

Deep Learning

Using a Convolutional Neural Network

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LECTURE 4

Convolutional Neural Networks Challenges

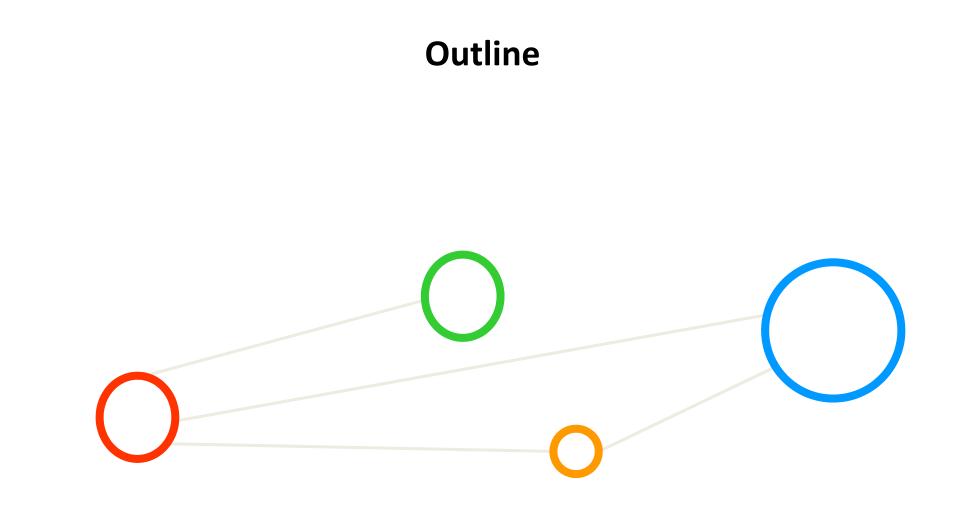
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UNIVERSITY OF ICELAND SCHOOL OF ENGINEERING AND NATURAL SCIENCES

FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE





Outline of the Course

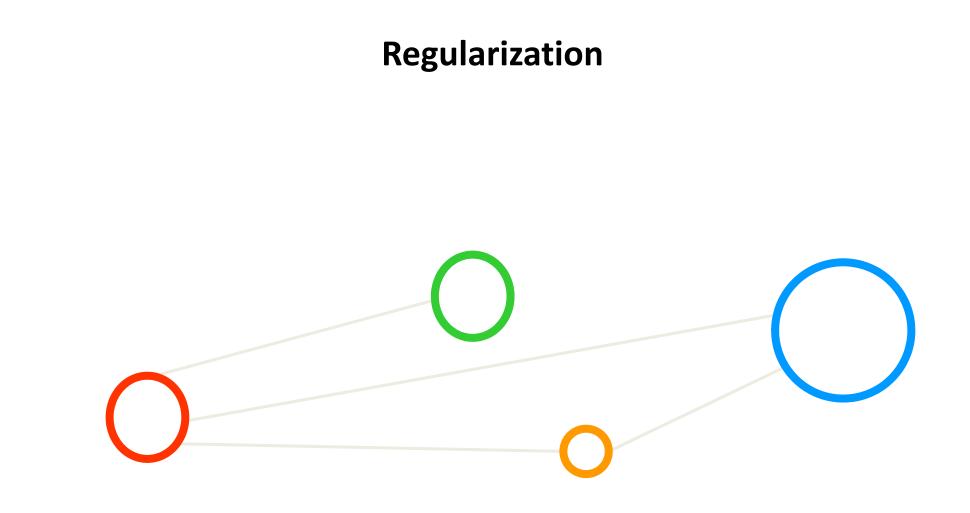
- 1. Deep Learning Fundamentals & GPGPUs
- 2. Convolutional Neural Networks & Tools
- 3. Convolutional Neural Network Applications
- 4. Convolutional Neural Network Challenges
- 5. Transfer Learning Technique
- 6. Other Deep Learning Models & Summary



Outline

- Regularization
 - Overfitting as Key Challenge
 - Fitting Noise & Noise Types
 - ANN & CNN Examples
 - Regularization Approaches
 - Weight Dropout and L2 Examples
- Validation and Model Selection
 - Many Parameters of Model Selection
 - Validation Approaches
 - ANN & CNN Examples
 - Complexity in Finding the right Parameters



