Machine Learning Tricks

Philipp Koehn

13 October 2020



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

• At some point, you will think:

Why are you telling us all this madness?

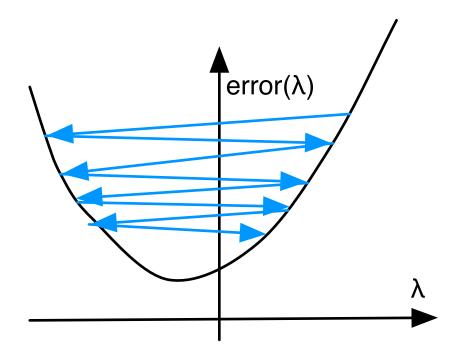
• Because pretty much all of it is commonly used



failures in machine learning

Failures in Machine Learning



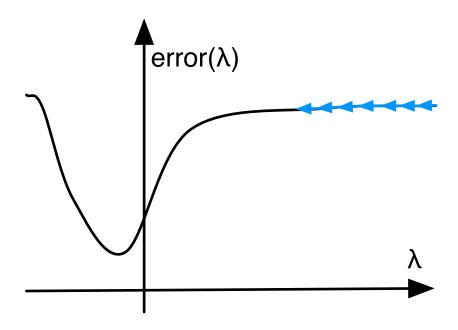


Too high learning rate may lead to too drastic parameter updates

→ overshooting the optimum

Failures in Machine Learning

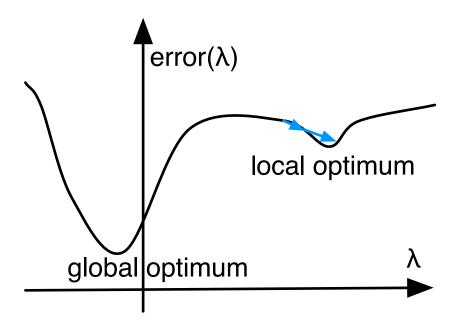




Bad initialization may require many updates to escape a plateau

Failures in Machine Learning





Local optima trap training

Learning Rate



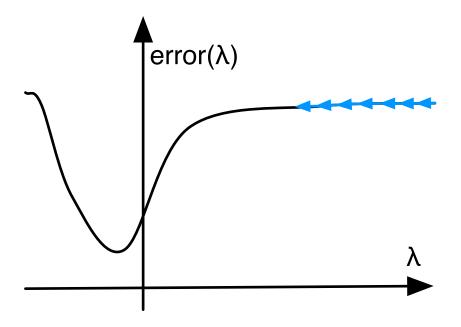
- Gradient computation gives direction of change
- Scaled by learning rate
- Weight updates

- Simplest form: fixed value
- Annealing
 - start with larger value (big changes at beginning)
 - reduce over time (minor adjustments to refine model)

Initialization of Weights

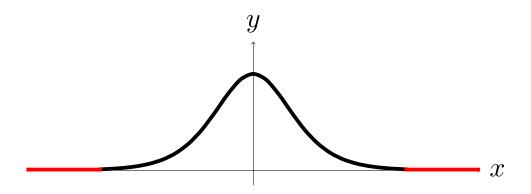


- Initialize weights to random values
- But: range of possible values matters



Sigmoid Activation Function



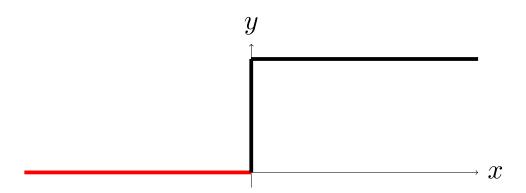


Derivative of sigmoid

Near zero for large positive and negative values

Rectified Linear Unit





Derivative of ReLU

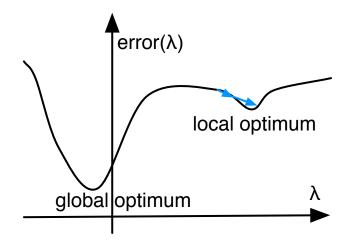
Flat and for large interval: Gradient is 0

