Contents

1 Machine Learning Basics

1.1 Un-/Supervised Learning

- Unsupervised Learning
  - No label or target class
  - Find out properties of the structure of the data
  - Clustering (k-means, PCA, etc.)
- Supervised Learning
  - Labels or target classes
- Reinforcement Learning

2 Linear Models

2.1 Regression, Classification

- **Regression:** Predicts a continuous output value
- **Classification:** Predicts a discrete value
  - **Binary Classification:** Output either 0 or 1
  - **Multi-class classification:** Set of N classes

2.2 Linear Regression

2.2.1 Linear Model

i:	Index of current sample
j:	Index of current weight
d:	Input dimension/number of weights
x_{ij}:	i-th Input data/feature of the j-th weight
θ_0:	Bias
θ_j:	Weights
$\hat{y}_i$:	i-th Prediction/Estimation (predicted label)

$$\hat{y}_i = \theta_0 + \sum_{j=1}^{d} x_{ij}\theta_j = \theta_0 + x_{i1}\theta_1 + \cdots + x_{id}\theta_d$$

Matrix Notation:

$$\hat{y} = X\theta$$

2.2.2 Loss function

Measures how good my estimation is and tells the optimization method how to make it better

2.2.2.1 Linear Least Squares:

n:	Number of training samples
y:	Ground truth labels
$\hat{y}$:	Estimated labels

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$$

Matrix Notation:

$$J(\theta) = (X\theta - y)^T(X\theta - y) = (\hat{y} - y)^T(\hat{y} - y)$$

2.2.3 Optimization

Changes the model in order to improve the loss function/estimation:

$$\theta = (X^TX)^{-1}X^Ty$$

2.3 Logistic Regression

2.3.1 Model

i:	Index of current sample
j:	Index of current weight
d:	Input dimension/number of weights
x_{ij}:	i-th Input data/feature of the j-th weight
θ_j:	Model parameters (Bias + Weights)
$\hat{y}_i$:	i-th Prediction/Estimation (predicted label)

$$\hat{y}_i = \sigma(x_i\theta) = \sigma\left(\theta_0 + \sum_{j=1}^{d} x_{ij}\theta_j\right)$$

with

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

2.3.2 Loss function

Measures how good my estimation is and tells the optimization method how to make it better

2.3.2.1 Binary Cross-Entropy:

y:	Ground truth labels
$\hat{y}$:	Estimated labels

$$\mathcal{L}(\hat{y}_i, y_i) = y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

2.3.3 Cost function

n:	Number of labels

$$C(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(\hat{y}_i, y_i)$$

2.3.4 Optimization

Changes the model in order to improve the loss function/estimation

- No closed-form solution
- Make use of an iterative method e.g. Gradient Descent

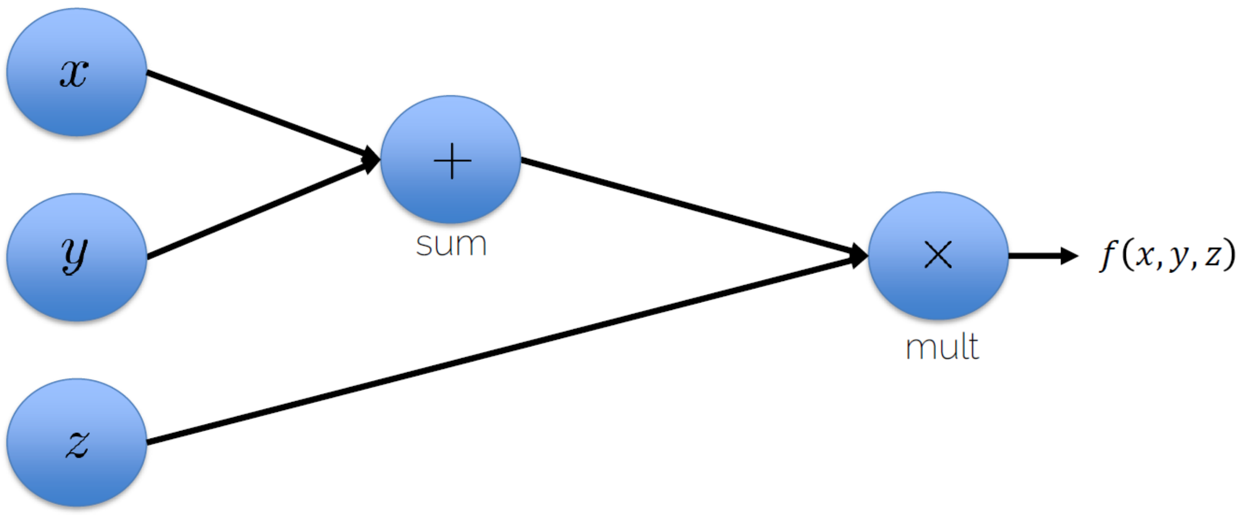
3 Computational Graphs

- Directional graph
- Matrix operations are represented as compute nodes
- Vertex nodes are variables or operators like $+, -, \cdot, /, log(), exp(), \dots$
- Directional edges show flow of inputs to vertices
- Neural network can be represented as computational graph

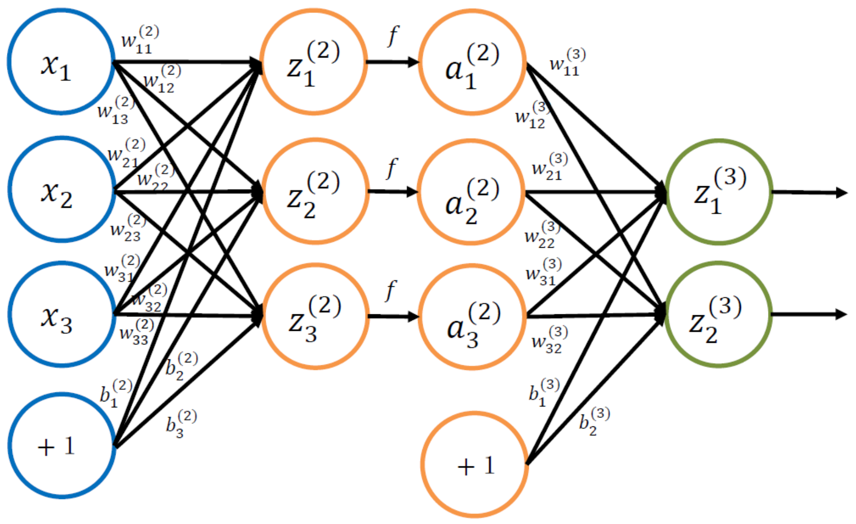
3.1 Graphical representation

Example

$$f(x, y, z) = (x + y) \cdot z$$



Neural Network as Computational Graph



$$z_k^{(2)} = \sum_i x_i w_{ik}^{(2)} + b_i^{(2)}$$

$$a_k^{(2)} = f(z_k^{(2)})$$

$$z_k^{(3)} = \sum_i a_i^{(2)} w_{ik}^{(3)} + b_i^{(3)}$$

...