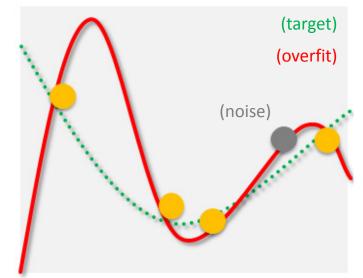


Exercises



Challenge Two – Problem of Overfitting

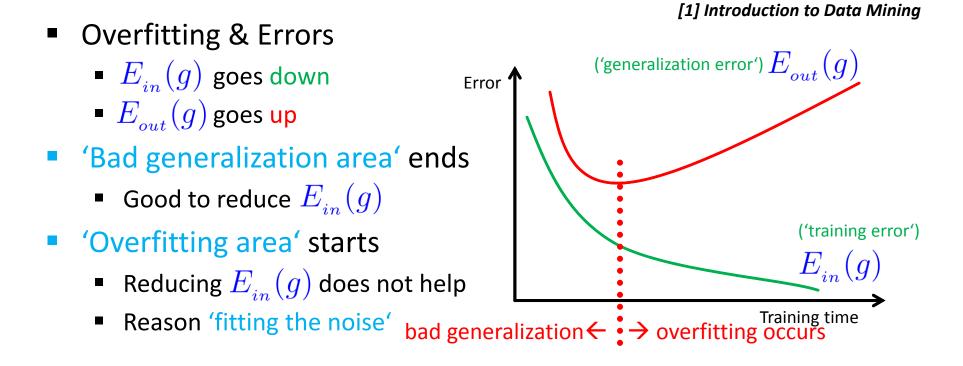
- Overfitting refers to fit the data too well more than is warranted thus may misguide the learning
- Overfitting is not just 'bad generalization' e.g. the VC dimension covers noiseless & noise targets
- Theory of Regularization are approaches against overfitting and prevent it using different methods
 - Key problem: noise in the target function leads to overfitting
 - Effect: 'noisy target function' and its noise misguides the fit in learning
 - There is always 'some noise' in the data
 - Consequence: poor target function ('distribution') approximation
 - Example: Target functions is second order polynomial (i.e. parabola)
 - Using a higher-order polynomial fit
 - Perfect fit: low $E_{\scriptscriptstyle in}(g)$, but large $E_{\scriptscriptstyle out}(g)$



(but simple polynomial works good enough) ('over': here meant as 4th order, a 3rd order would be better, 2nd best)

Problem of Overfitting – Clarifying Terms

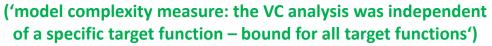
- A good model must have low training error (E_{in}) and low generalization error (E_{out})
- Model overfitting is if a model fits the data too well (E_{in}) with a poorer generalization error (E_{out}) than another model with a higher training error (E_{in})

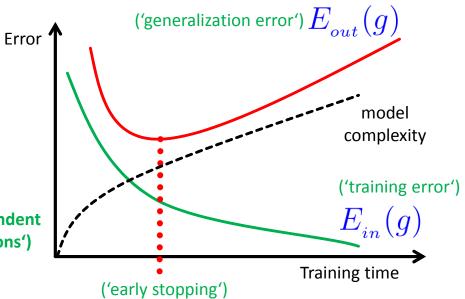


The two general approaches to prevent overfitting are (1) regularization and (2) validation

Problem of Overfitting – Model Relationships

- Review 'overfitting situations'
 - When comparing 'various models' and related to 'model complexity'
 - Different models are used, e.g. 2nd and 4th order polynomial
 - Same model is used with e.g. two different instances (e.g. two neural networks but with different parameters)
- Intuitive solution
 - Detect when it happens
 - 'Early stopping regularization term' to stop the training
 - Early stopping method (later)



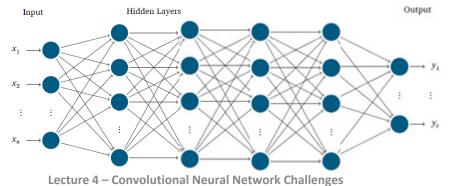


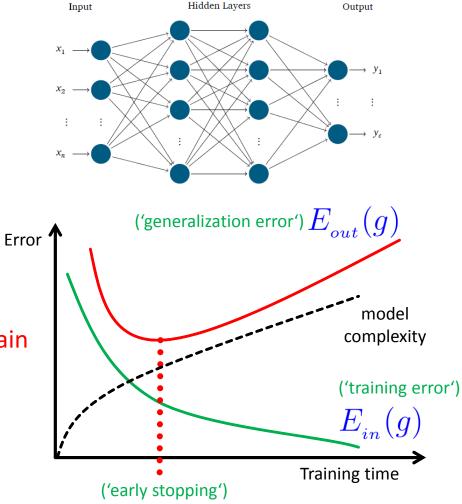
• 'Early stopping' approach is part of the theory of regularization, but based on validation methods

Problem of Overfitting – ANN Model Example

Two Hidden Layers

- Good accuracy and works well
- Model complexity seem to match the application & data
- Four Hidden Layers
 - Accuracy goes down
 - $E_{in}(g)$ goes down
 - $E_{out}(g)$ goes up
 - Significantly more weights to train
 - Higher model complexity

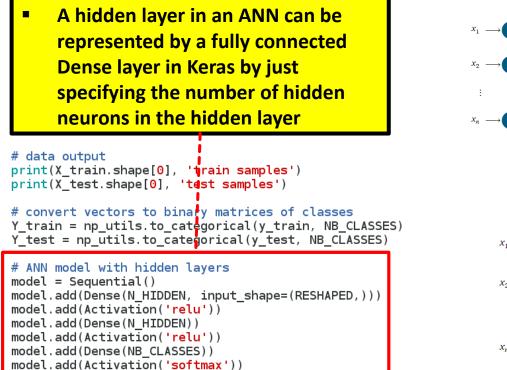


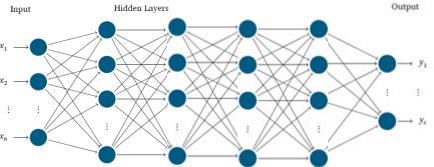


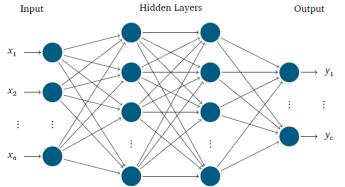
Exercises



ANN – MNIST Dataset – Add Two More Hidden Layers







model.summary()

