same story / debate)
- Online updating: last examples matter more



- Typical training data in machine translation
  - different types of corpora
    - \* European Parliament Proceedings
    - \* collection of movie subtitles
  - temporal structure in each corpus
  - similar sentences next too each other (e.g., same story / debate)
- Online updating: last examples matter more
- Convergence criterion: no improvement recently
  - → stretch of hard examples following easy examples: prematurely stopped



- Typical training data in machine translation
  - different types of corpora
    - \* European Parliament Proceedings
    - \* collection of movie subtitles
  - temporal structure in each corpus
  - similar sentences next too each other (e.g., same story / debate)
- Online updating: last examples matter more
- Convergence criterion: no improvement recently
  - → stretch of hard examples following easy examples: prematurely stopped
- ⇒ randomly shuffle the training data (maybe each epoch)

# Weight Initialization



- Initialize weights to random values
- Values are chosen from a uniform distribution
- Ideal weights lead to node values in transition area for activation function

# Weight Initialization



- Initialize weights to random values
- Values are chosen from a uniform distribution
- Ideal weights lead to node values in transition area for activation function

## For Example: Sigmoid



- Input values in range [-1; 1]
- $\Rightarrow$  Output values in range [0.269;0.731]

# For Example: Sigmoid



- Input values in range [-1; 1]
- $\Rightarrow$  Output values in range [0.269;0.731]
  - Magic formula (*n* size of the previous layer)

$$\big[-\frac{1}{\sqrt{n}},\frac{1}{\sqrt{n}}\big]$$

# For Example: Sigmoid



- Input values in range [-1; 1]
- $\Rightarrow$  Output values in range [0.269;0.731]
  - Magic formula (*n* size of the previous layer)

$$\left[-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}\right]$$

Magic formula for hidden layers

$$\left[-\frac{\sqrt{6}}{\sqrt{n_j+n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j+n_{j+1}}}\right]$$

- $n_j$  is the size of the previous layer
- $n_j$  size of next layer

#### **Problem: Overconfident Models**



- Predictions of the neural machine translation models are surprisingly confident
- Often almost all the probability mass is assigned to a single word (word prediction probabilities of over 99%)

#### **Problem: Overconfident Models**



- Predictions of the neural machine translation models are surprisingly confident
- Often almost all the probability mass is assigned to a single word (word prediction probabilities of over 99%)
- Problem for decoding and training
  - decoding: sensible alternatives get low scores, bad for beam search
  - training: overfitting is more likely

#### **Problem: Overconfident Models**



- Predictions of the neural machine translation models are surprisingly confident
- Often almost all the probability mass is assigned to a single word (word prediction probabilities of over 99%)
- Problem for decoding and training
  - decoding: sensible alternatives get low scores, bad for beam search
  - training: overfitting is more likely
- Solution: label smoothing

#### **Problem: Overconfident Models**



- Predictions of the neural machine translation models are surprisingly confident
- Often almost all the probability mass is assigned to a single word (word prediction probabilities of over 99%)
- Problem for decoding and training
  - decoding: sensible alternatives get low scores, bad for beam search
  - training: overfitting is more likely
- Solution: label smoothing
- Jargon notice
  - in classification tasks, we predict a *label*
  - jargon term for any output
  - $\rightarrow$  here, we smooth the word predictions

# **Label Smoothing during Decoding**



- Common strategy to combat peaked distributions: smooth them
- Recall
  - prediction layer produces numbers for each word
  - converted into probabilities using the softmax

$$p(y_i) = \frac{\exp s_i}{\sum_j \exp s_j}$$

# **Label Smoothing during Decoding**



- Common strategy to combat peaked distributions: smooth them
- Recall
  - prediction layer produces numbers for each word
  - converted into probabilities using the softmax

$$p(y_i) = \frac{\exp s_i}{\sum_j \exp s_j}$$

ullet Softmax calculation can be smoothed with so-called **temperature** T

$$p(y_i) = \frac{\exp s_i/T}{\sum_j \exp s_j/T}$$

 Higher temperature → distribution smoother (i.e., less probability is given to most likely choice)

# **Label Smoothing during Training**



- Root of problem: training
- Training object: assign all probability mass to single correct word