4 Neural Network

4.1 Activation Functions

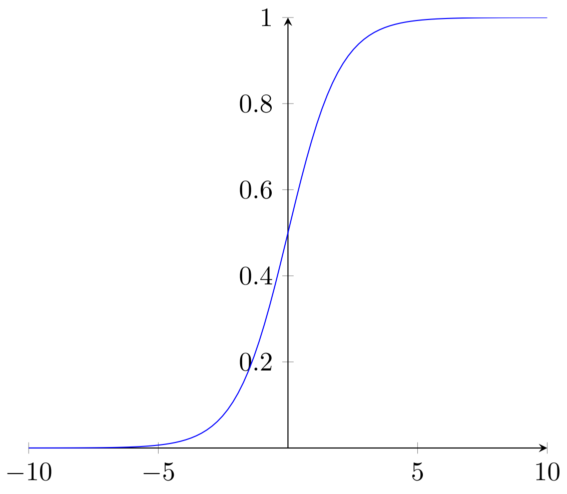
Parameters:

$\hat{y}$:	Prediction
$\hat{y}_j$:	Prediction of j-th output (j-th Neuron of output layer)
h:	Outputs of hidden layer
s:	Output of layer (before activation)
s_j:	Output of the j-th neuron in layer (before activation)
C:	Number of classes (number of neurons in output layer)

4.1.1 Sigmoid

- Used for Binary Classification to output a probability matching first or second class
- Output: $\hat{y} = (0, 1)$
- If used as activation function in hidden layer (typically it is not)
  - – Output is always positive
  - – Saturates for high positive or low negative values $\rightarrow$ kills the gradient flow

$$\sigma(s) = \frac{1}{1 + e^{-s}}$$



4.1.2 Softmax

- Used for Multiclass Classification to output a probability matching the i-th class
- Output: $\hat{y}_j = (0, 1)$

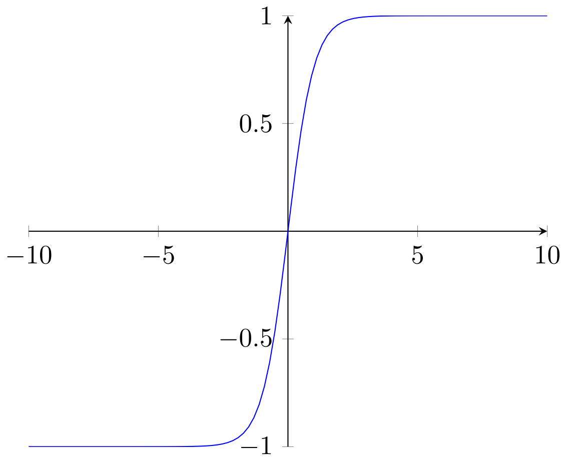
$$\hat{y}_j = \frac{e^{s_j}}{\sum_{k=1}^{C} e^{s_k}}$$

4.1.3 Tanh (Hyperbolic Tanjant Function)

+ Zero-centered

– Saturates for high positive or low negative values $\rightarrow$ kills the gradient flow

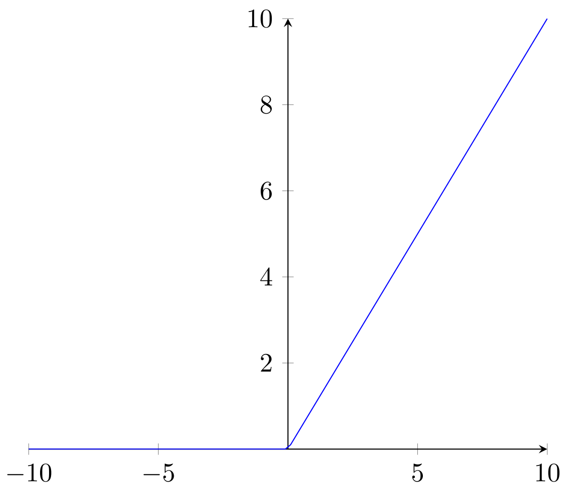
$$h = \tanh(s)$$



4.1.4 ReLU (Rectified Linear Units)

- ○ Standard choice for activation function
- + Does not saturate
- + Large and consistent gradients
- + Fast convergence
- − Dead ReLU if output is zero
- ○ Initialization of ReLU neurons with slightly positive biases (e.g. 0.01) $\to$ Likely to stay active for most inputs

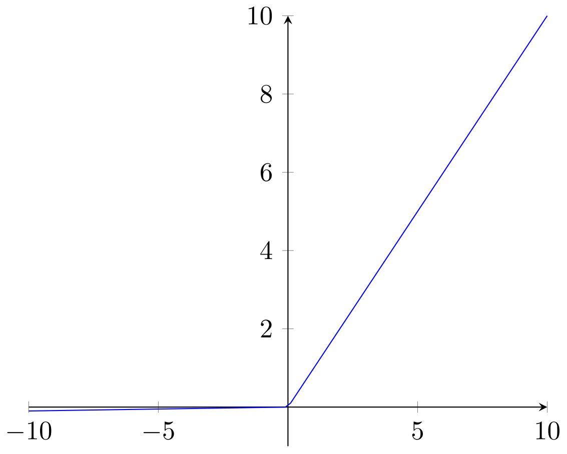
$$h = \max(0, s)$$



4.1.5 Leaky ReLU

- + Does not die

$$h = \max(0.01s, s)$$



4.1.6 Parametric ReLU

- ∘ α is a learnable parameter
- + Does not die

$$h = \max(\alpha s, s)$$

4.1.7 ELU

$$f(s) = \begin{cases} s & \text{if } s > 0 \\ \alpha(e^s - 1) & \text{if } s \leq 0 \end{cases}$$

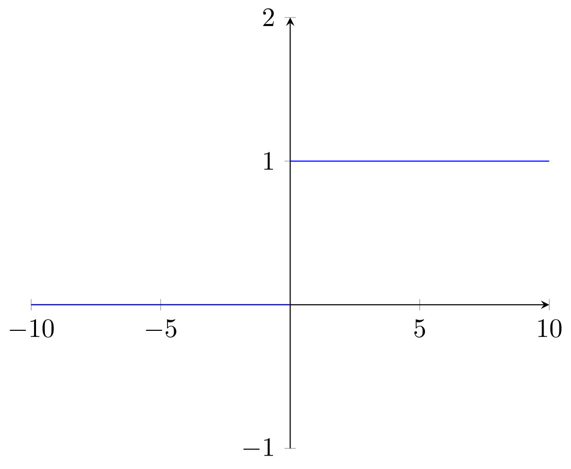
4.1.8 Maxout

- + Generalization of ReLUs
- + Linear regimes
- + Does not die
- + Does not saturate
- − Increases the number of parameters

$$h = \max(w_1^T s + b_1, w_2^T s + b_2)$$

4.1.9 Step Function

$$h = \begin{cases} 0 & \text{if } s < 0 \\ 1 & \text{if } s \geq 0 \end{cases}$$



4.2 Loss Function

4.2.1 Description

- A function to measure the goodness of the predictions
- Goal: Minimize the loss $\iff$ Find better predictions
- ○ Large loss $\implies$ bad predictions
- ○ Choice of the loss function depends on the concrete problem or the distribution of the target variable

4.2.2 Parameters

y_i:	Ground truth of i-th sample
$\hat{y}_i$:	Prediction of i-th sample
n:	number of training samples
k:	number of classes
$\hat{y}_{i,gt}$:	Prediction of ground truth class of i-th sample (where $y_{ij} = 1$)

4.2.3 L1 Loss

- Sum of absolute differences
- ○ Optimum is the median
- ○ Robust (cost of outliers is linear)
- − Costly to optimize

$$\mathcal{L}(y, \hat{y}; \theta) = \frac{1}{n} \sum_i^n ||y_i - \hat{y}_i||_1$$

4.2.4 L2/MSE Loss

- Sum of squared differences
- ○ Optimum is the mean
- ○ Prone to outliers
- + Compute-efficient optimization

$$\mathcal{L}(y, \hat{y}; \theta) = \frac{1}{n} \sum_i^n ||y_i - \hat{y}_i||_2^2$$

4.2.5 Binary Cross Entropy

$$\mathcal{L}(y, \hat{y}; \theta) = -\frac{1}{n} \sum_{i=1}^{n} (y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i))$$

4.2.6 Cross Entropy

- ○ Loss is typically always $> 0 \rightarrow$ Always improvement

$$\mathcal{L}(y, \hat{y}; \theta) = -\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} (y_{ij} \log \hat{y}_{ij})$$

4.2.7 Hinge Loss (SVM Loss)

- ○ Loss can become $= 0 \rightarrow$ Saturation

$$\mathcal{L}(y, \hat{y}; \theta) = \frac{1}{n} \sum_{i=1}^{n} \sum_{\substack{j=1, \\ j \neq gt}}^{k} \max(0, \hat{y}_{ij} - \hat{y}_{i,gt} + 1)$$

4.3 Optimization Functions

Changes the model in order to improve the loss function/estimation

4.3.1 General Optimization

- **Goal:** $\theta^* = \arg\min f(\theta, x, y)$
- **Linear Systems (Ax = b)**
  - LU, QU, Cholesky, Jacobi, Gauss-Seidel, CG, PCG, ...
- **Non-linear systems** (Gradient based methods):
  - First order methods:
    - ∗ Gradient Descent, SGD, SGD with Momemtum, RMSProp, Adam (Standard)
  - Second order methods (faster than first order methods, but only for full batch updates):
    - ∗ Newton, Gauss-Newton, Levenberg-Marquardt, (L)BFGS