Compilation
model.compile(loss='categorical_crossentropy', optimizer=0PTIMIZER, metrics=['accuracy'])

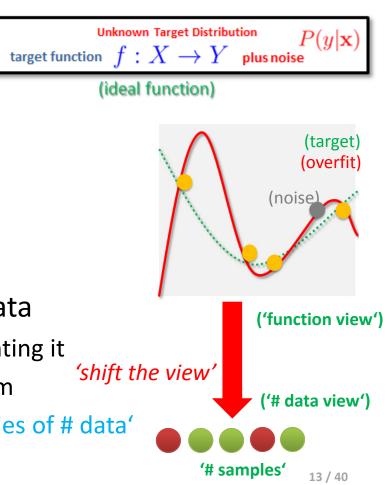
```
# Fit the model
```

history = model.fit(X_train, Y_train, batch_size=BATCH_SIZE, epochs=NB_EPOCH, verbose=VERBOSE, validation_split=VALIDATION_SPLIT)

```
# evaluation
score = model.evaluate(X_test, Y_test, verbose=VERBOSE)
print('Test score:', score[0])
print('Test accuracy:', score[1])
```

Problem of Overfitting – Noise Term Revisited

- '(Noisy) Target function' is not a (deterministic) function
 - Getting with 'same x in' the 'same y out' is not always given in practice
 - Idea: Use a 'target distribution' instead of 'target function'
 - Fitting some noise in the data is the basic reason for overfitting and harms the learning process
 - Big datasets tend to have more noise in the data so the overfitting problem might occur even more intense
- 'Different types of <u>some</u> noise' in data
 - Key to understand overfitting & preventing it
 - Shift of view': refinement of noise term
 - Learning from data: 'matching properties of # data'



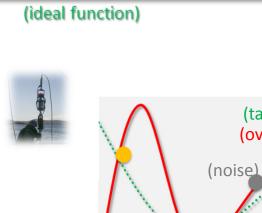
Problem of Overfitting – Stochastic Noise

- Stoachastic noise is a part 'on top of' each learnable function
 - Noise in the data that can not be captured and thus not modelled by f
 - Random noise : aka 'non-deterministic noise'
 - Conventional understanding established early in this course
 - Finding a 'non-existing pattern in noise not feasible in learning'
- Practice Example
 - Random fluctuations and/or measurement errors in data
 - Fitting a pattern that not exists 'out-of-sample'
 - Puts learning progress 'off-track' and 'away from f'
- Stochastic noise here means noise that can't be captured, because it's just pure 'noise as is' (nothing to look for) – aka no pattern in the data to understand or to learn from

 $P(y|\mathbf{x}$

(target) (overfit)





Unknown Target Distribution

target function $f: X \to Y$ plus noise





Problem of Overfitting – Deterministic Noise

- Part of target function f that H can not capture: $f(\mathbf{x}) h^*(\mathbf{x})$
 - Hypothesis set H is limited so best h* can not fully approximate f
 - h* approximates f, but fails to pick certain parts of the target f
 - 'Behaves like noise', existing even if data is 'stochastic noiseless'
- Different 'type of noise' than stochastic noise
 - Deterministic noise depends on \mathcal{H} (determines how much more can be captured by
 - E.g. same f, and more sophisticated H : noise is smaller*
 (stochastic noise remains the same, nothing can capture it)
 - Fixed for a given x, clearly measurable (stochastic noise may vary for values of x)

(f) (h*)

(learning deterministic noise is outside the ability to learn for a given h*)

 Deterministic noise here means noise that can't be captured, because it is a limited model (out of the league of this particular model), e.g. 'learning with a toddler statistical learning theory'

Problem of Overfitting – Impacts on Learning

- The higher the degree of the polynomial (cf. model complexity), the more degrees of freedom are existing and thus the more capacity exists to overfit the training data
- Understanding deterministic noise & target complexity
 - Increasing target complexity increases deterministic noise (at some level)
 - Increasing the number of data N decreases the deterministic noise
- Finite N case: \mathcal{H} tries to fit the noise
 - Fitting the noise straightforward (e.g. Perceptron Learning Algorithm)
 - Stochastic (in data) and deterministic (simple model) noise will be part of it
- Two 'solution methods' for avoiding overfitting
 - Regularization: 'Putting the brakes in learning', e.g. early stopping (more theoretical, hence 'theory of regularization')
 - Validation: 'Checking the bottom line', e.g. other hints for out-of-sample (more practical, methods on data that provides 'hints')