# **Label Smoothing during Training**



- Root of problem: training
- Training object: assign all probability mass to single correct word
- Label smoothing
  - truth gives some probability mass to other words (say, 10% of it)
  - uniformly distributed over all words
  - relative to unigram word probabilities
     (relative counts of each word in the target side of the training data)



# adjusting the learning rate

# **Adjusting the Learning Rate**



- Gradient descent training: weight update follows the gradient downhill
- Actual gradients have fairly large values, scale with a learning rate (low number, e.g.,  $\mu = 0.001$ )
- Change the learning rate over time
  - starting with larger updates
  - refining weights with smaller updates
  - adjust for other reasons
- Learning rate schedule

#### **Momentum Term**



- Consider case where weight value far from optimum
- Most training examples push the weight value in the same direction
- Small updates take long to accumulate

#### **Momentum Term**



- Consider case where weight value far from optimum
- Most training examples push the weight value in the same direction
- Small updates take long to accumulate

- Solution: momentum term  $m_t$ 
  - accumulate weight updates at each time step t
  - some decay rate for sum (e.g., 0.9)
  - combine momentum term  $m_{t-1}$  with weight update value  $\Delta w_t$

$$m_t = 0.9m_{t-1} + \Delta w_t$$

$$w_t = w_{t-1} - \mu \ m_t$$

# Adapting Learning Rate per Parameter



- Common strategy: reduce the learning rate  $\mu$  over time
- Initially parameters are far away from optimum → change a lot
- Later nuanced refinements needed → change little

• Now: different learning rate for each parameter

## **Adagrad**



- Different parameters at different stages of training
  - $\rightarrow$  different learning rate for each parameter
- Adagrad
  - record gradients for each parameter
  - accumulate their square values over time
  - use this sum to reduce learning rate

# Adagrad



- Different parameters at different stages of training
  - → different learning rate for each parameter
- Adagrad
  - record gradients for each parameter
  - accumulate their square values over time
  - use this sum to reduce learning rate
- Update formula
  - gradient  $g_t = \frac{dE_t}{dw}$  of error E with respect to weight w
  - divide the learning rate  $\mu$  by accumulated sum

$$\Delta w_t = \frac{\mu}{\sqrt{\sum_{\tau=1}^t g_\tau^2}} g_t$$

- Big changes in the parameter value (corresponding to big gradients  $g_t$ )
  - $\rightarrow$  reduction of the learning rate of the weight parameter

#### **Adam: Elements**



- Combine idea of momentum term and reduce parameter update by accumulated change
- Momentum term idea (e.g.,  $\beta_1 = 0.9$ )

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$

• Accumulated gradients (decay with  $\beta_2 = 0.999$ )

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

#### **Adam: Technical Correction**



- Initially, values for  $m_t$  and  $v_t$  are close to initial value of 0
- Adjustment

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

• With  $t \to \infty$  this correction goes away

$$\lim_{t\to\infty}\frac{1}{1-\beta^t}\to 1$$

#### Adam



- Given
  - learning rate  $\mu$
  - momentum  $\hat{m}_t$
  - accumulated change  $\hat{v}_t$
- Weight update per Adam (e.g.,  $\epsilon = 10^{-8}$ )

$$\Delta w_t = \frac{\mu}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$$



ullet Accumulate all weight updates for all the training example o update (converges slowly)



- ullet Accumulate all weight updates for all the training example o update (converges slowly)
- Process each training example → update (stochastic gradient descent)
   (quicker convergence, but last training disproportionately higher impact)



- Accumulate all weight updates for all the training example → update (converges slowly)
- Process each training example → update (stochastic gradient descent)
   (quicker convergence, but last training disproportionately higher impact)
- Process data in batches
  - compute all their gradients for individual word predictions errors
  - use sum over each batch to update parameters
  - → better parallelization on GPUs



- Accumulate all weight updates for all the training example → update (converges slowly)
- Process each training example → update (stochastic gradient descent)
   (quicker convergence, but last training disproportionately higher impact)
- Process data in batches
  - compute all their gradients for individual word predictions errors
  - use sum over each batch to update parameters
  - → better parallelization on GPUs
- Process data on multiple compute cores
  - batch processing may take different amount of time
  - asynchronous training: apply updates when they arrive
  - mismatch between original weights and updates may not matter much



# avoiding local optima

# **Avoiding Local Optima**



- One of hardest problem for designing neural network architectures and optimization methods
- Ensure that model converges to at least to a set of parameter values that give results close to this optimum on unseen test data.
- There is no real solution to this problem.
- It requires experimentation and analysis that is more craft than science.
- Still, this section presents a number of methods that generally help avoiding getting stuck in local optima.