4.3.2 Gradient Descent

- Finds local minimum
- Does gradient steps in direction of negative gradient
- ○ Does not guarantee to find global optimum
- – Requires a lot of memory $\implies$ extremely expensive

Parameters:

$f(\theta, x_{1..n}, y_{1..n})$:	Function describing the neural network (including loss function)
$x_{1..n}$:	Input vectors for all n training samples
$y_{1..n}$:	Ground truth for all n training samples
$\theta^k = \{W, b\}$:	Model Parameters at step k
α:	Learning rate

Gradient Step:

$$\theta^{k+1} = \theta^k - \alpha \nabla_\theta f(\theta^k, x_{1..n}, y_{1..n})$$

4.3.3 Stochastic Gradient Descent

- Split training set into several minibatches
- Minibatch size:
  - Is a hyperparameter
  - Is typically a power of 2
  - Smaller batch size $\implies$ Greater variance in the gradients
  - Is mostly limited by GPU memory
- ◦ Epoch: Complete pass through training set
- – Cannot independently scale directions
- – Need to have conservative min learning rate to avoid divergence
- – Is slower than necessary

Parameters:

n:	Number of total training samples
m:	Minibatch size (number of training samples per minibatch)
n/m:	Number of minibatches
$f(\theta, x_{1..m}, y_{1..m})$:	Function describing the neural network (including loss function)
$x_{1..m}$:	Input vectors for one minibatch
$y_{1..m}$:	Ground truth for one minibatch
$\theta^k = \{W, b\}$:	Model Parameters at iteration k
k:	Iteration in current epoch
α:	Learning rate

Gradient Step:

$$\theta^{k+1} = \theta^k - \alpha \nabla_\theta f(\theta^k, x_{1..m}, y_{1..m})$$

4.3.3.1 Convergence of Stochastic Gradient Descent

$f(\theta, x, y)$ converges to a local (global) minimum if:

1. $\alpha_n \geq 0, \forall n \geq 0$
2. $\sum_{n=1}^{\infty} \alpha_n = \infty$
3. $\sum_{n=1}^{\infty} \alpha_n^2 < \infty$
4. $f(\theta, x, y)$ ist strictly convex

where $\alpha_1, \ldots, \alpha_n$ is a sequence of positive step-sizes

4.3.4 Gradient Descent with Momentum

- Step will be largest when a sequence of gradients all point to the same direction

Parameters:

$f(\theta, x, y)$:	Function describing the neural network (including loss function)
x:	Input vectors
y:	Ground truth
$\theta^k = \{W, b\}$:	Model Parameters at step k
α:	Learning rate
β:	Accumulation rate (friction, momentum), default: 0.9
v^k:	Velocity at step k

Gradient step:

$$v^{k+1} = \beta \cdot v^k - \alpha \cdot \nabla_\theta f(\theta^k, x, y)$$
$$\theta^{k+1} = \theta^k + v^{k+1}$$

4.3.5 Nesterov Momentum

- Look-ahead momentum
- Steps:
  1. Make a big jump in the direction of the previous accumulated gradient
  2. Measure the gradient where you end up
  3. Make a correction

Parameters:

$f(\theta, x, y)$:	Function describing the neural network (including loss function)
x:	Input vectors
y:	Ground truth
$\theta^k = \{W, b\}$:	Model Parameters at step k
α:	Learning rate
β:	Accumulation rate (friction, momentum), default: 0.9
v^k:	Velocity at step k

Gradient step:

$$\tilde{\theta}^{k+1} = \theta^k + \beta \cdot v^k$$
$$v^{k+1} = \beta \cdot v^k - \alpha \cdot \nabla_\theta f(\tilde{\theta}^{k+1}, x, y)$$
$$\theta^{k+1} = \theta^k + v^{k+1}$$

4.3.6 Root Mean Squared Prop (RMSProp)

- Divides the learning rate by an exponentially-decaying average of squared gradients
- Damps the oscillations for high-variance directions

+ Can increase learning rate because it is less likely to diverge → Speeds up learning speed

Parameters:

$f(\theta, x, y)$:	Function describing the neural network (including loss function)
x:	Input vectors
y:	Ground truth
$\theta^k = \{W, b\}$:	Model Parameters at step k
α:	Learning rate
β:	Accumulation rate (friction, momentum), default: 0.9
ϵ:	Prevents division by zero, default: 10^{-8}
s^k:	Second momentum (uncentered variance of gradients)

Gradient step:

$$s^{k+1} = \beta \cdot s^k + (1 - \beta)(\nabla_\theta f(\theta^k, x, y) \circ \nabla_\theta f(\theta^k, x, y))$$
$$\theta^{k+1} = \theta^k - \alpha \cdot \frac{\nabla_\theta f(\theta^k, x, y)}{\sqrt{s^{k+1}} + \epsilon}$$

where $a \circ b$ is an element-wise multiplication

4.3.7 Adaptive Momemt Estimation (Adam)

- Combines Momentum and RMSProp
- Combines first and second order momentum

Parameters:

$f(\theta, x, y)$:	Function describing the neural network (including loss function)
x:	Input vectors
y:	Ground truth
$\theta^k = \{W, b\}$:	Model Parameters at step k
α:	Learning rate
β_1:	Accumulation rate 1, default: 0.9
β_2:	Accumulation rate 2, default: 0.999
ϵ:	Prevents division by zero, default: 10^{-8}
s^k:	Second momentum (uncentered variance of gradients)

Gradient step:

$$\hat{m}^{k+1} = \frac{\beta_1 \cdot m^k + (1-\beta_1) \cdot \nabla_\theta f(\theta^k, x, y)}{1-\beta_1^{k+1}}$$
$$\hat{v}^{k+1} = \frac{\beta_2 \cdot v^k + (1-\beta_2)(\nabla_\theta f(\theta^k, x, y) \circ \nabla_\theta f(\theta^k, x, y))}{1-\beta_2^{k+1}}$$
$$\theta^{k+1} = \theta^k - \alpha \cdot \frac{\hat{m}^{k+1}}{\sqrt{\hat{v}^{k+1}} + \epsilon}$$

where $m^0 = v^0 = 0$

4.3.8 Newton's Method

- Computation complexity of inversion per iteration: $\mathcal{O}(k^3)$

Parameters:

$f(\theta)$:	Function describing the neural network (including loss function)
$\theta = \{W, b\}$:	Model Parameters
$\nabla_\theta f(\theta)$:	Gradient (first derivative)
$H(\theta)$:	Hessian matrix (second derivative)

Approximate the function by a second-order Taylor series expansion

$$f(\theta) \approx f(\theta_0) + (\theta-\theta_0)^T \nabla_\theta f(\theta_0) + \frac{1}{2}(\theta-\theta_0)^T H(\theta-\theta_0)$$

Update step:

$$\theta^* = \theta_0 - H^{-1}\nabla_\theta f(\theta)$$

4.3.9 Broyden-Fletcher-Goldfarb-Shanno algorithm (BFGS and L-BFGS)

- Belongs to the family of quasi-Newton methods
- Have an approximation of the inverse of the Hessian
- Computation complexity of inversion per iteration:
  - BFGS: $\mathcal{O}(n^2)$
  - L-BFGS: $\mathcal{O}(n)$

Update step:

$$\theta^* = \theta_0 - H^{-1}\nabla_\theta f(\theta)$$

4.3.10 Gauss-Newton

- Approximates 2nd derivatives since there are often hard to obtain

Parameters:

$\theta = \{W, b\}$:	Model Parameters
$\nabla_\theta f(\theta)$:	Gradient (first derivative)
$\mathcal{J}(\theta)$:	Jacobian matrix

$$H(\theta) \approx 2\mathcal{J}^T(\theta)\mathcal{J}(\theta)$$

Linear equation:

$$2(\mathcal{J}^T(\theta_k)\mathcal{J}(\theta_k)) \cdot (\theta_k - \theta_{k+1}) = \nabla_\theta f(\theta)$$

