THE UNIVERSITY *of* EDINBURGH
informatics

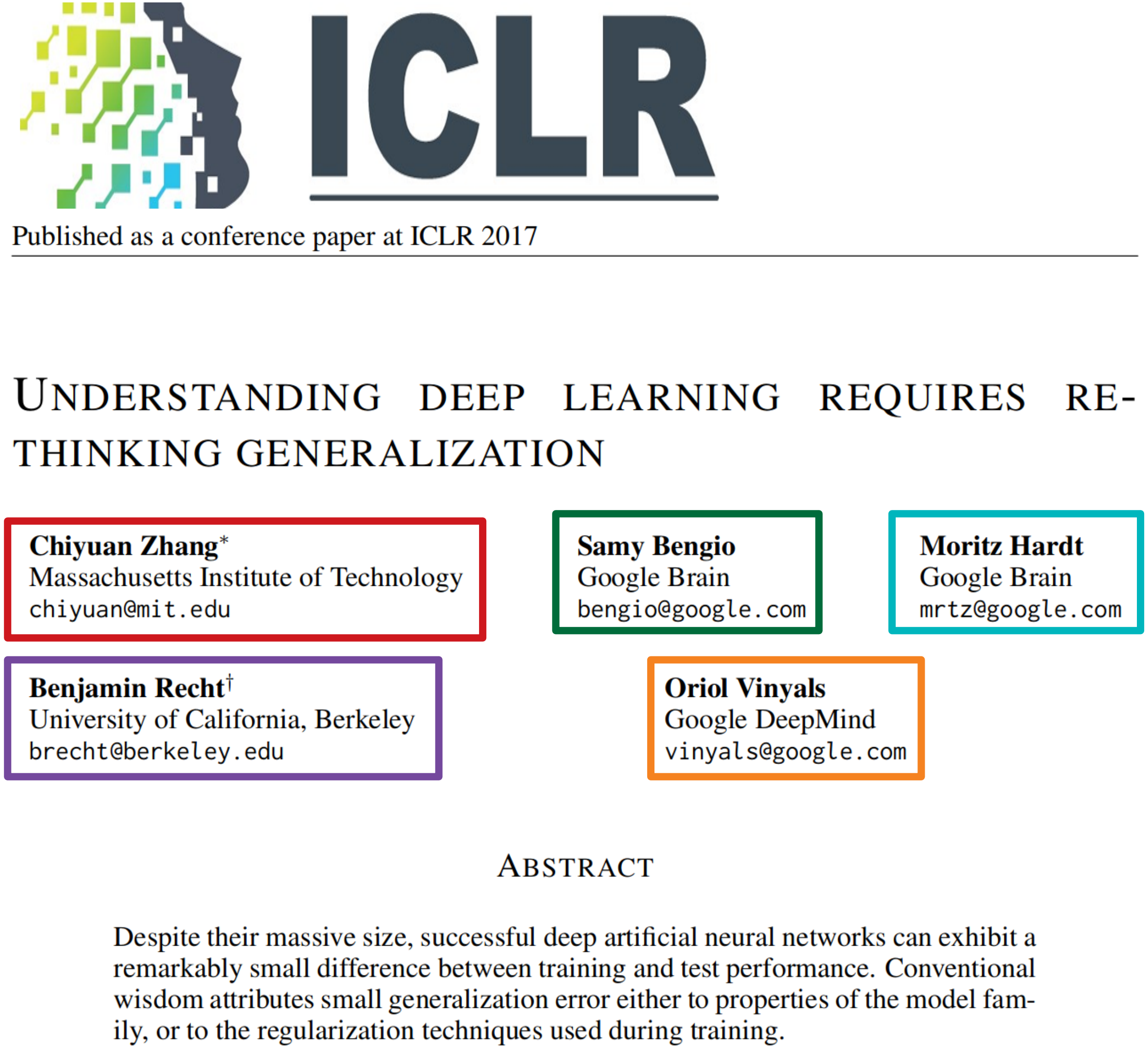
CSTR

Understanding Deep Learning Requires Rethinking Generalisation

Erfan Loweimi

Centre for Speech Technology Research (CSTR)

Listen! 12.3.2019



Published as a conference paper at ICLR 2017

UNDERSTANDING DEEP LEARNING REQUIRES RETHINKING GENERALIZATION

Chiyuan Zhang[*]
Massachusetts Institute of Technology
chiyuan@mit.edu

Samy Bengio
Google Brain
bengio@google.com

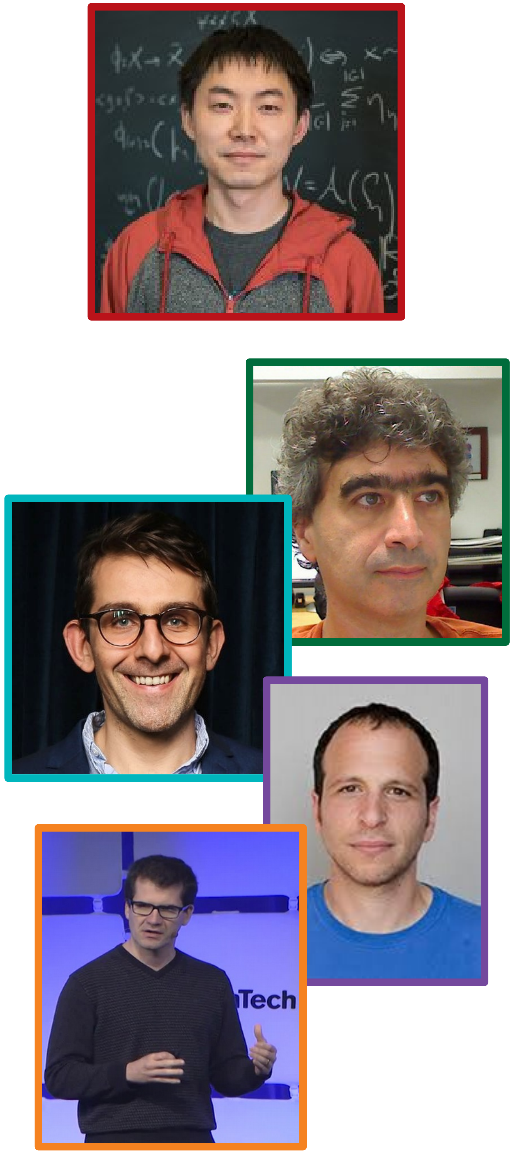
Moritz Hardt
Google Brain
mrtz@google.com

Benjamin Recht[†]
University of California, Berkeley
brecht@berkeley.edu

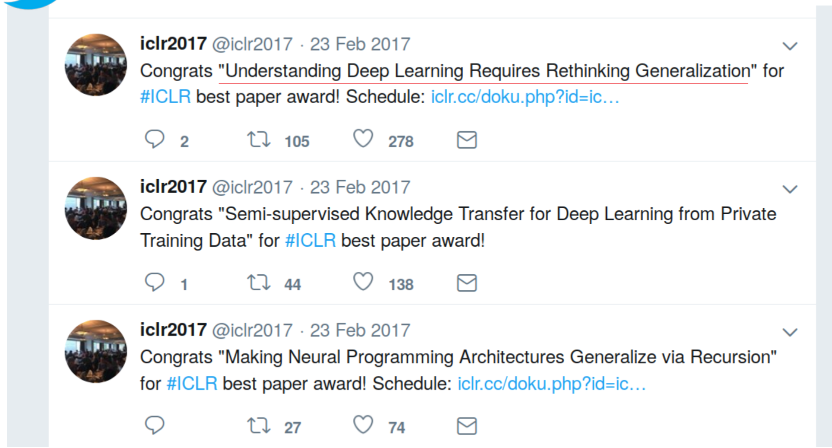
Oriol Vinyals
Google DeepMind
vinyals@google.com

ABSTRACT

Despite their massive size, successful deep artificial neural networks can exhibit a remarkably small difference between training and test performance. Conventional wisdom attributes small generalization error either to properties of the model family, or to the regularization techniques used during training.



Important Paper ...