High-level Tools – Keras – Regularization Techniques

- Keras is a high-level deep learning library implemented in Python that works on top of existing other rather low-level deep learning frameworks like Tensorflow, CNTK, or Theano
- The key idea behind the Keras tool is to enable faster experimentation with deep networks
- Created deep learning models run seamlessly on CPU and GPU via low-level frameworks

keras.layers.Dropout(rate, **Dropout is randomly setting a fraction** noise shape=None, of input units to 0 at each update seed=None) during training time, which helps prevent overfitting (using parameter rate) from keras import regularizers L2 regularizers allow to apply penalties model.add(Dense(64, input dim=64, on layer parameter or layer activity kernel regularizer=regularizers.l2(0.01), during optimization itself – therefore activity regularizer=regularizers.l1(0.01))) the penalties are incorporated in the lost function that the network

[5] Keras Python Deep Learning Library

optimizes

Lecture 4 – Convolutional Neural Network Challenges

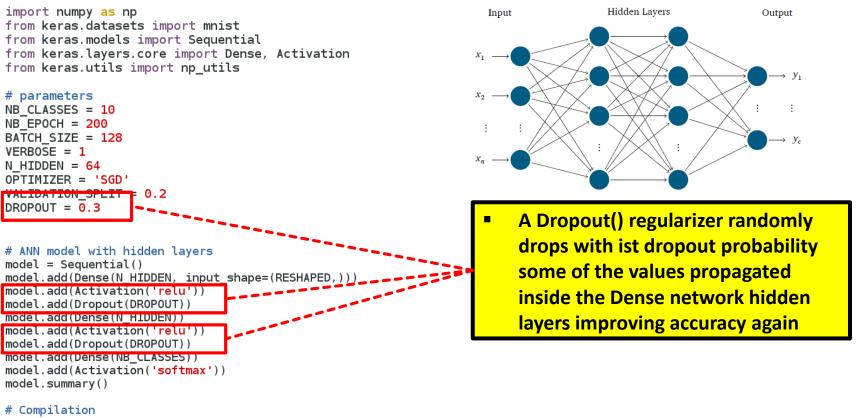
K Keras

Exercises – Underfitting & Dropout Regularizer

- Run with 20 Epochs first (not trained enough); then 250 Epochs
 - Training accuracy should be above the test accuracy otherwise 'underfitting'



ANN – MNIST Dataset – Add Weight Dropout Regularizer



model.compile(loss='categorical_crossentropy', optimizer=OPTIMIZER, metrics=['accuracy'])

Fit the model

history = model.fit(X_train, Y_train, batch_size=BATCH_SIZE, epochs=NB_EPOCH, verbose=VERBOSE, validation_split=VALIDATION_SPLIT)

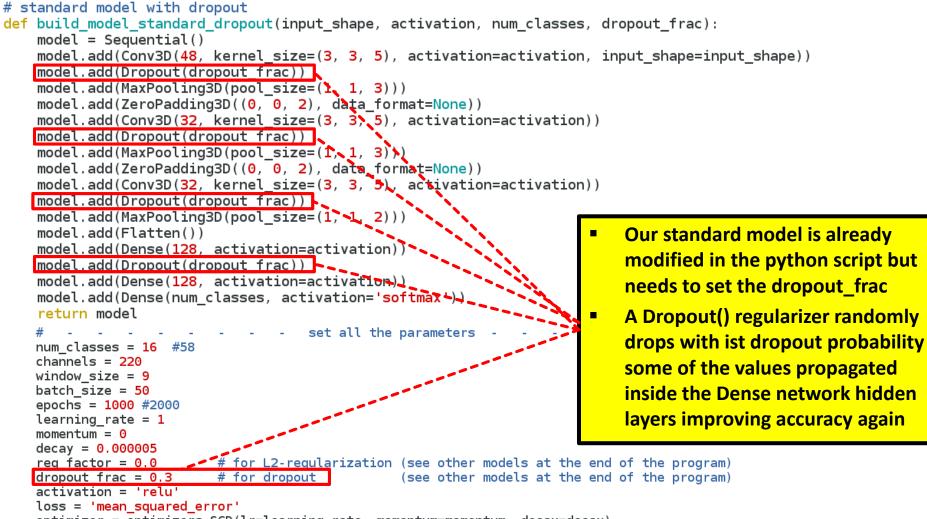
evaluation

```
score = model.evaluate(X_test, Y_test, verbose=VERBOSE)
print('Test score:', score[0])
print('Test accuracy:', score[1])
```