4.3.11 Levenberg

- Damped version of Gauss-Newton
- Damping factor is adjusted in each iteration, so that: $f(\theta_k) > f(\theta_{k+1})$

Parameters:

$\theta = \{W, b\}$:	Model Parameters
$\nabla_\theta f(\theta)$:	Gradient (first derivative)
$\mathcal{J}(\theta)$:	Jacobian matrix
λ:	Damping factor

Linear equation:

$$(\mathcal{J}^T(\theta_k)\mathcal{J}(\theta_k) + \lambda I) \cdot (\theta_k - \theta_{k+1}) = \nabla_\theta f(\theta)$$

4.3.12 Levenberg-Marquardt

- Scales each component of the gradient according to the curvature

+ Avoids slow convergence in components with a small gradient

Parameters:

$\theta = \{W, b\}$:	Model Parameters
$\nabla_\theta f(\theta)$:	Gradient (first derivative)
$\mathcal{J}(\theta)$:	Jacobian matrix
λ:	Damping factor

Linear equation:

$$(\mathcal{J}^T(\theta_k)\mathcal{J}(\theta_k) + \lambda \cdot \mathrm{diag}(\mathcal{J}^T(\theta_k)\mathcal{J}(\theta_k))) \cdot (\theta_k - \theta_{k+1}) = \nabla_\theta f(\theta)$$

4.4 Learning rate

- Goal: High learning rate in the beginning, then low learning rate

4.4.1 Learning Rate Decay

α_0:	Initial learning rate (e.g. 0.1)
t:	Factor by which the learning rate is decayed
$epoch$:	Epoch of current run

Learning rate decays:

$$\alpha = \frac{1}{1 + t \cdot epoch} \cdot \alpha_0, \qquad \text{default: } t = 0.1$$

Step decay:

$$\alpha = \alpha - t \cdot \alpha, \qquad \text{default: } t = 0.5$$

Exponential decay:

$$\alpha = t^{epoch} \cdot \alpha_0, \qquad t < 1.0$$

$$\alpha = \frac{t}{\sqrt{epoch}} \cdot \alpha_0$$

4.4.2 Training Schedule

- Manually set learning rate every n epochs

4.5 Regularization Techniques

- Increasing training error
- Lower validation error

4.5.1 L1/L2 Regularization

L:	Loss
$\mathcal{L}(y, \hat{y}, \theta)$:	Loss function (without generalization)
λ:	Regularization rate
$\theta = \{W, b\}$:	Model parameters

Add regularization term to loss function:

$$L = \mathcal{L}(y, \hat{y}, \theta) + \lambda R(\theta)$$

L1 Regularization
Enforces sparsity

$$R(\theta) = \sum_{i=1}^{n} |\theta_i|$$

L2 Regularization
Enforces that the weights have similar values

$$R(\theta) = \sum_{i=1}^{n} \theta_i^2$$

4.5.2 Weight Decay

- ○ Penalizes large weights
- ○ Improves generalization

Parameters:

$f(\theta, x_{1..n}, y_{1..n})$:	Function describing the neural network (including loss function)
$x_{1..n}$:	Input vectors for all n training samples
$y_{1..n}$:	Ground truth for all n training samples
$\theta^k = \{W, b\}$:	Model Parameters at step k
α:	Learning rate
λ:	Regularization rate
$R(\theta^k)$:	L2 Regularization

Add regularization term to Gradient step:

$$\theta^{k+1} = \theta^k - \alpha \nabla_\theta f(\theta^k, x_{1..n}, y_{1..n}) - \lambda R(\theta^k)$$

4.5.3 Early Stopping

Stop training as soon as the model begins overfitting

4.5.4 Bagging and Ensemble Methods

- Train multiple models and average their results
- Use different optimization functions, loss functions, ... for each model
- + If errors are uncorrelated, the expected combined error will decrease linearly with the ensemble size

4.5.5 Dropout

- Disable a random set of neurons with probability p (default: $p = 50\%$)
- ○ Intuition: Use half of the network:
  - → Redundant representations
  - → Base your scores on more features
  - → Reducing co-adaptations between neurons
- Testing:
  - – Disable dropout (all neurons are turned on)
  - – Multiply with dropout probability: $s_j' = s_j \cdot p$
- – Reduces the effective capacity of a model → More training time

4.5.6 Batch Normalization (BN)

- Goal: Activations do not die out
- Normalizes the mean and the variance of the inputs to the activation functions
- Is applied after Fully Connected (or Convolutional) Layers and before non-linear activation functions
- + Very deep nets are much easier to train → more stable gradients
- ○ Can be undone by the network with: $\gamma^{(k)} = \sqrt{Var[s^{(k)}]}, \beta^{(k)} = \mathbb{E}[s^{(k)}]$
- ○ All biases of the layers before BN can be set to zero, since they will be canceled out by BN anyway
- Testing:
  - – Compute mean μ_{test} and variance σ^2_{test} by running an exponentially weighted averaged across training minibatches:
    $Var_{running} = \beta_m \cdot Var_{running} + (1 - \beta_m) \cdot Var_{minibatch}$
    $\mu_{running} = \beta_m \cdot \mu_{running} + (1 - \beta_m) \cdot \mu_{minibatch}$

Parameters:

s^k:	Output of the Fully Connected or Convolutional Layer before the Batch Normalization Layer
$\mathbb{E}[s^k]$:	Mean of the mini-batch examples over feature k
$Var[s^k]$:	Variance of the mini-batch examples over feature k
$\gamma^{(k)}, \beta^{(k)}$:	Parameters optimized during Backpropagation

1. Normalize:

$$\hat{s}^{(k)} = \frac{s^{(k)} - \mathbb{E}[s^{(k)}]}{\sqrt{Var[s^{(k)}]}}$$

2. Allow the network to change the range:

$$s'^{(k)} = \gamma^{(k)}\hat{s}^{(k)} + \beta^{(k)}$$

4.5.7 Other Normalizations

- Layer Norm
- Instance Norm
- Group Norm

4.5.8 Data Augmentation

- Classifier has to be invariant to a wide variety of transformations $\rightarrow$ Synthesize data simulating plausible transformations
- ○ Training: Random Crops, Testing: Fixed Set of Crops
- ○ Use same data augmentation when comparing two networks
- ○ Consider data augmentation a part of your network design
- Augmentations:
  - Flip
  - Crop
  - Brightness and contrast changes
  - ...

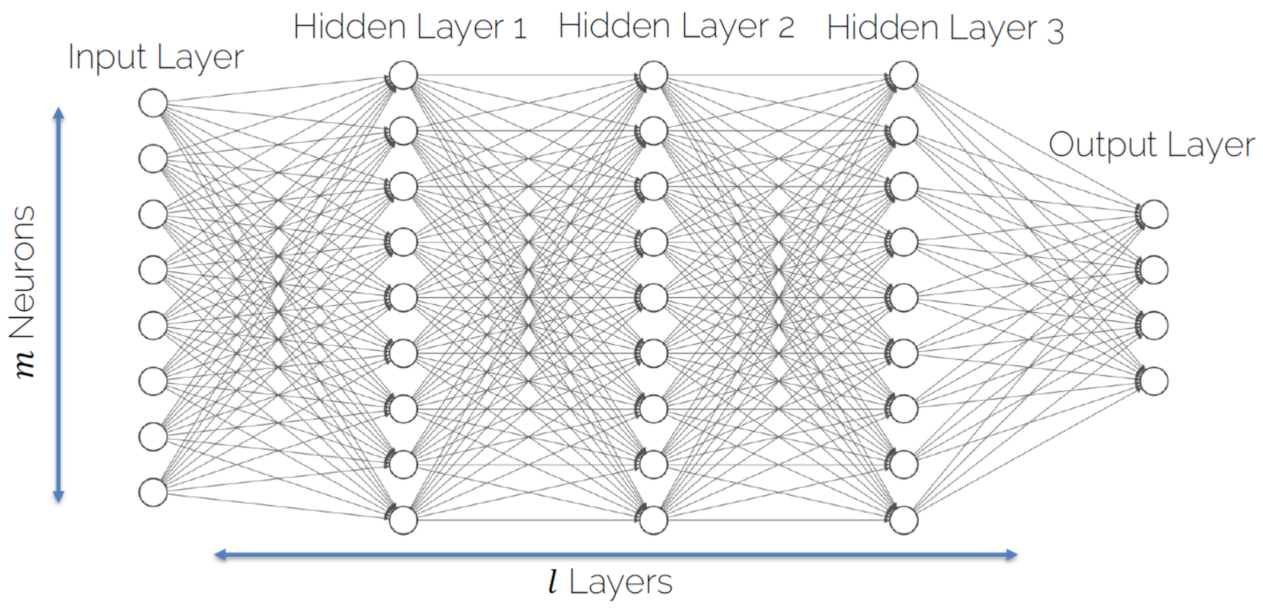
5 Fully Connected Neural Network

5.1 Structure

Parameters:

x_k:	Input variables
$\theta = \{W, b\}$:	Model parameters
$w_{i,j,k}$:	Network weights
$b_{i,j}$:	Network biases
	i: Index of layer
	j: Index of neuron in layer (neuron of next layer)
	k: Index of weight in neuron (neuron of previous layer)
l:	Depth: number of layers (All hidden and the output layer - no input layer)
m_j:	Width: number of neurons in layer i (Can be different for each layer)
$\hat{y}_i$:	Computed output/Prediction
y_i:	Ground truth targets
$\mathcal{L}(y, \hat{y}, \theta)$:	Loss function
$a(s)$:	Activation function

Graphical Representation



Mathematical Representation

$$L = \mathcal{L}(y_j, \hat{y}_j, \theta)$$

$$\hat{y}_j = a(s_{l,j})$$

$$h_{i,j} = a(s_{i,j})$$

$$s_{i,j} = b_{i,j} + \sum_{k=1}^{m_{i-1}} h_{i-1,k} \cdot w_{i,j,k}$$

$$s_{1,j} = b_{1,j} + \sum_{k=1}^{m_{i-1}} x_k \cdot w_{1,j,k}$$

5.2 Number of weights

l:	Depth: number of layers
m_i:	Width: number of neurons in layer i (Here: layer 0 is the input layer)
a	Number of parameters of the activation functions

Number of weights is defined as:

$$a + \sum_{i=1}^{l} m_i \cdot m_{i-1} + m_i$$

5.3 Forward and Backward Pass

5.3.1 Forward Pass/ Forward Propagation

Use formulas to calculate loss:

$$s_{1,1} = b_{1,1} + \sum_{k=1}^{m_0} x_k \cdot w_{1,1,k} \qquad \dots \qquad L = \mathcal{L}(y_j, \hat{y}_j, \theta)$$

5.4 Backward Pass/Backward Propagation

Weights of last layer:

$$\frac{\partial L}{\partial w_{l,j,k}} = \frac{\partial L}{\partial \hat{y}_j} \cdot \frac{\partial \hat{y}_j}{\partial s_{l,j}} \cdot \frac{\partial s_{l,j}}{\partial w_{l,j,k}}$$

Weights of second last layer:

$$\frac{\partial L}{\partial w_{l-1,j,k}} = \sum_{o=1}^{m_l} \frac{\partial L}{\partial \hat{y}_o} \cdot \frac{\partial \hat{y}_o}{\partial s_{l,o}} \cdot \frac{\partial s_{l,o}}{\partial h_{l-1,j}} \cdot \frac{\partial h_{l-1,j}}{\partial s_{l-1,j}} \cdot \frac{\partial s_{l-1,j}}{\partial w_{l-1,j,k}}$$

General:

$$\frac{\partial L}{\partial w_{i,j,k}} = \sum_{o_1=1}^{m_{i+1}} \cdots \sum_{o_{l-i}=1}^{m_l} \frac{\partial L}{\partial \hat{y}_{o_1}} \cdot \frac{\partial \hat{y}_{o_1}}{\partial s_{l,o_1}} \quad \cdot \quad \frac{\partial s_{l,o_1}}{\partial h_{l-1,o_2}} \cdot \frac{\partial h_{l-1,o_2}}{\partial s_{l-1,o_2}} \cdot \ldots \cdot \frac{\partial s_{i+1,o_{l-i}}}{\partial h_{i,j}} \cdot \frac{\partial h_{i,j}}{\partial s_{i,j}} \cdot \frac{\partial s_{i,j}}{\partial w_{i,j,k}}$$

6 Convolutional Neural Network

6.1 Advantages over FCNNs

Using deep networks:

- Fully Connected Neural Networks:
  - – No structure
  - – Just brute force
  - – Optimization becomes hard
  - – Performance plateaus/drops
- Convolutional Neural Network
  - + Layers with structure
  - + Weight sharing (using the same weights for different parts of the image)

6.2 2D - Convolution

6.2.1 General

- Stride = 1
- Padding = 0

6.2.1.1 Mathematical representation

Parameters:

$x_{i,j,k}$:	Value of the pixel of the input image at position i, j, k
$w_{i,j,k}$:	Value of the pixel of the kernel at position i, j, k
$z_{i,j,k}$:	Value of the pixel of the output image (feature map) at position i, j, k
	i: Index of channel
	j: Index of height
	k: Index of width
C:	Depth of the input image (number of channels)
H_i:	Height of the input image (number of pixels (vertical))
W_i:	Width of the input image (number of pixels (horizontal))
H_K:	Height of the kernel
W_K:	Width of the kernel
H_o:	Height of the output image
W_o:	Width of the output image
$b_{j,k}$:	Bias at position j, k

Input image:
Image with the pixels: $x_{1,1,1}$ to x_{C,H_i,W_i}

Kernel:
Filter image with the pixels: $w_{1,1,1}$ to w_{C,H_K,W_K}

Output image:
Image with the pixels: $z_{1,1,1}$ to z_{1,H_o,W_o} where:

$$z_{1,j,k} = b_{j,k} + \sum_{l=1}^{C} \sum_{m=j}^{H_K+j-1} \sum_{n=k}^{W_K+k-1} w_{l,m-j+1,n-k+1} \cdot x_{l,m,n}$$

6.2.1.2 Graphical representation

Image:

Channel 1:

$x_{1,1,1}$	$x_{1,1,2}$	$\dots$	$x_{1,1,W}$
$x_{1,2,1}$	$x_{1,2,2}$	$\dots$	$x_{1,2,W}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$
$x_{1,H,1}$	$x_{1,H,2}$	$\dots$	$x_{1,H,W}$

$\dots$

Channel C:

$x_{C,1,1}$	$x_{C,1,2}$	$\dots$	$x_{C,1,W}$
$x_{C,2,1}$	$x_{C,2,2}$	$\dots$	$x_{C,2,W}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$
$x_{C,H,1}$	$x_{C,H,2}$	$\dots$	$x_{C,H,W}$

Kernel:

Channel 1:

$w_{1,1,1}$	$\dots$	$w_{1,1,W_K}$
$\vdots$	$\ddots$	$\vdots$
$w_{1,H_K,1}$	$\dots$	w_{1,H_K,W_K}

$\dots$

Channel C:

$w_{C,1,1}$	$\dots$	$w_{C,1,W_K}$
$\vdots$	$\ddots$	$\vdots$
$w_{C,H_K,1}$	$\dots$	w_{C,H_K,W_K}

Output image:

Channel 1:

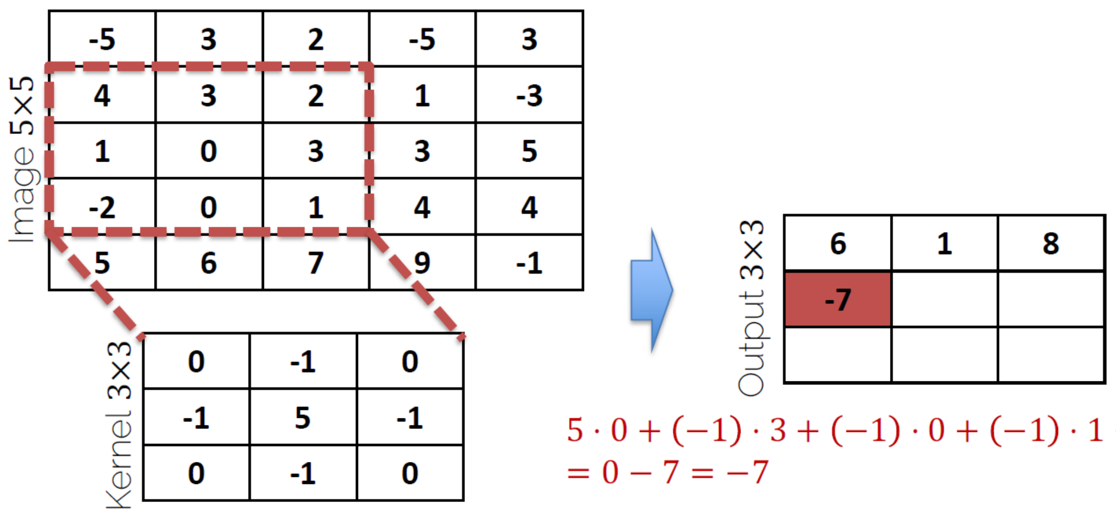
$z_{1,1,1}$	$\dots$	$z_{1,1,W_K}$
$\vdots$	$\ddots$	$\vdots$
$z_{1,H_K,1}$	$\dots$	z_{1,H_K,W_K}

$\dots$

Channel C:

$z_{C,1,1}$	$\dots$	$z_{C,1,W_K}$
$\vdots$	$\ddots$	$\vdots$
$z_{C,H_K,1}$	$\dots$	z_{C,H_K,W_K}

6.2.1.3 Graphical Example



$$5 \cdot 0 + (-1) \cdot 3 + (-1) \cdot 0 + (-1) \cdot 1 + (-1) \cdot 3$$
$$= 0 - 7 = -7$$

6.2.2 Stride

- Apply filter every S-th spatial location
- ∘ Must hold $(H_i - H_K)/S, (W_i - W_K)/S \in \mathbb{N}_0$

Parameters:

$z_{j,k}$:	Value of the pixel of the original output image (with stride 1) at position j, k
$z'_{j,k}$:	Value of the pixel of the output image with stride S at position j, k
j:	Index of height
k:	Index of width
H_i:	Height of the original image (number of pixels (vertical))
W_i:	Width of the original input image (number of pixels (horizontal))
H_o:	Height of the new output image (number of pixels (vertical))
W_o:	Width of the new output image (number of pixels (horizontal))
H_K:	Height of the kernel
W_K:	Width of the kernel
S:	Stride

Original output image:
Original Output image with the pixels: $z_{1,1}$ to z_{H_i,W_i}

New output image:
Output image with stride with the pixels: $z'_{1,1}$ to z'_{H_o,W_o} where

$$z'_{j,k} = z_{2j-1,2k-1}$$

and

$$H_o = \frac{H_i - 1}{S} + 1, \qquad W_o = \frac{W_i - 1}{S} + 1$$

6.2.3 Padding

- Surround original input image with pixels with value 0
  - Allows the output image to have the same number of pixels as the input image

6.2.3.1 Mathematical representation

Parameters:

$x_{i,j,k}$:	Value of the pixel of the original input image (with padding 0) at position i, j, k
$x'_{i,j,k}$:	Value of the pixel of the input image with Padding P at position i, j, k
i:	Index of channel
j:	Index of height
k:	Index of width
C_i:	Depth of the input image (number of channels)
H_i:	Height of the original image (number of pixels (vertical))
W_i:	Width of the original input image (number of pixels (horizontal))
H_o:	Height of the new input image (number of pixels (vertical))
W_o:	Width of the new input image (number of pixels (horizontal))
P:	Padding

Original input image:
Original input image with the pixels: $x_{1,1,1}$ to z_{C,H_i,W_i}

New input image:
Input image with padding with the pixels: $x'_{1,1,1}$ to z'_{C,H_o,W_o} where

$$x'_{i,j,k} = \begin{cases} x_{i,j-P,k-P} & \text{for } P < j \leq j + P, P < k \leq k + P \\ 0 & \text{sonst} \end{cases}$$

and

$$H_o = H_i + 2 \cdot P, \qquad W_o = W_i + 2 \cdot P$$

6.2.3.2 Graphical representation for P = 1

Original input image:

Channel 1:

$x_{1,1,1}$	$\dots$	$x_{1,1,W_K}$
$\vdots$	$\ddots$	$\vdots$
$x_{1,H_K,1}$	$\dots$	x_{1,H_K,W_K}

$\dots$

Channel C:

$x_{C,1,1}$	$\dots$	$x_{C,1,W_i}$
$\vdots$	$\ddots$	$\vdots$
$x_{C,H_i,1}$	$\dots$	x_{C,H_i,W_i}

New input image:

Channel 1:

0	0	$\dots$	0	0
0	$x_{1,1,1}$	$\dots$	$x_{1,1,W_i}$	0
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
0	$x_{1,H_i,1}$	$\dots$	x_{1,H_i,W_i}	0
0	0	$\dots$	0	0

$\dots$

Channel C:

0	0	$\dots$	0	0
0	$x_{C,1,1}$	$\dots$	$x_{C,1,W_K}$	0
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
0	$x_{C,H_K,1}$	$\dots$	x_{C,H_K,W_K}	0
0	0	$\dots$	0	0

6.3 Convolution Layer

- Contains several filters of size $C_i * H_K * W_K$
- Output image is the concatenations of the images generated by a 2D-Convolution with each filter

◦ Each filter captures a different image characteristics

◦ Numer of output channels is equal to the number of filters

◦ Filter values are learnable by the network

◦ Feature Extraction: Computes a feature in a given region

6.3.1 Mathematical representation

Parameters:

$x_{i,j,k}$:	Value of the pixel of the input image at position i, j, k	
$w_{i,o,j,k}$:	Value of the pixel of the kernel at position i, o, j, k	
$z_{i,j,k}$:	Value of the pixel of the output image at position i, j, k	
	i:	Index of channel
	j:	Index of height
	k:	Index of width
	o:	Index of the filters
C_i:	Depth of the input image (number of channels)	
H_i:	Height of the input image (number of pixels (vertical))	
W_i:	Width of the input image (number of pixels (horizontal))	
H_K:	Height of the kernel	
W_K:	Width of the kernel	
C_o:	Depth of the output image	
H_o:	Height of the output image	
W_o:	Width of the output image	
$b_{j,k}$:	Bias at position j, k	
S:	Stride	
P:	Padding	

Input image:
Image with the pixels: $x_{1,1,1}$ to x_{C,H_i,W_i}

Kernel:
Weight tensor with the pixels: $w_{1,1,1,1}$ to w_{C_i,C_o,H_K,W_K} where $w_{1,o,1,1}$ to w_{C_i,o,H_K,W_K} is the o-th filter image

Output image:
Image with the pixels: $z_{1,1,1}$ to z_{C_o,H_o,W_o} where:

$$z_{i,j,k} = b_{j,k} + \sum_{l=1}^{C_i} \sum_{m=j}^{H_K+j-1} \sum_{n=k}^{W_K+k-1} w_{l,i,m-j+1,n-k+1} \cdot x_{l,m,n}$$

6.3.2 Output dimension

Output dimensions:

$$H_o = \left(\left\lfloor \frac{H_i + 2 \cdot P - H_K}{S} \right\rfloor + 1 \right)$$
$$W_o = \left(\left\lfloor \frac{W_i + 2 \cdot P - W_K}{S} \right\rfloor + 1 \right)$$

Output dimension for $N = H_i = W_i$ and $F = H_K = W_K$ (default):

$$\left(\left\lfloor \frac{N + 2 \cdot P - F}{S} \right\rfloor + 1 \right) \times \left(\left\lfloor \frac{N + 2 \cdot P - F}{S} \right\rfloor + 1 \right)$$

6.3.3 Number of parameters

C_K:	Depth of the kernel (number of channels)
H_K:	Height of the kernel
W_K:	Width of the kernel
C_o:	Depth of the output image (number of filters)

$$\text{number of parameters} = (C_K \cdot H_K \cdot W_K + 1) \cdot C_o$$

6.3.4 Types of convolutions

Valid convolution:

$$P = 0$$

Same convolution:
Output size = input size:

$$P = (F - 1)/2$$

where $F = H_K = W_K$ (filter size)