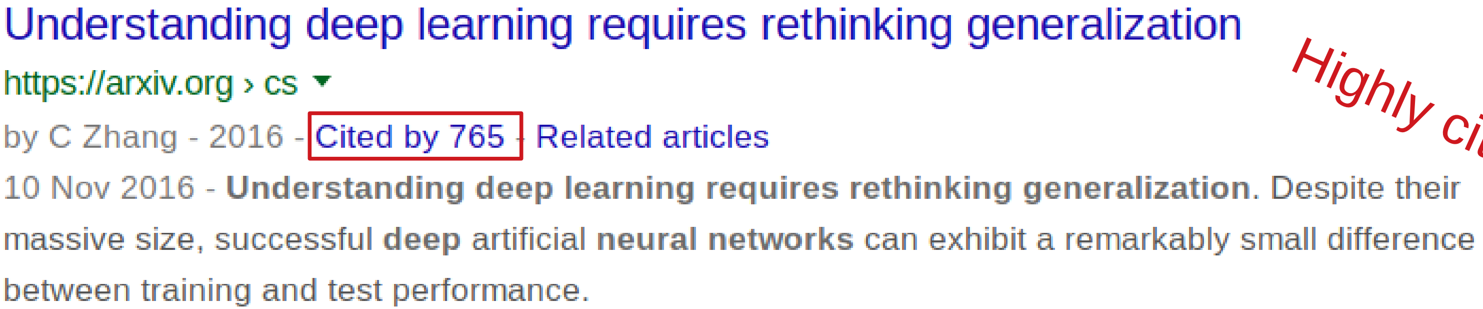
iclr2017 @iclr2017 · 23 Feb 2017
Congrats "Understanding Deep Learning Requires Rethinking Generalization" for #ICLR best paper award! Schedule: iclr.cc/doku.php?id=ic…
2 105 278

iclr2017 @iclr2017 · 23 Feb 2017
Congrats "Semi-supervised Knowledge Transfer for Deep Learning from Private Training Data" for #ICLR best paper award!
1 44 138

iclr2017 @iclr2017 · 23 Feb 2017
Congrats "Making Neural Programming Architectures Generalize via Recursion" for #ICLR best paper award! Schedule: iclr.cc/doku.php?id=ic…
27 74

Understanding deep learning requires rethinking generalization

ICLR 2017 Best Paper Award



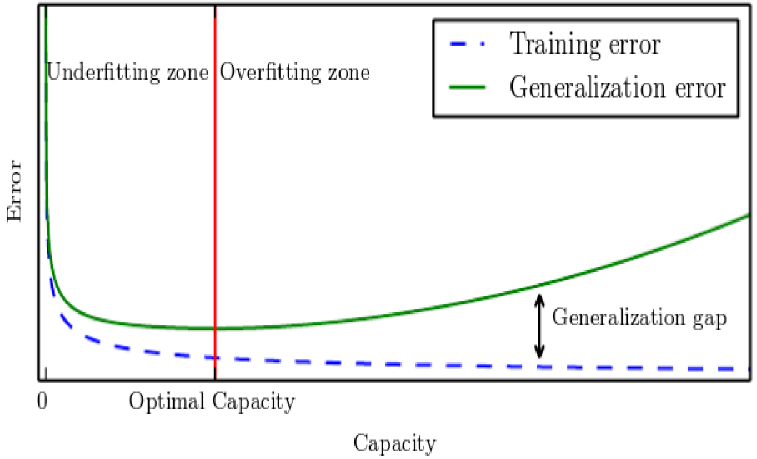
Understanding deep learning requires rethinking generalization
https://arxiv.org › cs
by C Zhang - 2016 - Cited by 765 - Related articles
10 Nov 2016 - **Understanding deep learning requires rethinking generalization**. Despite their massive size, successful **deep** artificial **neural networks** can exhibit a remarkably small difference between training and test performance.

11/3/2019 →

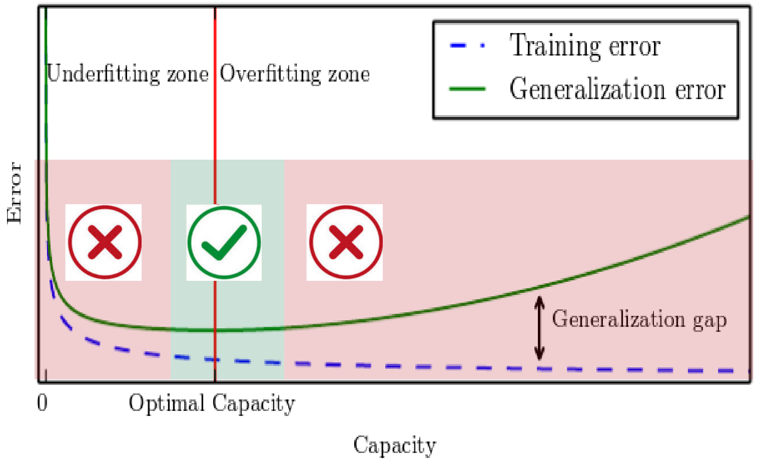
Highly cited

- Why DNNs work/generalise well
- Interpretability/understanding

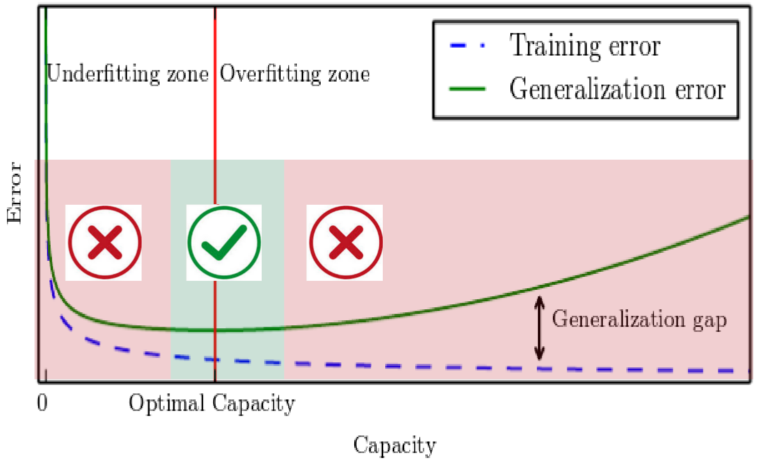
- Why DNNs work/generalise well
- Interpretability/understanding



- Why DNNs work/generalise well
- Interpretability/understanding



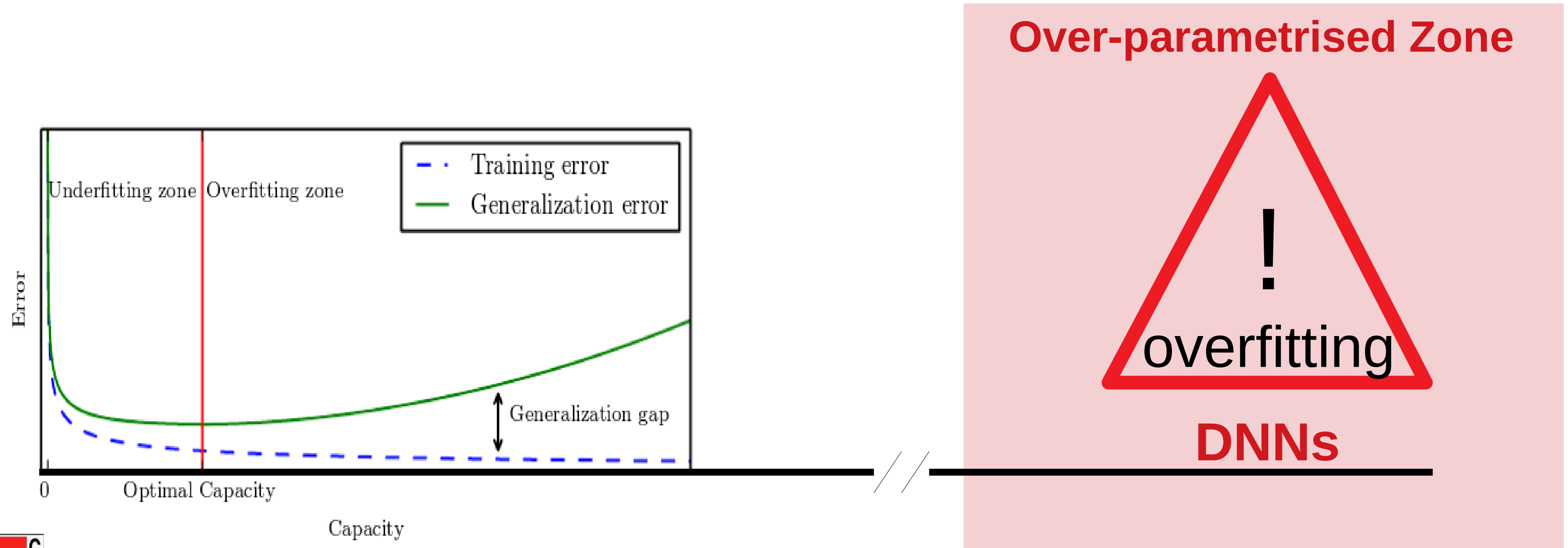
- Why DNNs work/generalise well
- Interpretability/understanding



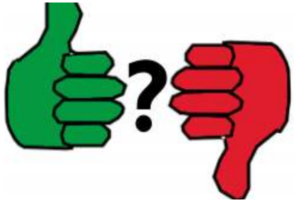
Underfitting: High Bias ✗

Overfitting: High Variance ✗

- Why DNNs work/generalise well

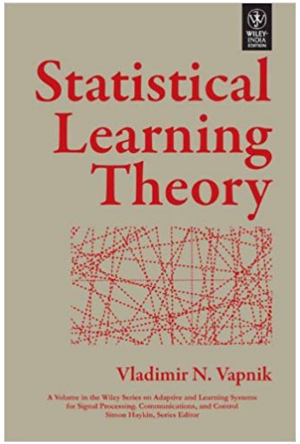


Over-parametrisation is Good or Bad?