Exercises – Regularizers in non-Standard CNN Model



Remote Sensing Dataset – CNN Script – Dropout Regularizer



Remote Sensing Dataset – CNN Script – L2 Regularizer

standard model with L2-regularization def build model standard L2(input shape, activation, num classes, reg factor): model = Sequential() model.add(Conv3D(48, kernel_size=(3, 3, 5), activation=activation, kernel_regularizer=regularizers.l2(reg_factor), nput_shape=input_shape)) model.add(MaxPooling3D(pool size=(1, 1, 3))) model.add(ZeroPadding3D((0, 0, 2), data format=None)) model.add(Conv3D(32, kernel_size=(3, 3, 5), activation=activation_kernel_regularizer=regularizers.l2(reg_factor))) model.add(MaxPooling3D(pool size=(1, 1, 3))) model.add(ZeroPadding3D((0, 0, 2), data format=None model.add(Conv3D(32, kernel_size=(3, 3, 5), activation_activation_kernel_regularizer=regularizers.l2(reg_factor))) model.add(MaxPooling3D(pool size=(1, 1, 2))) model.add(Flatten()) model.add(Dense(128, activation=activation, kernel_regularizer=regularizers.l2(reg_factor))) model.add(Dense(128, activation=activation, kernel_regularizer=regularizers.l2(reg_factor))) model.add(Dense(num_classes, activation='softmax')) return model

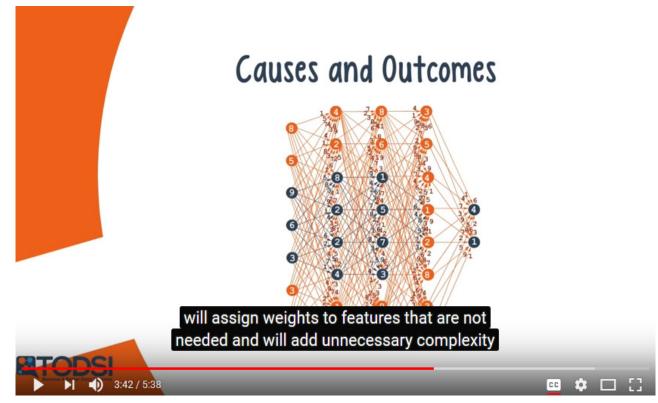
- Our standard model is already modified in the python script but needs to set the reg_factor
- L1 regularization (also known as lasso): The complexity of the model is expressed as the sum
- L2 regularization (also known as ridge): The complexity of the model is expressed as the sum of the squares of the weights
- Elastic net regularization: The complexity of the model is captured by a combination of the two preceding techniques

<pre>#</pre>		-	set	all	the	param	eters	-	-	-	-	-
reg_factor = 0.01	# fo	r L2-re	egula	ariza	atior	ı (see	othei	r mod	els	at	the	end
dropout_frac = 0.0 activation = 'relu'	# tor	dropo	ut			(see	other	mode	ls a	at t	he	end

loss = 'mean_squared_error'

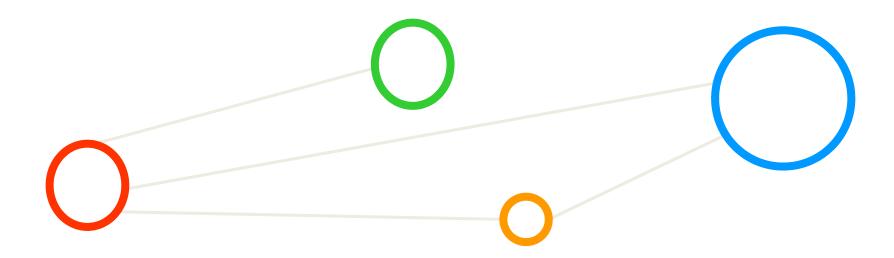
optimizer = optimizers.SGD(lr=learning_rate, momentum=momentum, decay=decay)

[Video] Overfitting in Deep Neural Networks

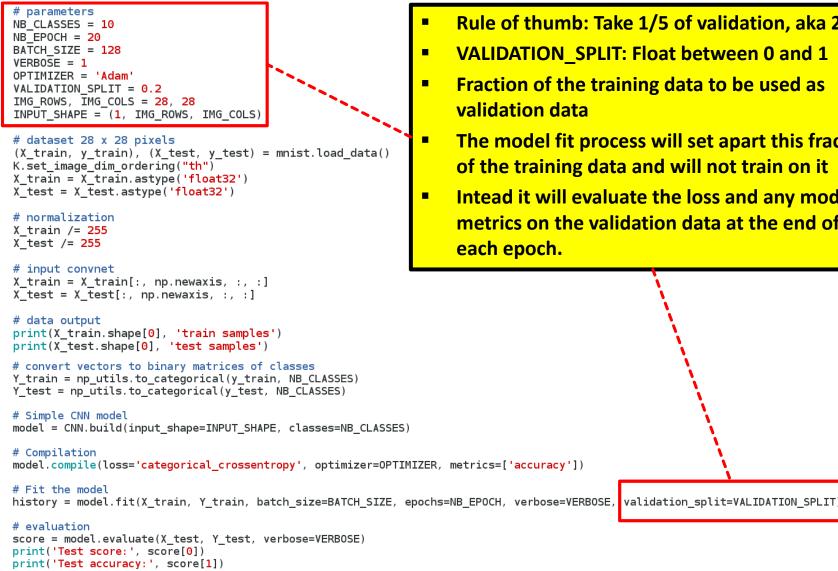


[2] How good is your fit?, YouTube

Validation and Model Selection



MNIST Dataset – CNN Python Script – Validation Data



- Rule of thumb: Take 1/5 of validation, aka 20%
- VALIDATION SPLIT: Float between 0 and 1
- Fraction of the training data to be used as
- The model fit process will set apart this fraction of the training data and will not train on it
- Intead it will evaluate the loss and any model metrics on the validation data at the end of