"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

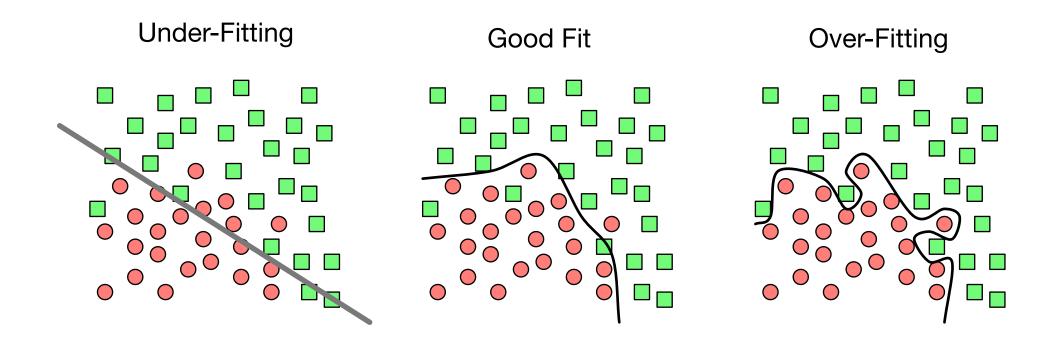




- Repeated multiplication with same values
- If gradients are too low $\rightarrow 0$
- If gradients are too big $\to \infty$

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

- 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)

Shuffling the Training Data



- 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

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_i is the size of the previous layer
- n_{j+1} 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 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

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

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
 - 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

- 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 Δw_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 μ 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
 - → 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 μ 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)
 - → 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 μ
 - momentum \hat{m}_t
 - accumulated change \hat{v}_t
- Weight update per Adam (e.g., $\epsilon = 10^{-8}$)

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

Batched Gradient Updates



- 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

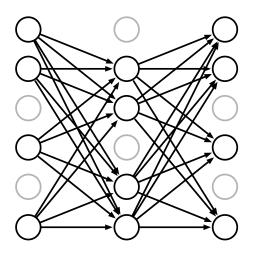
Dropout

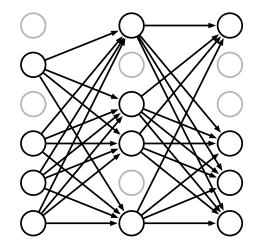


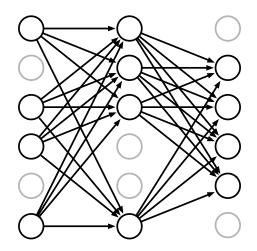
- Training may get stuck in local optima
 - some properties of task have been learned
 - discovery of other properties would take it too far out of its comfort zone.
- Machine translation example
 - model learned the language model aspects
 - but cannot figure out role of input sentence
- Drop out: for 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 (τ)
 - 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 μ^l and variance σ^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

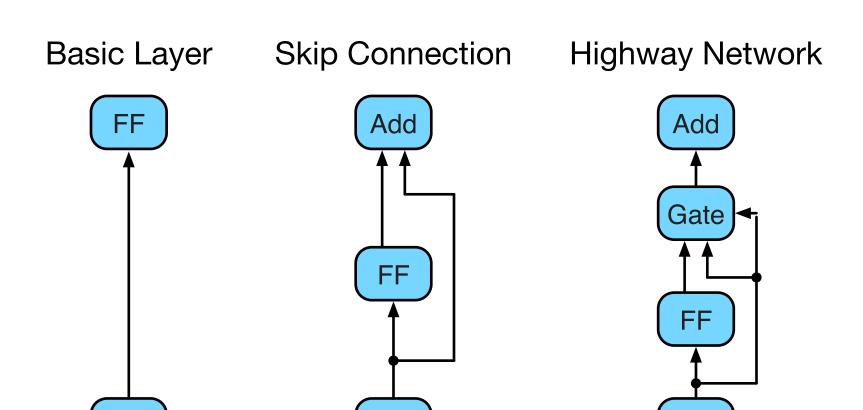


- Regulate how much information from f(x) and x should impact the output y
- Gate t(x) (typically computed by a feed-forward layer)

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

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