E. Loweimi

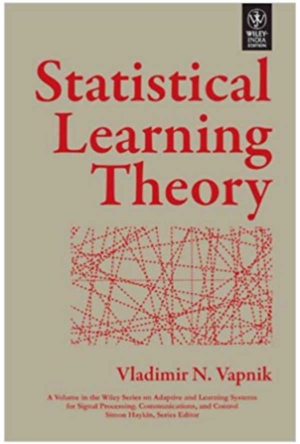
Generalisation Error


WILEY INDIA EDITION
Statistical Learning Theory
Vladimir N. Vapnik
A Volume in the Wiley Series on Adaptive and Learning Systems
for Signal Processing, Communications, and Control
Simon Haykin, Series Editor

- Definition: $E_{gen} = E_{test} – E_{train}$
- Statistical Learning Theory
  - Complexity measures ↔ upper bound for E_{gen}

$$E_{gen} = E_{test} - E_{train} \overset{\leq}{\propto} \frac{f_1(\#parameters)}{f_2(N)}$$

Generalisation Error



Statistical Learning Theory

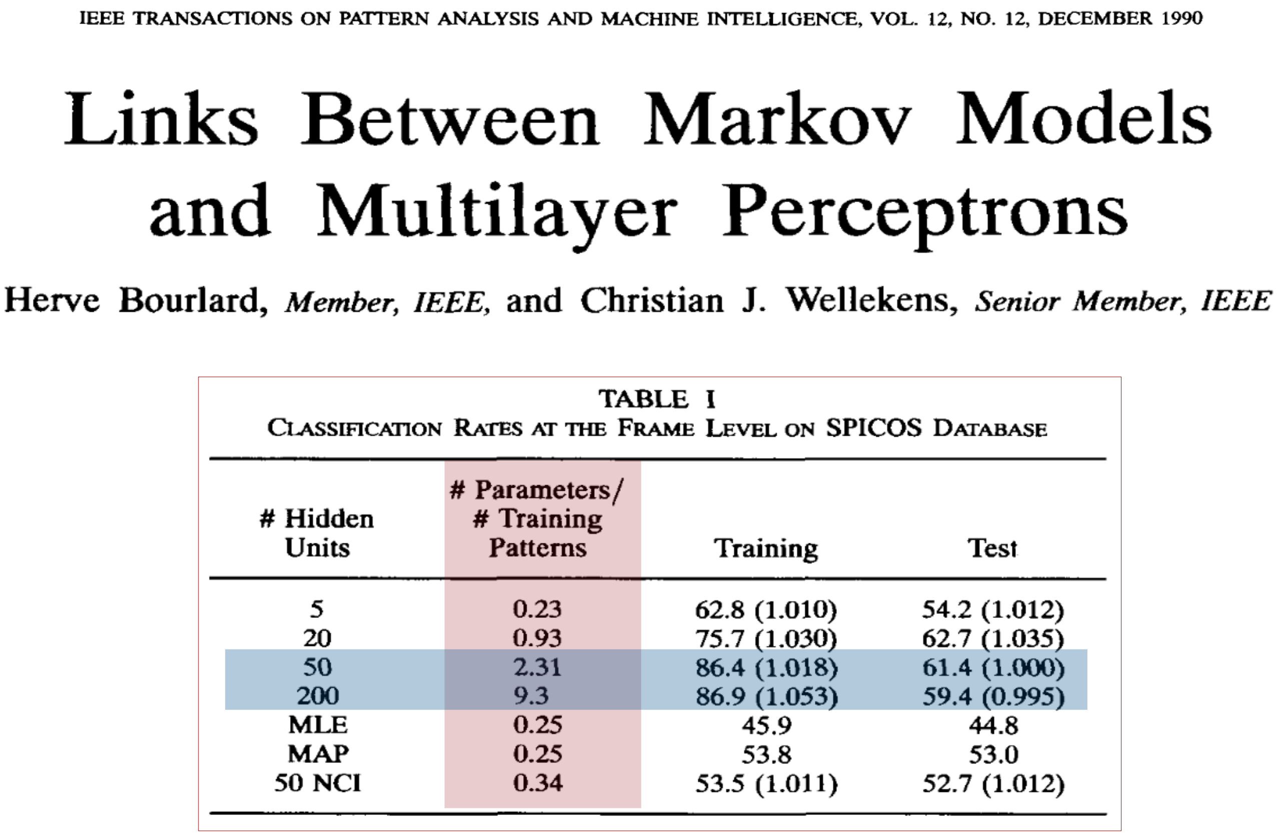
Vladimir N. Vapnik

A Volume in the Wiley Series on Adaptive and Learning Systems
for Signal Processing, Communications, and Control
Simon Haykin, Series Editor

- Definition: $E_{gen} = E_{test} – E_{train}$
- Statistical Learning Theory
  - Complexity measures ↔ upper bound for E_{gen}
  - Examples: VC-dim, Rademacher, Uniform stability

$$E_{gen} = E_{test} - E_{train} \overset{\leq}{\propto} \frac{f_1(\#parameters)}{f_2(N)} \overset{\text{e.g.}}{=} f\left(\frac{VC\text{-}dim}{N}\right)$$

Over-parametrisation is Good or Bad?



IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. 12, NO. 12, DECEMBER 1990

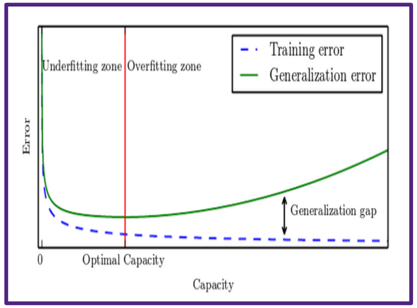
Links Between Markov Models and Multilayer Perceptrons

Herve Bourlard, *Member, IEEE,* and Christian J. Wellekens, *Senior Member, IEEE*

TABLE I
CLASSIFICATION RATES AT THE FRAME LEVEL ON SPICOS DATABASE

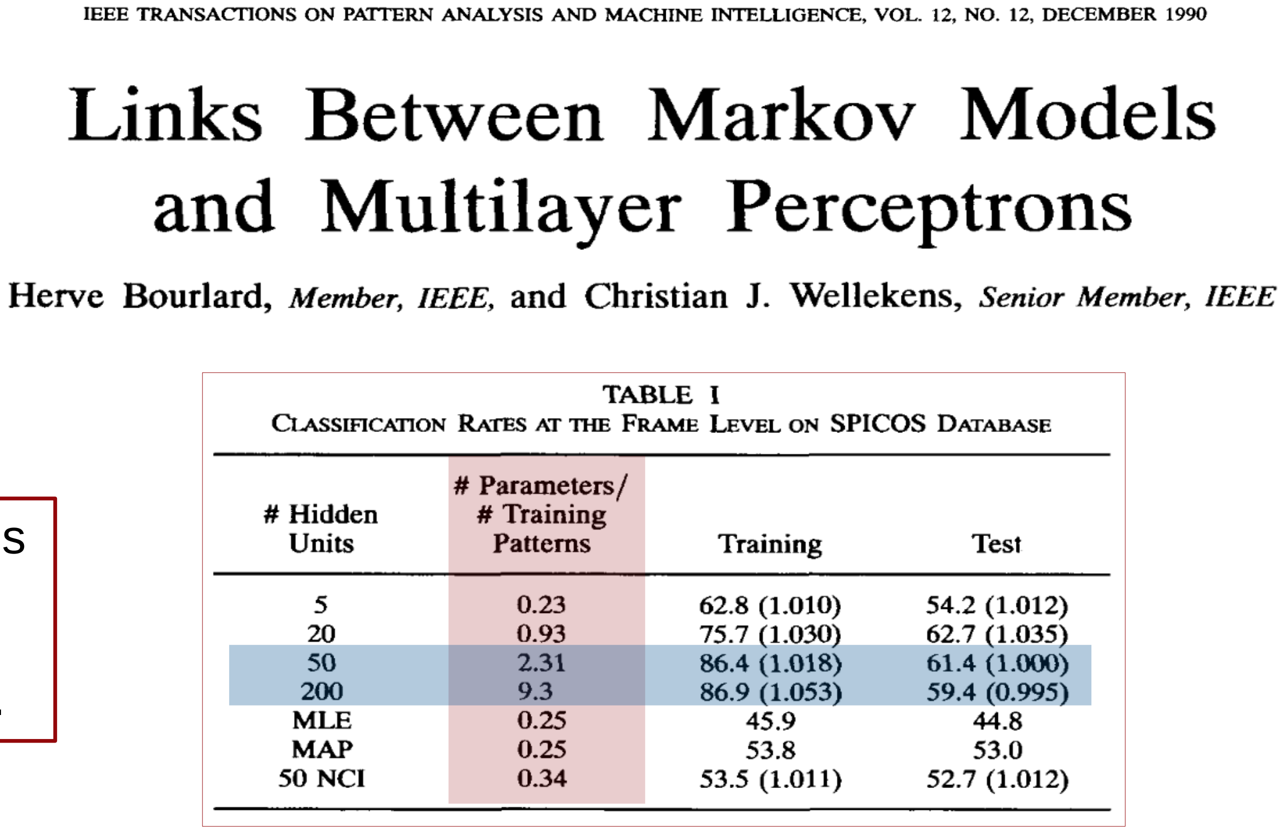
# Hidden Units	# Parameters/ # Training Patterns	Training	Test
5	0.23	62.8 (1.010)	54.2 (1.012)
20	0.93	75.7 (1.030)	62.7 (1.035)
50	2.31	86.4 (1.018)	61.4 (1.000)
200	9.3	86.9 (1.053)	59.4 (0.995)
MLE	0.25	45.9	44.8
MAP	0.25	53.8	53.0
50 NCI	0.34	53.5 (1.011)	52.7 (1.012)

Over-parametrisation is Good or **Bad**?