MNIST Dataset – CNN Model – Output using Validation

[vsc42544@gligar01 deeplearning]\$ head KERAS_MNIST_CNN.o1179880
60000 train samples

10000 train samples

10000 test samples

Train on 48000 samples, validate on 12000 samples

Epoch 1/20

128/48000 []	- ETA: 10:06 - loss: 2.2997 - acc: 0.1250
256/48000 []	- ETA: 7:46 - loss: 2.2578 - acc: 0.1992
384/48000 []	- ETA: 6:58 - loss: 2.2127 - acc: 0.2083
512/48000 []	- ETA: 6:35 - loss: 2.1632 - acc: 0.2598
640/48000 []	- ETA: 6:20 - loss: 2.0934 - acc: 0.3234

[vsc42544@gligar01 deeplearning]\$ tail KERAS_MNIST_CNN.o1179880

9824/10000 [======>] - ETA: 0s 9856/10000 [=====>] - ETA: 0s 9888/10000 [=====>] - ETA: 0s 9920/10000 [=====>] - ETA: 0s 9952/10000 [======>] - ETA: 0s 9984/10000 [=======]] - ETA: 0s 10000/10000 [=====]] - 41s 4ms/step Test score: 0.0483192791523 Test accuracy: 0.99

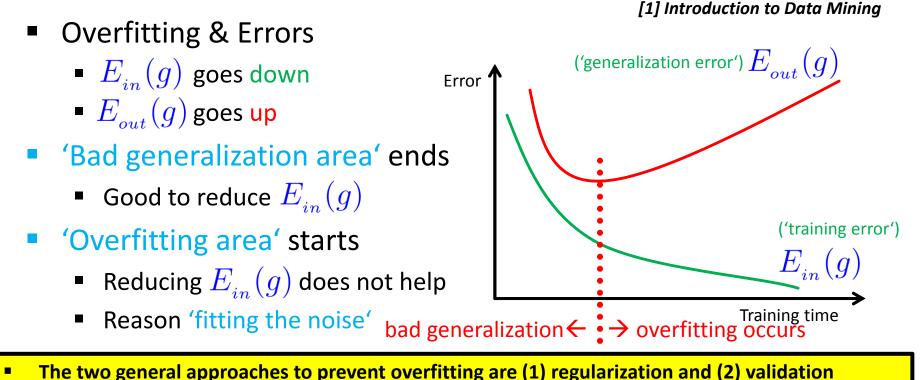
Working directory was /user/scratch/gent/vsc425/vsc42544/KERAS_MNIST_CNN_1179880.master19.golett.gent.vsc

Exercises – Change the Validation to 80% - What happens?



Problem of Overfitting – Clarifying Terms – Revisited

- A good model must have low training error (E_{in}) and low generalization error (E_{out})
- Model overfitting is if a model fits the data too well (E_{in}) with a poorer generalization error (E_{out}) than another model with a higher training error (E_{in})



- The two general approaches to prevent overhitting are (1) regularization and (2) validation

(Decisions about the model are related to the problem of overfitting – need another method to 'select model well')

Problem of Overfitting – Impacts on Learning Revisited

- The higher the degree of the polynomial (cf. model complexity), the more degrees of freedom are existing and thus the more capacity exists to overfit the training data
- Understanding deterministic noise & target complexity
 - Increasing target complexity increases deterministic noise (at some level)
 - Increasing the number of data N decreases the deterministic noise
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 - Fitting the noise straightforward (e.g. with linear regression)
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- Two 'solution methods' for avoiding overfitting
 - Regularization: 'Putting the brakes in learning', e.g. early stopping (more theoretical, hence 'theory of regularization')
 - Validation: 'Checking the bottom line', e.g. other hints for out-of-sample (more practical, methods on data that provides 'hints')

(Decisions about the model are related to the model complexity – need another method to 'select model well')

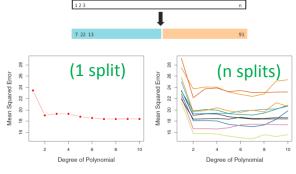
Validation & Model Selection – Terminology

- The 'Validation technique' should be used in all machine learning or data mining approaches
- Model assessment is the process of evaluating a models performance
- Model selection is the process of selecting the proper level of flexibility for a model

modified from [4] 'An Introduction to Statistical Learning'

- 'Training error'
 - Calculated when learning from data (i.e. dedicated training set)
- 'Test error'
 - Average error resulting from using the model with 'new/unseen data'
 - 'new/unseen data' was not used in training (i.e. dedicated test set)
 - In many practical situations, a dedicated test set is not really available
- Validation Set'
 - Split data into training & validation set
- Variance' & 'Variability'
 - Result in different random splits (right)

(split creates a two subsets of comparable size)