6.4 Pooling Layer

- Common used to shrink size of the image
- Feature Selection: Picks the strongest activation in a region

Parameters:

$x_{i,j,k}$:	Value of the pixel of the input image at position i, j, k
$z_{i,j,k}$:	Value of the pixel of the output image at position i, j, k
	i: Index of channel
	j: Index of height
	k: Index of width
C_i:	Depth of the input image (number of channels)
H_i:	Height of the input image (number of pixels (vertical))
W_i:	Width of the input image (number of pixels (horizontal))
H_K:	Height of the kernel
W_K:	Width of the kernel
C_o:	Depth of the output image (number of channels)
H_o:	Height of the output image
W_o:	Width of the output image
S:	Stride
$F = H_K = W_K$:	Filter size (if $H_K = W_K$)

6.4.1 Output dimension:

$$C_o = C_i$$
$$H_o = \frac{H_i - H_K}{S} + 1$$
$$W_o = \frac{W_i - H_K}{S} + 1$$

6.4.2 Max Pooling

- Takes the maximum value of a region in the input image
- ○ Common settings: $F = 2, S = 2$ or $F = 3, S = 2$

Input image:
Image with the pixels: $x_{1,1,1}$ to x_{C,H_i,W_i}

Output image:
Image with the pixels: $z_{1,1,1}$ to z_{1,H_o,W_o} where:

$$z_{i,j,k} = \max(x_{i,j,k}, \ldots, x_{i,j,W_K+k-1}, \ldots, x_{i,H_K+j-1,k}, \ldots, x_{i,H_K+j-1,W_K+k-1})$$

6.4.3 Average Pooling

- Takes the average value of a region in the input image
- ○ Common settings: $F = 2, S = 2$ or $F = 3, S = 2$
- ○ Typically used deeper in the network

Input image:
Image with the pixels: $x_{1,1,1}$ to x_{C,H_i,W_i}

Output image:
Image with the pixels: $z_{1,1,1}$ to z_{1,H_o,W_o} where:

$$z_{i,j,k} = (x_{i,j,k} + \cdots + x_{i,j,W_K+k-1} + \cdots + x_{i,H_K+j-1,k} + \cdots + x_{i,H_K+j-1,W_K+k-1})/H_K \cdot W_K$$

6.5 ConvNet

- Is a concatenation of Conv Layers and activations

6.5.1 Typically network architecture

    - ∗ Convolution Layer
    - ∗ Activation Function

      ⋮
    - ∗ Convolution Layer
    - ∗ Activation Function
  - – Pool Layer

    ⋮
    - ∗ Convolution Layer
    - ∗ Activation Function

      ⋮
    - ∗ Convolution Layer
    - ∗ Activation Function
  - – Pool Layer
- 1 or 2 Fully Connected Layer

7 Training

7.1 Learning

- Learning means generalization to unknown dataset, i.e. train on known dataset, test with optimized parameters on unknown dataset

7.2 Dataset

- Split dataset into
  - Training set (e.g. 60%, 80%) - Used to train the neural network
  - Validation set (e.g. 20%, 10%) - Validate the current model to find the best hyperparameters
  - Test set (e.g. 20%, 10%) - Is only used once in the end

7.3 Obtaining the model

1. Estimating using current model
2. Calculating loss
3. Optimizing the model

7.4 Weight initialization

Bad choice:

- All weights $= 0 \rightarrow$ No symmetry breaking
- Small Random Numbers $\rightarrow$ Output becomes zero using tanh as activation function $\rightarrow$ Vanishing gradient
- Big Random Numbers $\rightarrow$ Output saturates to -1 and 1 using tanh as activation function $\rightarrow$ Vanishing gradient

7.4.1 Xavier Initialization

- Gaussian with zero mean and $Var(w) = \frac{1}{n}$ (n: number of input neurons)
- For ReLU: $Var(w) = \frac{2}{n}$

7.5 Errors

- Ground truth error
  - Faults in dataset, e.g. wrong classification of sample image
  - Underfitting
- Training set error
  - Underfitting
- Validation/test set error
  - Overfitting

7.6 Hyperparameters

- Hyperparameters = Learning Setup + Optimization, i.e.,
  - Network architecture (number of layers, number of weights, ...)
  - Number of iterations
  - Learning rate(s)
  - Regularization
  - Batch size
  - ...

7.6.1 Hyperparameter Tuning Methods

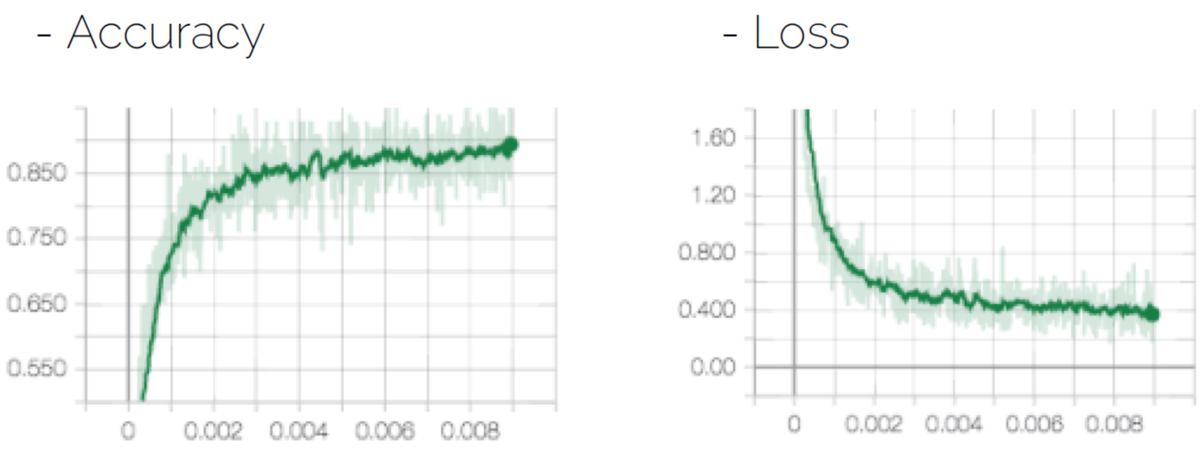
- Manual search:
  - Find out the optimal hyperparameters manually
  - Most common
- Grid search:
  - Define ranges for all parameters spaces and select points
  - Iterates over all possible configurations
- Random search:
  - Like grid search but one picks points at random in the predefined ranges

7.7 Learning Curves

7.7.1 Ideal Training

- Small gap between training and validation loss
- Training and validation loss go down at the same rate (stable without fluctuations)

Example:

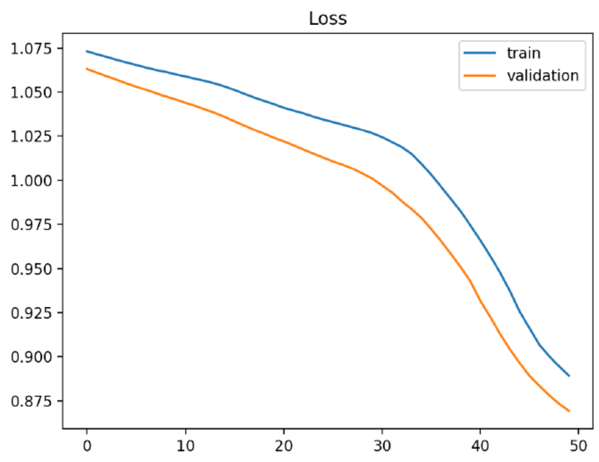


7.7.2 Underfitting

- Training and validation losses decreases even at the end of training

◦ Reasons:
  - Model is still learning

Example:



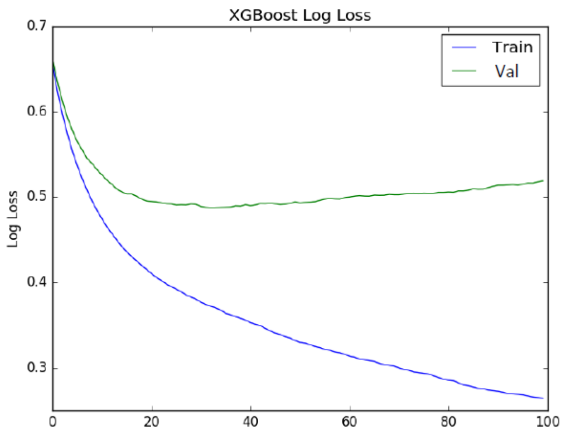
7.7.3 Overfitting

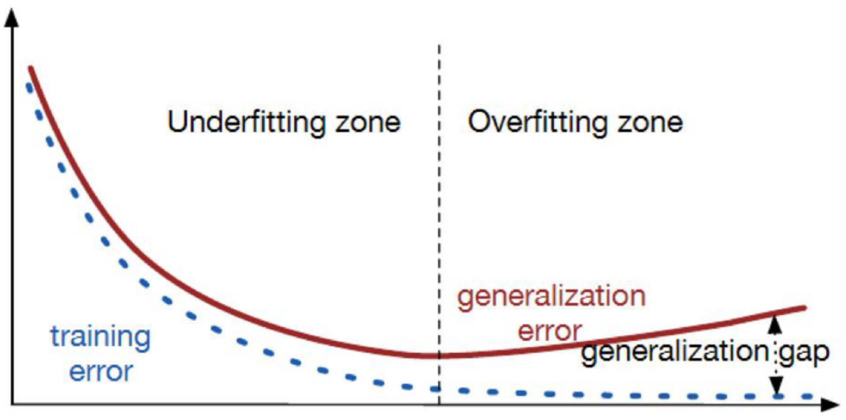
- Training loss decreases and validation loss increases

◦ Reasons:

  – Model is memorizing the training samples instead of generalizing

Example:





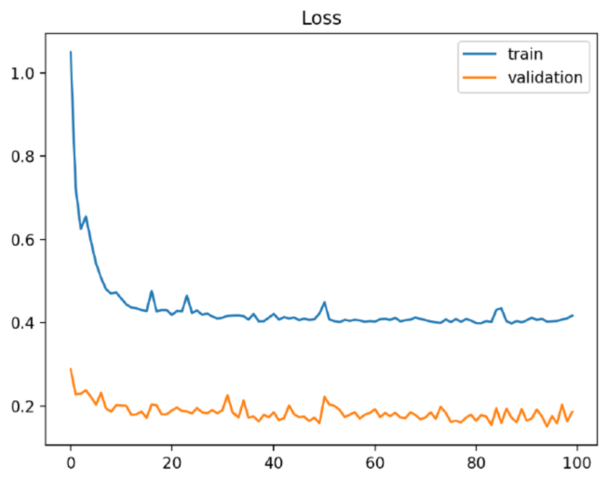
7.7.4 Other Examples

Validation set easier than training set:

- Validation loss is lower than training loss

- ◦ Reasons:
  - Validation set is easier than the training set
  - Bug in the implementation

Example:

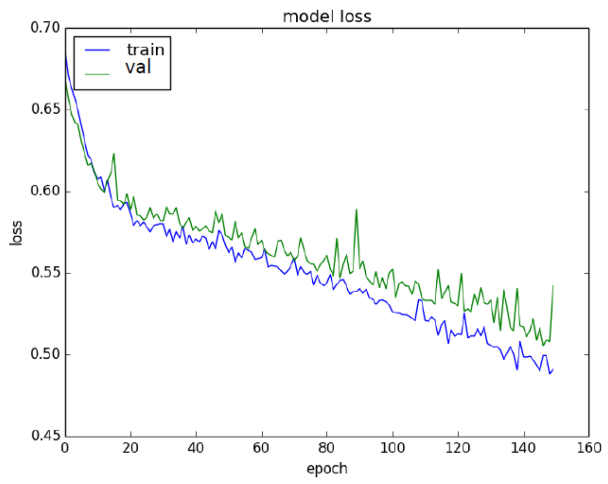


Learning rate to low:

- Loss curves decrease almost linearly

- ◦ Reasons:
  - The initial Learning rate is too low

Example:

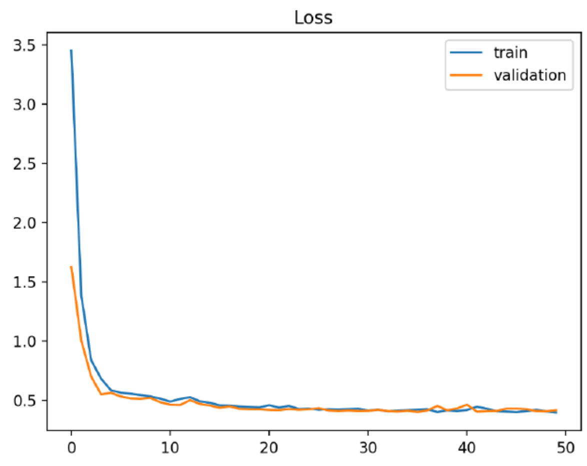


Learning rate to high:

- Loss curves decrease very quickly at the beginning and then remain on plateaus

- ◦ Reasons:
  - Learning rate is too big
  - Inconsistent dataset

Example:



7.8 How To

7.8.1 Network Architecture

- Start with the simplest network possible

7.8.2 Training samples

1. Start with a single training sample
    - Check if output is correct
    - Should overfit
    - Train accuracy should be 100%
2. Increase to handful of samples (e.g., 4)
    - Check if input is handled correctly
3. Move to more samples
    - 5, 10, 100, 1000, ...
    - At some point, you should see generalization

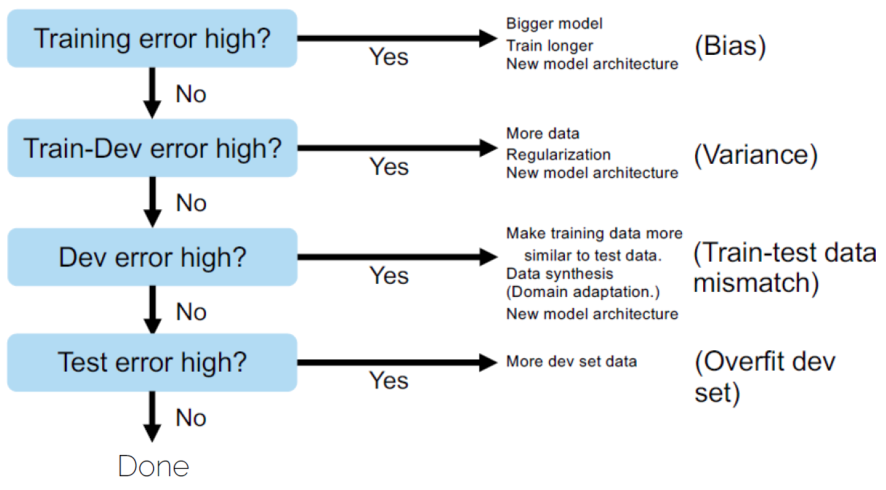
7.8.3 Learning rate

- Find a learning rate that makes the loss drop significantly within 100 iterations
- Good learning rates to try: $1e-1, 1e-2, 1e-3, 1e-4$
- Good weight decay to try: $1e-4, 1e-5, 0$
- Use Grid/Random search

7.8.4 Timings

- Measure how long each iteration takes (should be $< 500ms$)
- Look for bottlenecks (e.g. Dataloading, Backpropagation)
- Estimate total time

7.8.5 Basic Recipe



7.8.6 Bad Signs

- Training error not going down
- Validation error not going down
- Performance on validation better than on training set
- Tests on train set different than during training

7.8.7 Good/Bad Practice

Good Practice:

- Use train/validation/test curves
  - Evaluation needs to be consistent
  - Numbers need to be comparable
- Only make one change at a time

Bad Practice/Common Mistakes

- Using single batch, it did not overfit
- Forgot to toggle train/eval mode for network
- Forgot to call `.zero_grad()` (in PyTorch) before calling `.backward()`
- Passed softmaxed outputs to a loss function that expects raw logits
- Training set contains test data
- Debug algorithm on test data

Notes

This is a summary of the lecture Introduction to Deep Learning of the Technical University Munich. This lecture was presented by Nießner M. in the summer semester 2020. This summary was created by Gaida B. All provided information is without guarantee.