1. Over-parametrisation increases test error.

2. Results match traditional view.



IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE INTELLIGENCE, VOL. 12, NO. 12, DECEMBER 1990

Links Between Markov Models and Multilayer Perceptrons

Herve Bourlard, *Member, IEEE*, and Christian J. Wellekens, *Senior Member, IEEE*

TABLE I
CLASSIFICATION RATES AT THE FRAME LEVEL ON SPICOS DATABASE

# Hidden Units	# Parameters/ # Training Patterns	Training	Test
5	0.23	62.8 (1.010)	54.2 (1.012)
20	0.93	75.7 (1.030)	62.7 (1.035)
50	2.31	86.4 (1.018)	61.4 (1.000)
200	9.3	86.9 (1.053)	59.4 (0.995)
MLE	0.25	45.9	44.8
MAP	0.25	53.8	53.0
50 NCI	0.34	53.5 (1.011)	52.7 (1.012)

Size of the Model & Databases

CIFAR-10	#train: 50,000
Inception	1,649,402
AlexNet	1,387,786
MLP 1x512	1,209,866
ImageNet	#train: 1,200,000
Inception V3	23,885,392
AlexNet	61,100,840
ResNet-{18; 152}	11,689,512; 60,192,808
VGG-{11;19}	132,863,336; 143,667,240

Size of the Model & Databases

CIFAR-10	#train: 50,000	#parameter/#train
Inception	1,649,402	33
AlexNet	1,387,786	28
MLP 1x512	1,209,866	24
ImageNet	#train: 1,200,000	
Inception V3	23,885,392	20
AlexNet	61,100,840	51
ResNet-{18; 152}	11,689,512; 60,192,808	10; 50
VGG-{11;19}	132,863,336; 143,667,240	110; 120

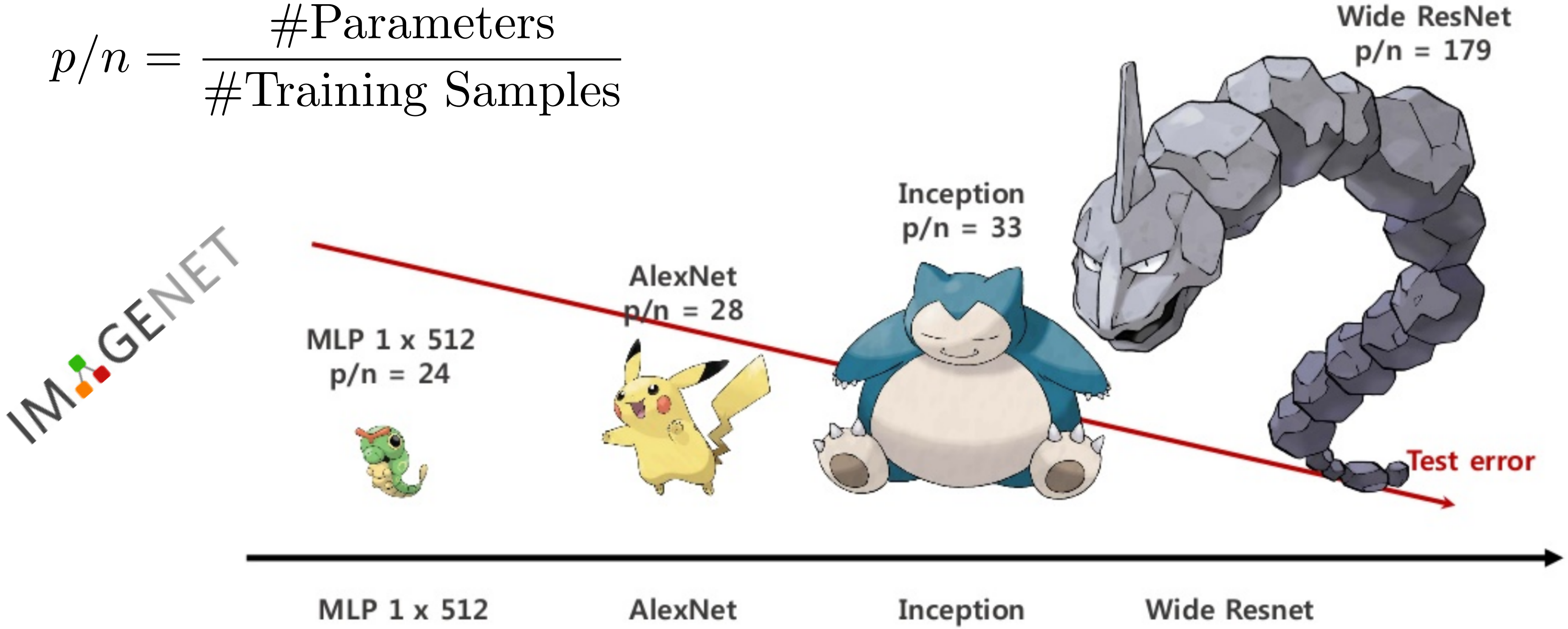
Size of the Model & Databases

CIFAR-10	#train: 50,000	#parameter/#train
Inception	1,649,402	33
AlexNet	1,387,786	28
MLP 1x512	1,209,866	24
ImageNet	#train: 1,200,000	
Inception V3	23,885,392	20
AlexNet	61,100,840	51
ResNet-{18; 152}	11,689,512; 60,192,808	10; 50
VGG-{11;19}	132,863,336; 143,667,240	110; 120

Overparametrised

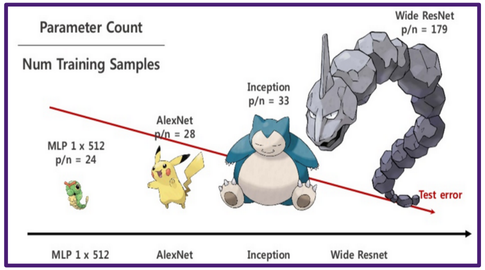
Over-parametrisation is **Good** or Bad?

$$p/n = \frac{\#\text{Parameters}}{\#\text{Training Samples}}$$

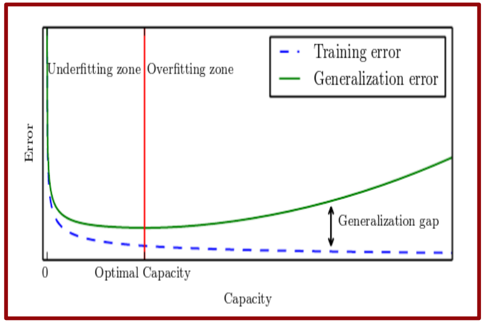


Over-parametrisation is Good or Bad?

- High #parameters does **NOT** necessarily …
  - degrade the generalisation performance
  - reflect model complexity



- Traditional views are **NOT** enough for explaining generalisation in the over-parameterised models (p>n).



The Puzzle

- Over-parametrisation is good or bad?
  - Both!

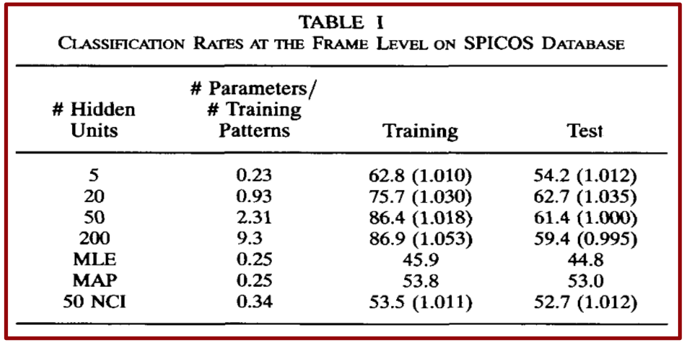
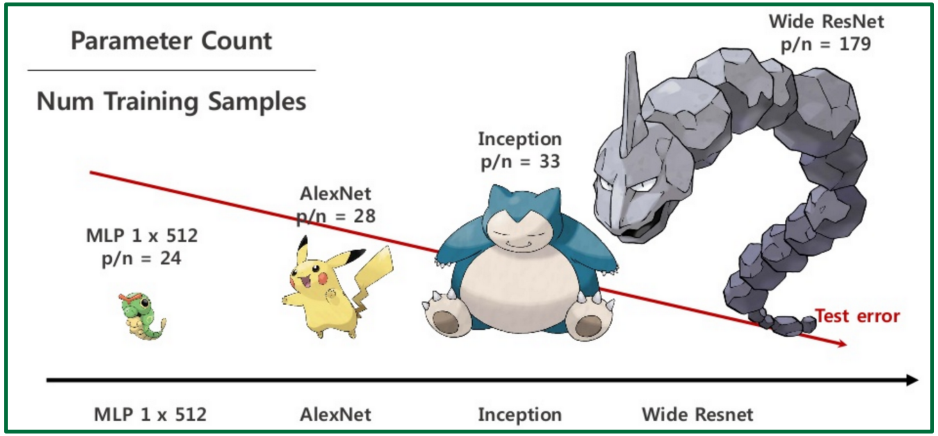
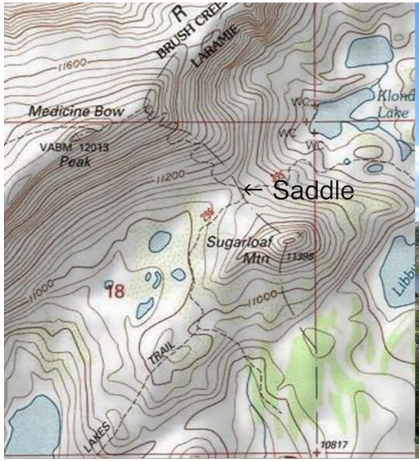