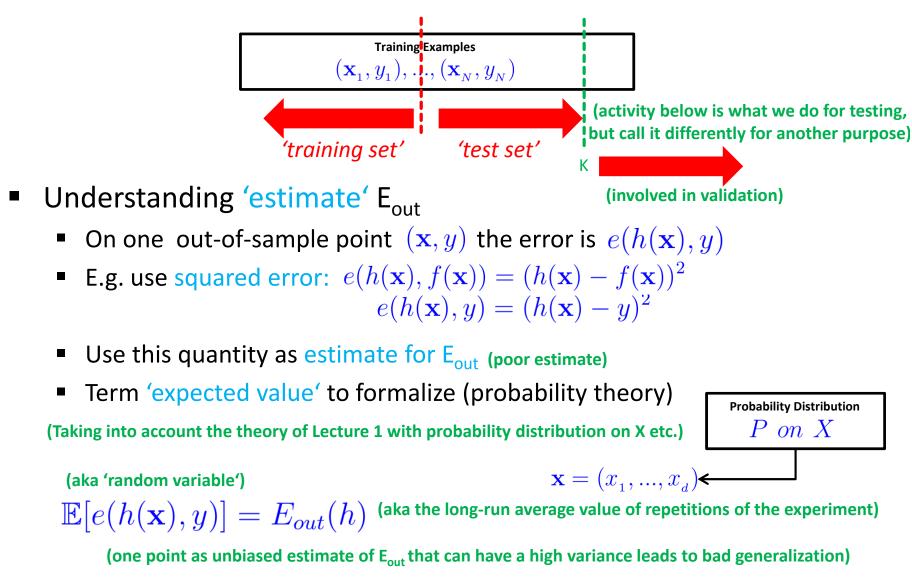
Validation Technique – Formalization & Goal

- Validation is a very important technique to estimate the out-of-sample performance of a model
 Main utility of regularization & validation is to control or avoid overfitting via model selection
- Regularization & Validation
 - Approach: introduce a 'overfit penalty' that relates to model complexity
 - Problem: Not accurate values: 'better smooth functions'

 $E_{out}(h) = E_{in}(h) + \begin{array}{c} \mathbf{overfit} \ \mathbf{penalty} \\ \uparrow \\ (validation \ estimates \\ this \ quantity) \end{array}$ (regularization uses a term that captures the overfit \ penalty \\ (minimize \ both \ to \ be \ better \ proxy \ for \ \mathbf{E}_{out}) \\ \uparrow \\ (regularization \ estimates \\ this \ quantity) \end{array}

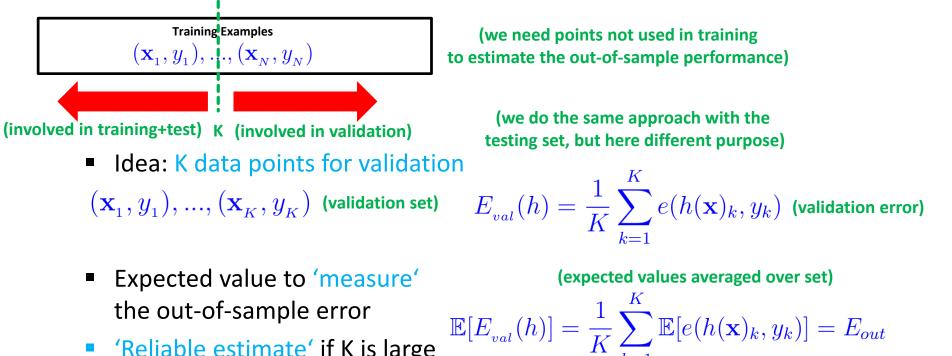
- Validation (measuring E_{out} is not possible as this is an unknown quantity, another quantity is needed that is measurable that at least estimates it)
 - Goal 'estimate the out-of-sample error' (establish a quantity known as validation error)
 - Distinct activity from training and testing (testing also tries to estimate the E_{out})

Validation Technique – Pick one point & Estimate E_{out}



Validation Technique – Validation Set

- Validation set consists of data that has been not used in training to estimate true out-of-sample
- Rule of thumb from practice is to take 20% (1/5) for validation of the learning model
- Solution for high variance in expected values $\mathbb{E}[e(h(\mathbf{x}), y)] = E_{out}(h)$
 - Take a 'whole set' instead of just one point (x, y) for validation