# **Overfitting and Underfitting**



- Neural machine translation models
  - 100s of millions of parameters
  - 100s of millions of training examples (individual word predictions)
- No hard rules for relationship between these two numbers
- Too many parameters and too few training examples → overfitting
- Too few parameters and many training examples → underfitting

## Regularization



- Motivation: prefer as few parameters as possible
- Strategy: set un-needed paramters a value of 0
- Method
  - adjust training objective
  - add cost for any non-zero parameter
  - typically done with L2 norm
- Practical impact
  - derivative of L2 norm is value of parameter
  - if not signal from training: reduce value of parameter
  - alsp called weight decay
- Not common in deep learning, but other methods understood as regularization

# **Curriculum Learning**



- Human learning
  - learn simple concepts first
  - learn more complex material later
- Early epochs: only easy training examples
  - only short sentences
  - create artificial data by extracting smaller segments
     (similar to phrase pair extraction in statistical machine translation)
  - Later epochs: all training data
- Not easy to callibrate

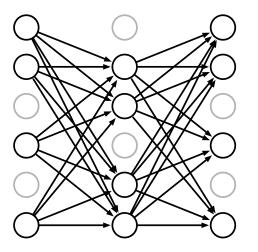
# **Dropout**

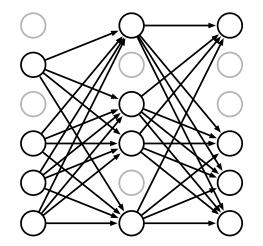


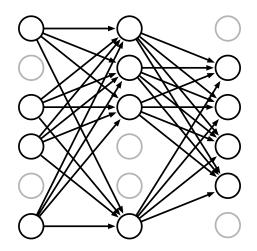
- Training may get stuck in local optima
  - some properties of task have been learned
  - discovery of other properties would take it too far out of its comfort zone.
- Machine translation example
  - model learned the language model aspects
  - but cannot figure out role of input sentence
- Drop out: for each batch, eliminate some nodes

## **Dropout**









#### Dropout

- For each batch, different random set of nodes is removed
- Their values are set to 0 and their weights are not updated
- 10%, 20% or even 50% of all the nodes
- Why does this work?
  - robustness: redundant nodes play similar nodes
  - ensemble learning: different subnetworks are different models

# **Gradient Clipping**



- Exploding gradients: gradients become too large during backward pass
- $\Rightarrow$  Limit total value of gradients for a layer to threshold ( $\tau$ )
  - Use of L2 norm of gradient values *g*

$$L2(g) = \sqrt{\sum_{j} g_j^2}$$

• Adjust each gradient value  $g_i$  for each element i in the vector

$$g_i' = g_i \times \frac{\tau}{\max(\tau, L2(g))}$$

## **Layer Normalization**



- During inference, average node values may become too large or too small
- Has also impact on training (gradients are multiplied with node values)
- ⇒ Normalize node values
  - During training, learn bias layer

## **Layer Normalization: Math**



• Feed-forward layer  $h^l$ , weights W, computed sum  $s^l$ , activation function

$$s^{l} = W h^{l-1}$$
  
 $h^{l} = \operatorname{sigmoid}(h^{l})$ 

• Compute mean  $\mu^l$  and variance  $\sigma^l$  of sum vector  $s^l$ 

$$\mu^l = \frac{1}{H} \sum_{i=1}^H s_i^l$$

$$\sigma^l = \sqrt{\frac{1}{H} \sum_{i=1}^{H} (s_i^l - \mu^l)^2}$$

# **Layer Normalization: Math**



• Normalize  $s^l$ 

$$\hat{s^l} = \frac{1}{\sigma^l} (s^l - \mu^l)$$

• Learnable bias vectors *g* and *b* 

$$\hat{s^l} = \frac{g}{\sigma^l}(s^l - \mu^l) + b$$

## **Shortcuts and Highways**



- Deep learning: many layers of processing
- ⇒ Error propagation has to travel farther
  - All parameters in processing change have to be adjusted
  - Instead of always passing through all layers, add connections from first to last
  - Jargon alert
    - shortcuts
    - residual connections
    - skip connections