TABLE I
CLASSIFICATION RATES AT THE FRAME LEVEL ON SPICOS DATABASE

# Hidden Units	# Parameters/ # Training Patterns	Training	Test
5	0.23	62.8 (1.010)	54.2 (1.012)
20	0.93	75.7 (1.030)	62.7 (1.035)
50	2.31	86.4 (1.018)	61.4 (1.000)
200	9.3	86.9 (1.053)	59.4 (0.995)
MLE	0.25	45.9	44.8
MAP	0.25	53.8	53.0
50 NCI	0.34	53.5 (1.011)	52.7 (1.012)



The Puzzle



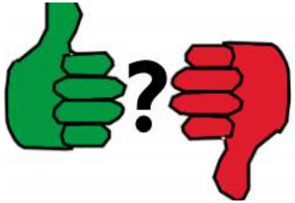
If the map and the terrain disagree, trust the terrain.

Swiss Army Aphorism

The Puzzle

- Over-parametrisation is good or bad?
  - Both!

- “*What is it then that distinguishes NNs that generalise well from those that don’t?*”



Experimental Setup

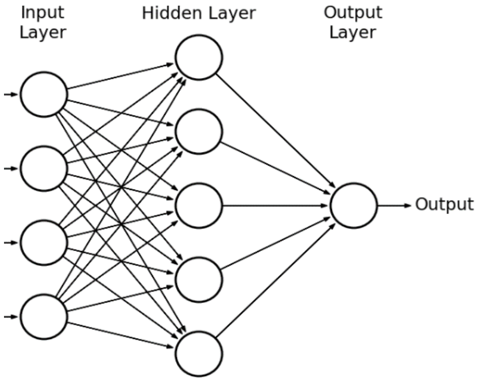
Experiments – Datasets

- CIFAR-10
  - 10 classes
  - 60k images, 32x32
    - 50k train + 10k test
- ImageNet (ILSVRC 2012)
  - 1000 classes
  - 1.35M images, 299x299
    - 1.2 M train + 150k val/test

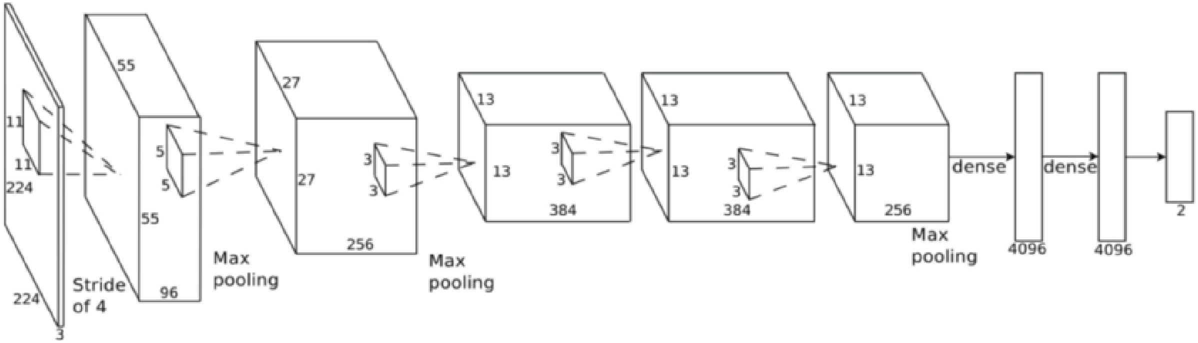
Architectures

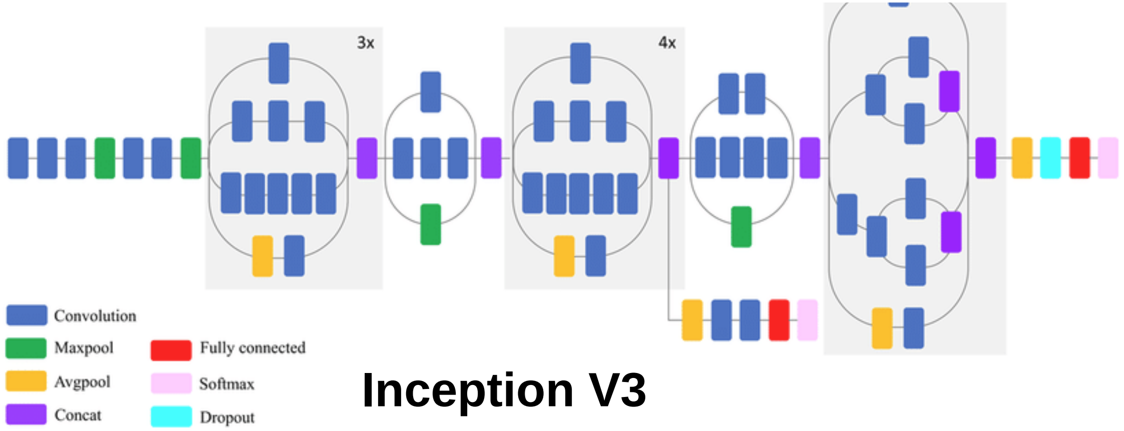
MLP1: 1x512

MLP2: 3x512



Alexnet





Inception V3

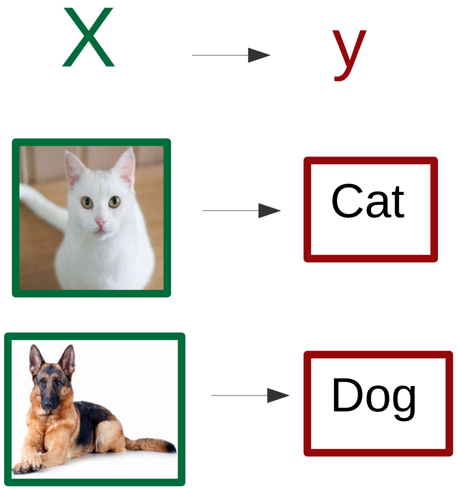
Experiments – Optimisation

- Stochastic Gradient Descend (SGD)
- Momentum: 0.9
- Learning rate:
  - MLP & Alexnet: 0.01, Inception: 0.1
- Learning rate annealing: 0.95 per epoch
- Mini-batch size: 128

Experiments – Randomizations Tests

- Label levels (y)

- Data level (X)



X → y

→ Cat

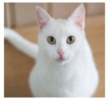
→ Dog

Randomizations Tests – Labels

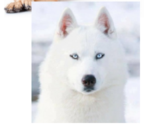
- Inspired from Non-parametric statistics

Label Randomisation

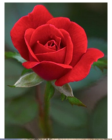
Cat


Cat

Dog


Dog

Horse

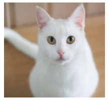

Flower

Car

Fish

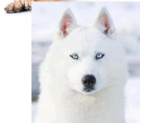
Label Randomisation

Cat [1]



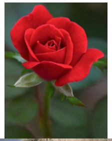
Cat [1]

Dog [2]



Dog [2]

Horse [3]



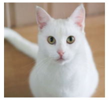
Flower [4]

Car [5]

Fish [6]

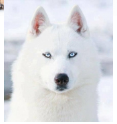
Label Randomisation

Cat [1]



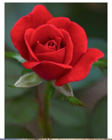
Cat [1]

Dog [2]



Dog [2]

Horse [3]



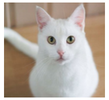
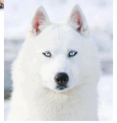
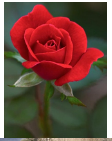
Flower [4]

Car [5]

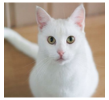
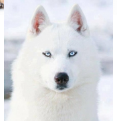
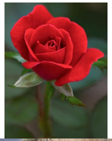
Fish [6]

Uniform sampling
(non-parametric)