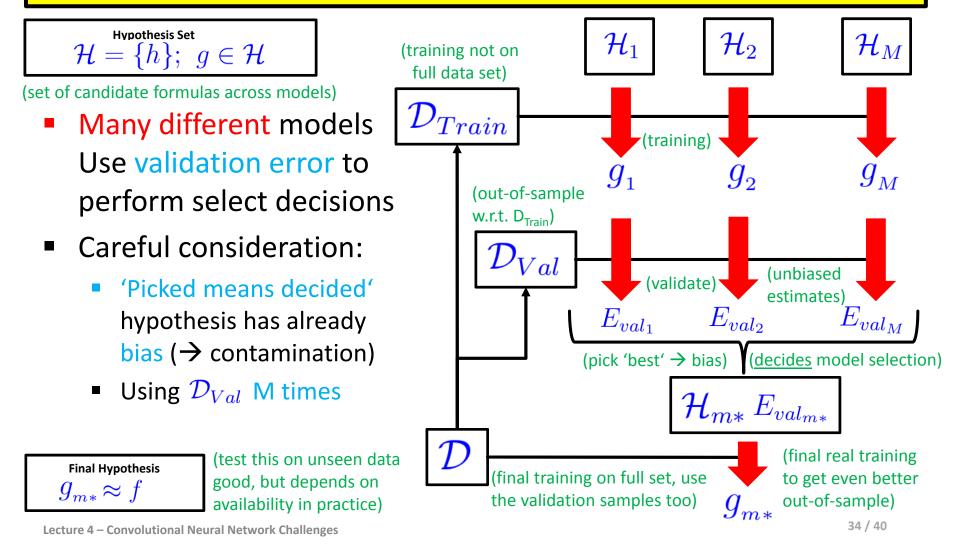
'Reliable estimate' if K is large



(this gives a much better (lower) variance than on a single point given K is large)

Validation Technique – Model Selection Process

- Model selection is choosing (a) different types of models or (b) parameter values inside models
- Model selection takes advantage of the validation error in order to decide \rightarrow 'pick the best'



Remote Sensing - Experimental Setup @ JSC - Revisited

- CNN Setup
 - Table overview
- HPC Machines used
 - Systems JURECA and JURON
- GPUs
 - NVIDIA Tesla K80 (JURECA)
 - NVIDIA Tesla P100 (JURON)
 - While Using MathWorks' Matlab for the data
- Frameworks
 - Keras library (2.0.6) was used
 - Tensorflow (0.12.1 on Jureca, 1.3.0rc2 on Juron) as back-end
 - Automated usage of the GPU's of these machines via Tensorflow

Feature	Representation / Value					
Conv. Layer Filters	48, 32, 32					
Conv. Layer Filter size	(3,3,5), (3,3,5), (3,3,5)					
Dense Layer Neurons	128, 128					
Optimizer	SGD					
Loss Function	mean squared error					
Activation Functions	ReLU					
Training Epochs	600					
Batch Size	50					
Learning Rate	1					
Learning Rate Decay	5×10^{-6}					

(adding regularization values adds even more complexity in finding the right parameters)

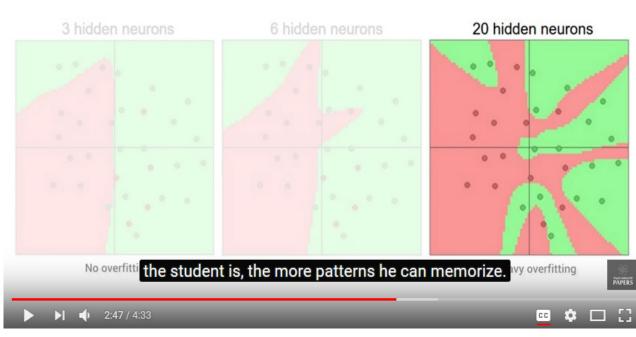
(having the validation with the full grid search of all parameters and all combinations is quite compute – intensive → ~infeasable)

Remote Sensing Data – Group Exercises L2 Values / Dropouts

- Add Validation (20%) and different L2 / dropouts per group
 - Which group performs best?



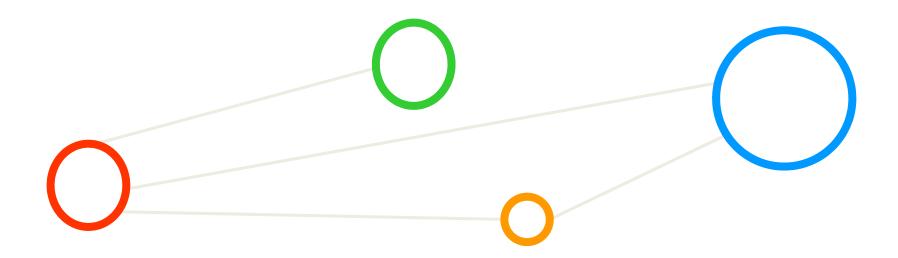
[Video] Overfitting in Deep Neural Networks



[3] Overfitting and Regularization For Deep Learning, YouTube

Source: Andrej Karpathy

Lecture Bibliography



Lecture Bibliography

- [1] Introduction to Data Mining, Pang-Ning Tan, Michael Steinbach, Vipin Kumar, Addison Wesley, ISBN 0321321367, English, ~769 pages, 2005
- [2] YouTube Video, 'How good is your fit? Ep. 21 (Deep Learning SIMPLIFIED)', Online: <u>https://www.youtube.com/watch?v=cJA5IHIIL30</u>
- [3] YouTube Video, 'Overfitting and Regularization For Deep Learning | Two Minute Papers #56', Online: <u>https://www.youtube.com/watch?v=6aF9sJrzxaM</u>
- [4] An Introduction to Statistical Learning with Applications in R, Online: <u>http://www-bcf.usc.edu/~gareth/ISL/index.html</u>
- [5] Keras Python Deep Learning Library, Online: <u>https://keras.io/</u>