#### **Shortcuts**



• Feed-forward layer

$$y = f(x)$$

• Pass through input *x* 

$$y = f(x) + x$$

• Note: gradient is

$$y' = f'(x) + 1$$

• Constant  $1 \rightarrow$  gradient is passed through unchanged

# **Highways**

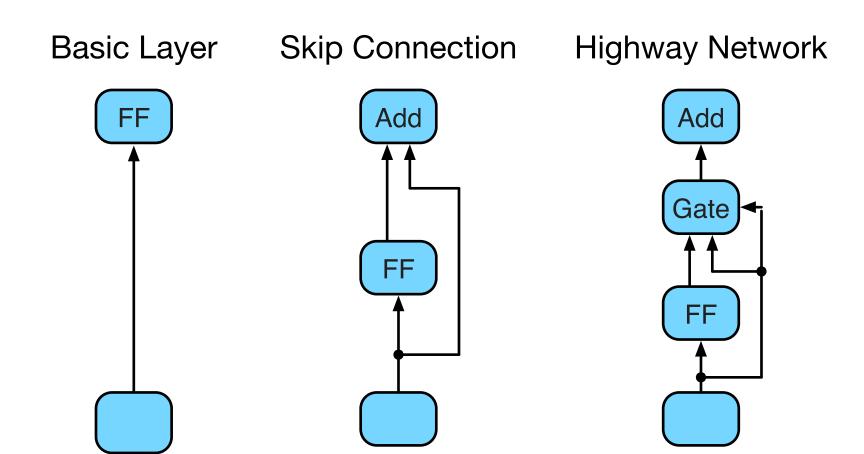


- Regulate how much information from f(x) and x should impact the output y
- Gate t(x) (typically computed by a feed-forward layer)

$$y = t(x) f(x) + (1 - t(x)) x$$

## **Shortcuts and Highways**





## LSTM and Vanishing Gradients



- Recall: Long short term memory (LSTM) cells
- Pass through of memory

$$memory^{t} = gate_{input} \times input^{t} + gate_{forget} \times memory^{t-1}$$

ullet Forget gate has values close to  $1 \rightarrow$  gradient passed through nearly unchanged



# generative adversarial training

# **Sequence-Level Training**



- Traditional training
  - predict one word at a time
  - compare against correct word
  - proceed training with correct word
- Sequence-level training
  - predict entire sequence
  - measure translation with sentence-level metric (e.g., BLEU)
- May use n-best translations, beam search, etc.

#### **Generative Adversarial Networks (GAN)**



- Game between two players
  - generator proposes a translation
  - discriminator distinguishes between generator's translation and human translation
  - generator tries to fool discriminator
- Training example: input sentence *x* and output sentence *y*
- Generator
  - traditional neural machine translation model
  - generates full sentence translations t for each input sentence
- Discriminator
  - is trained to classify (x, y) as correct example
  - is trained to classify (x, t) as generated example

#### **Generative Adversarial Networks (GAN)**



- 1. First train generator to some maturity
- 2. Train discriminator on generator predictions and human reference translations
- 3. Train jointly
  - generator with additional objective to fool discriminator
  - discriminator to do well on detecting generator's output as such

• In practice, this is hard to callibrate correctly

# Relationship to Reinforcement Learning



- No immediate feedback
  - chess playing: quality of move only revealed at end of game
  - walk through maze to avoid monsters and find gold
- Policy: decision process to which steps to take (here: generator, traditional neural machine translation model)
- Reward: end result (here: ability to fool discriminator)
- Popular technique: Monte Carlo search (here: Monte Carlo decoding)
- Training is called policy search