Label Randomisation

	Cat [1]	⚂	3 → Horse
	Cat [1]	⚄	5 → Car
	Dog [2]	⚃	4 → Flower
	Dog [2]	⚁	2→ Dog
	Horse [3]	⚂	3 → Horse
	Flower [4]	⚄	5 → Car
	Car [5]	⚅	6 → Fish
	Fish [6]	⚀	1 → Cat

Label Randomisation

	Cat [1]	⚂	3 → Horse
	Cat [1]	⚄	5 → Car
	Dog [2]	⚃	4 → Flower
	Dog [2]	⚁	2→ Dog
	Horse [3]	⚂	3 → Horse
	Flower [4]	⚄	5 → Car
	Car [5]	⚅	6 → Fish
	Fish [6]	⚀	1 → Cat

Randomizations Tests – Labels

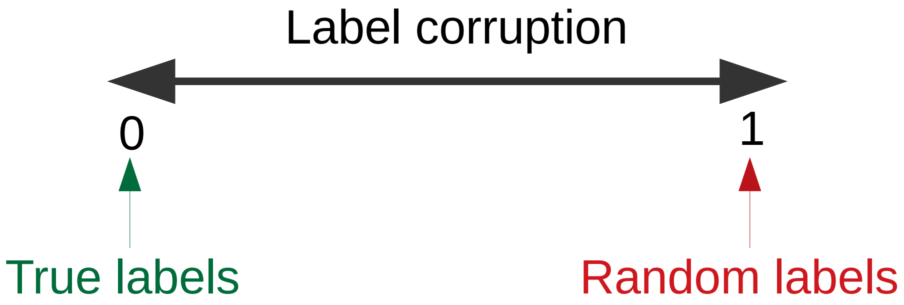
- Non-parametric statistics
- Test conditions
  - True labels
  - Random Labels

Randomizations Tests – Labels

- Non-parametric statistics
- Test conditions
  - True labels
  - Random Labels
    - Nothing (mapping/relationship/abstraction) to learn!
    - Does learning/optimisation algorithm converge?

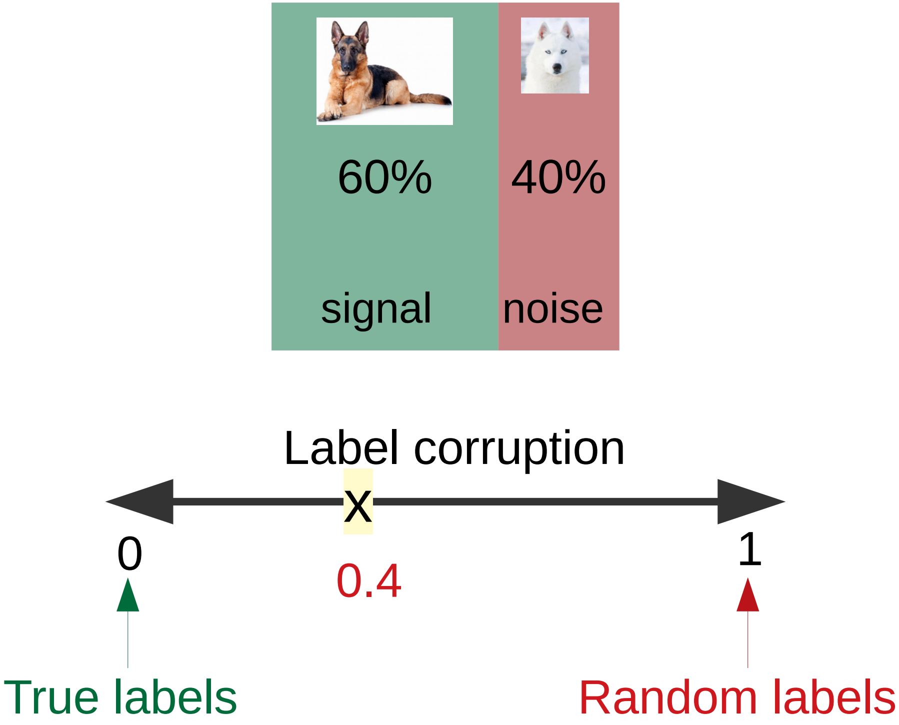
Randomizations Tests – Labels

- Non-parametric statistics
- Test conditions
  - True labels
  - Partially corrupted labels
  - Random Labels



Randomizations Tests – Labels

- Non-parametric statistics
- Test conditions
  - True labels
  - Partially corrupted labels
  - Random Labels

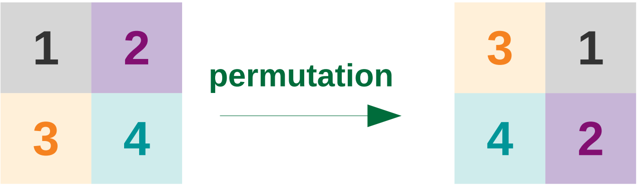


Randomizations Tests – Data

- Shuffled pixels
- Random pixels
- Gaussian

Randomizations Tests – Data

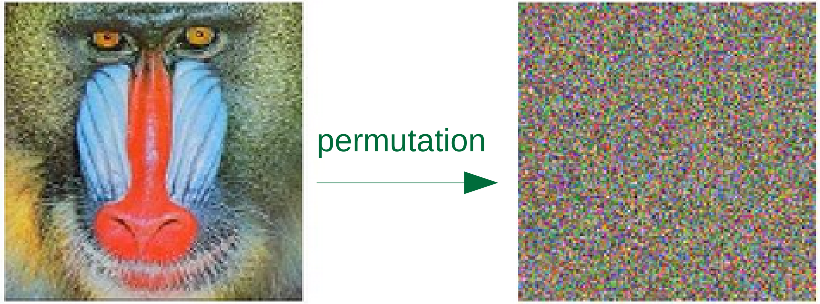
- Shuffled pixels → one permutation trans.
- Random pixels → Many permutation trans.
- Gaussian (parametric) → database mean & variance



1	2
3	4

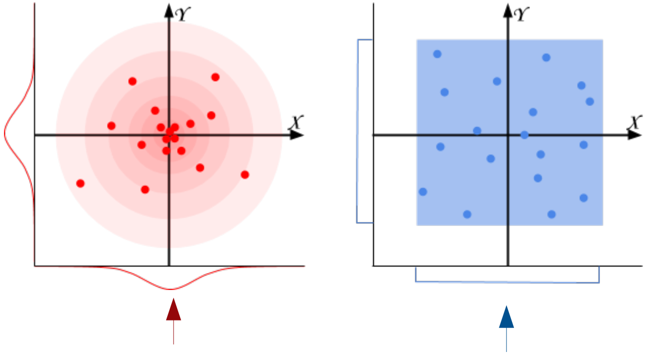
permutation

3	1
4	2



Randomizations Tests – Data

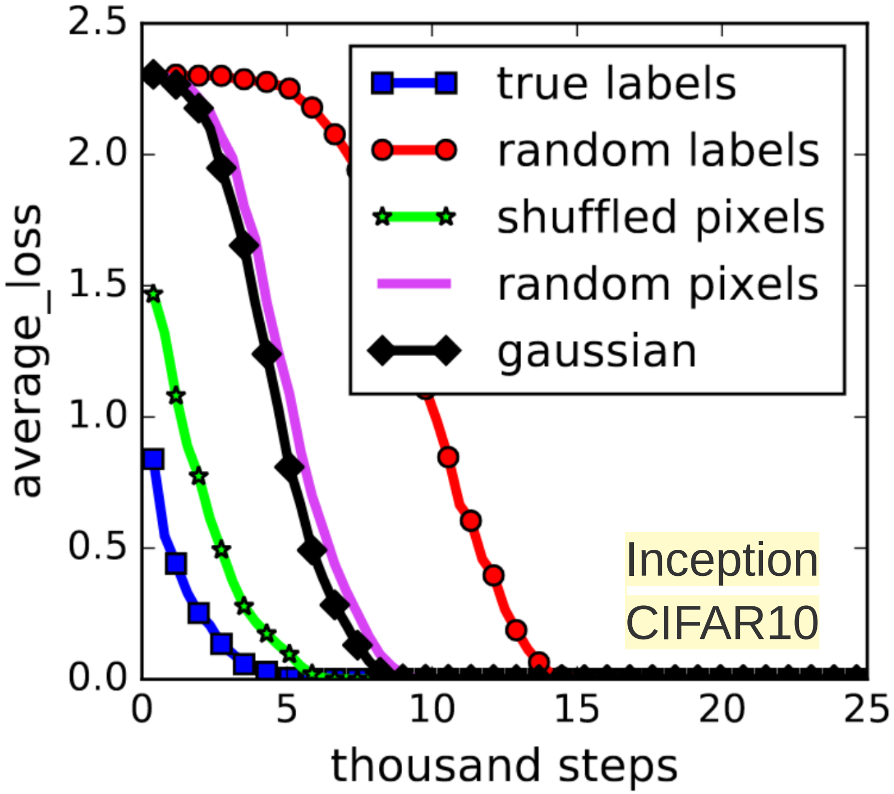
- Shuffled pixels → one permutation trans.
- Random pixels → Many permutation trans.
- Gaussian (parametric) → database mean & variance



parametric non-parametric

Learning Dynamics – Training Data

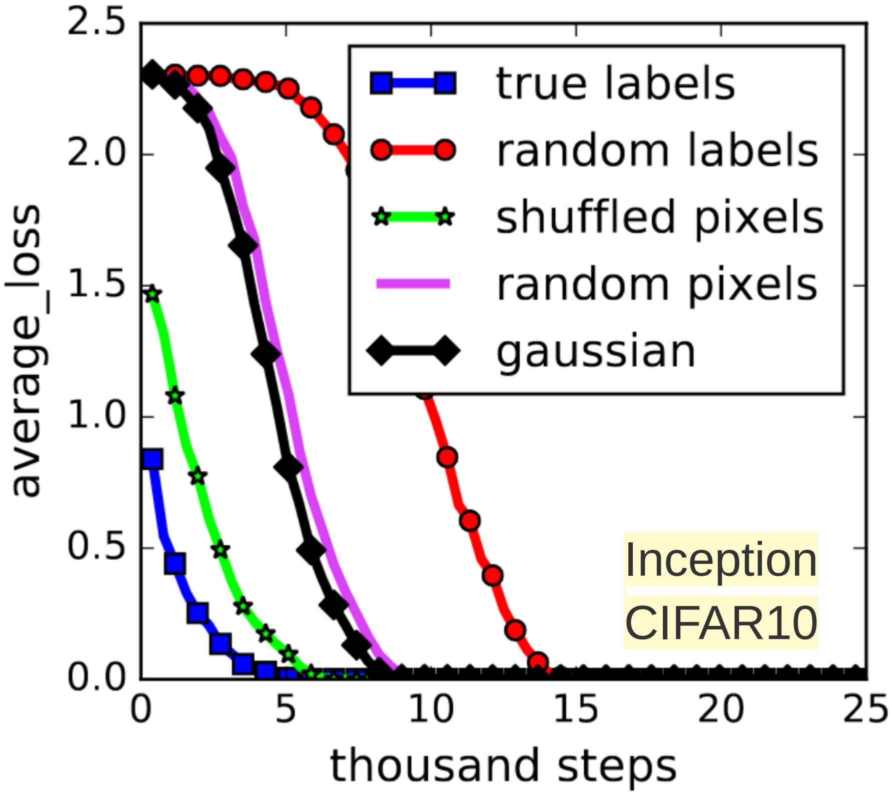
NOTE:
Hyperparameters are identical



Inception
CIFAR10

Learning Dynamics – Training Data

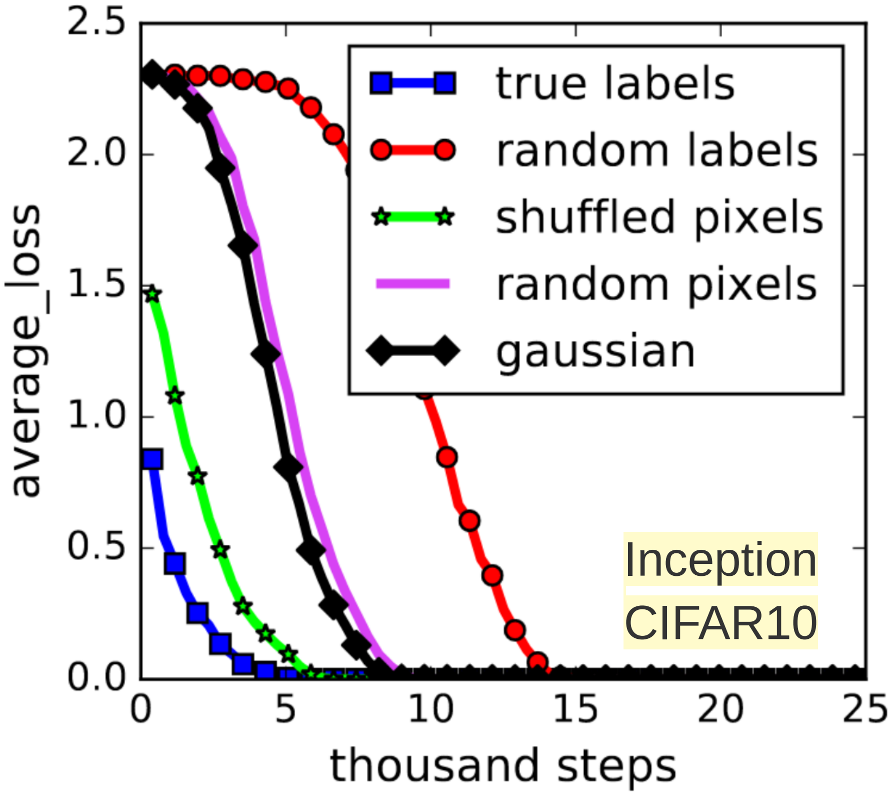
DNN shatters training data,
even with random data/labels.



Learning Dynamics – Training Data

DNN shatters training data, even with **random data/labels**.

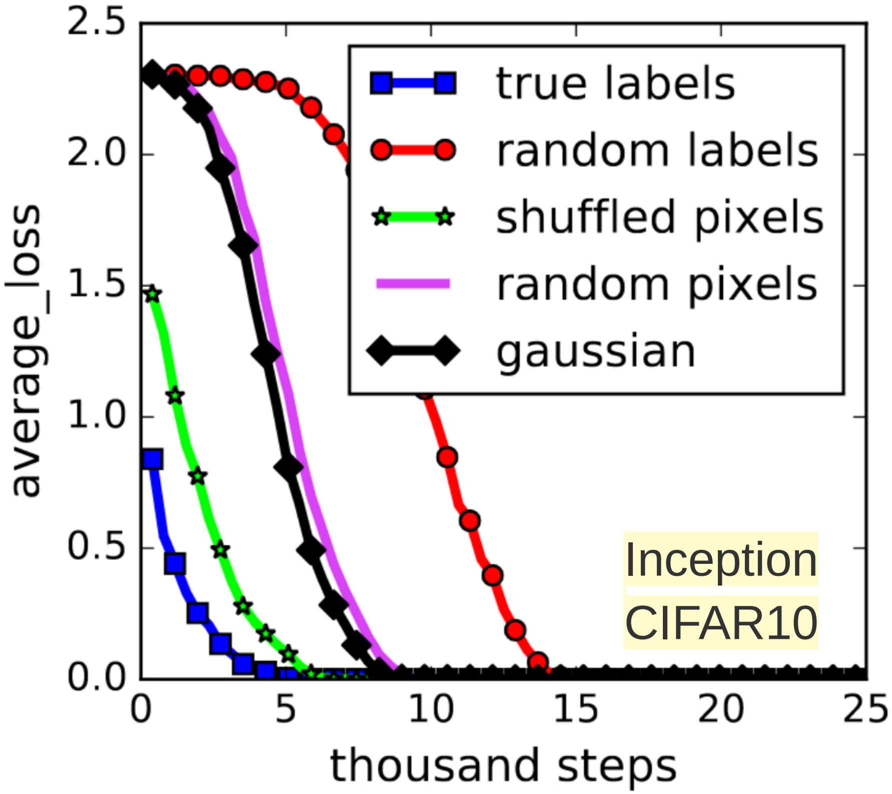
This is memorisation not learning.



Learning Dynamics – Training Data

Optimisation remains easy, even when learning is hard → Although slower, it converges

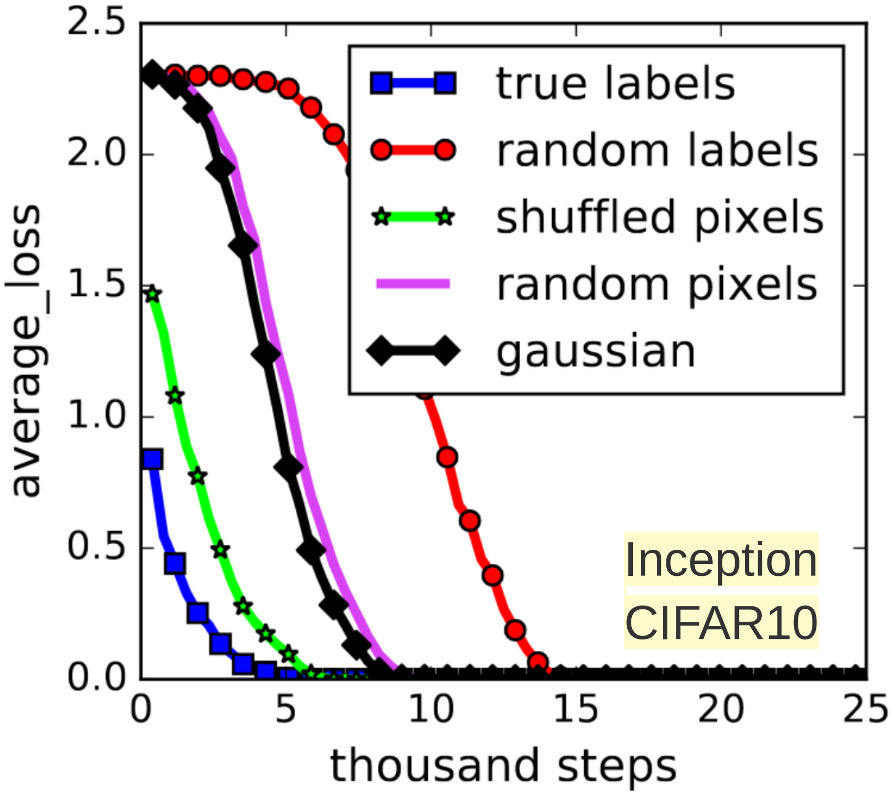
– Optimisation-Learning relationship?



Learning Dynamics – Training Data

Convergence for data randomisation happens earlier than label randomisation. Y?

- – better separation (paper)
- – randomisation level (I think)

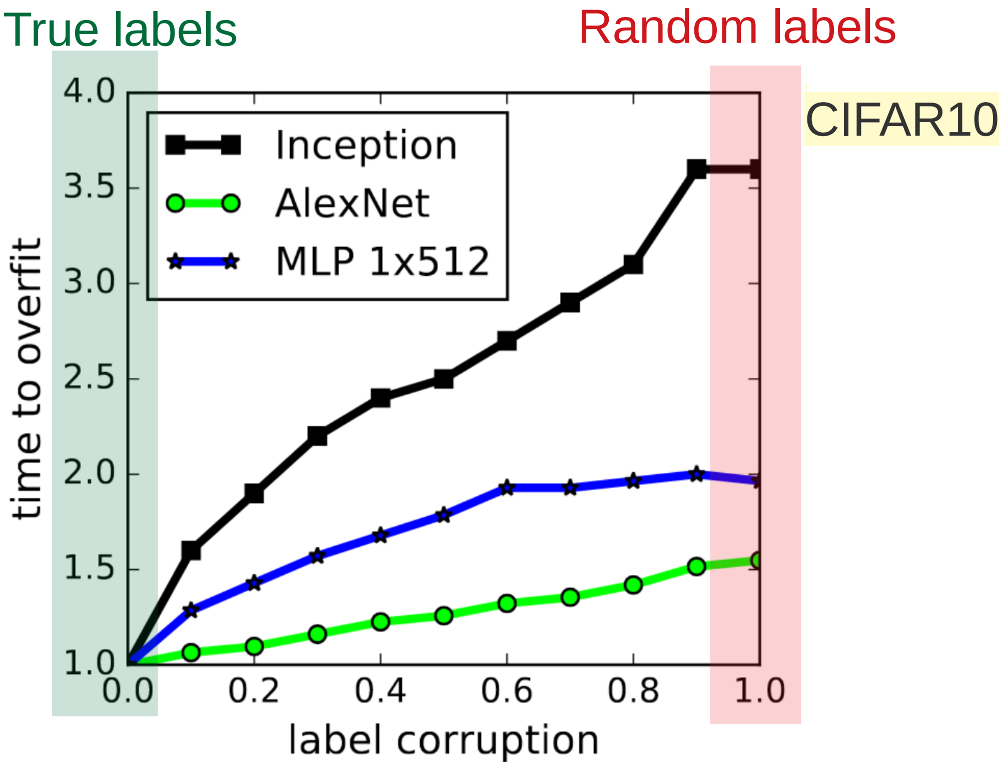


Convergence Slowdown
after Label Corruption

Label corruption

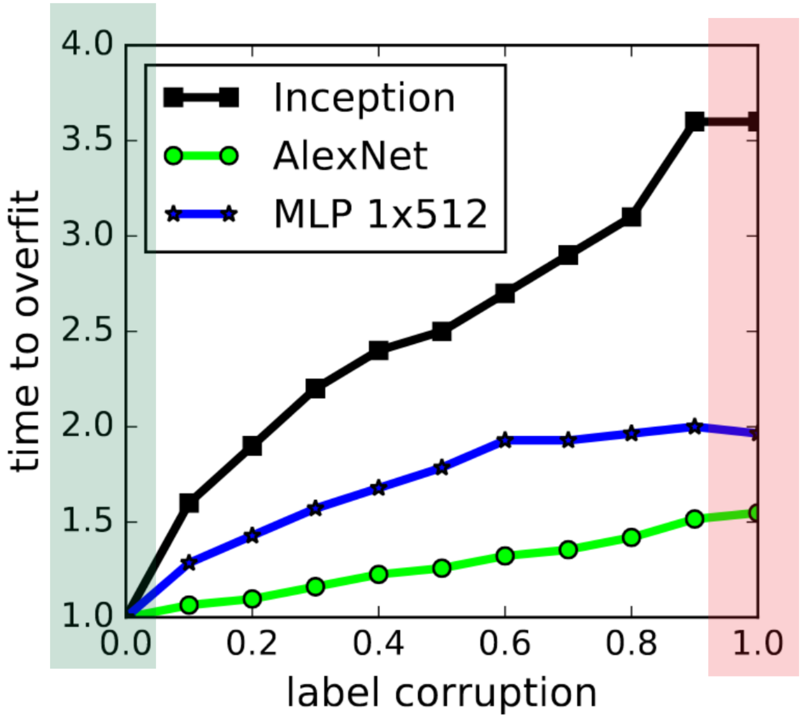
↓

slower convergence



Convergence Slowdown for
Different Label Corruption Rations

Slower convergence is proportional with **#parameters,** although **architecture** matters, too.



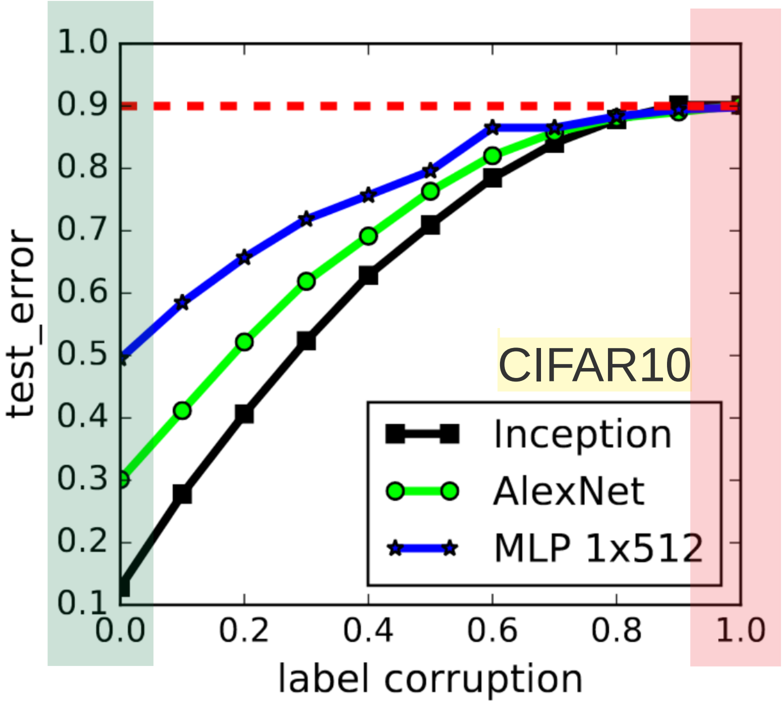
CIFAR10

Generalisation Error Growth

Architectures matters a lot!

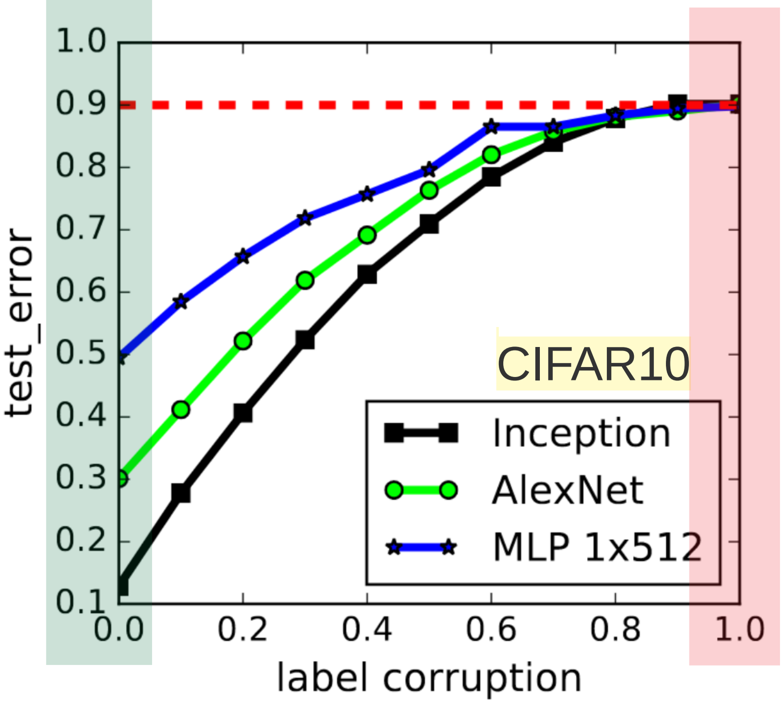
– Generalisaition performance

Inception > Alexnet > MLP



New Complexity Measures Required!

Steady increase in generalisation error by label corruption.

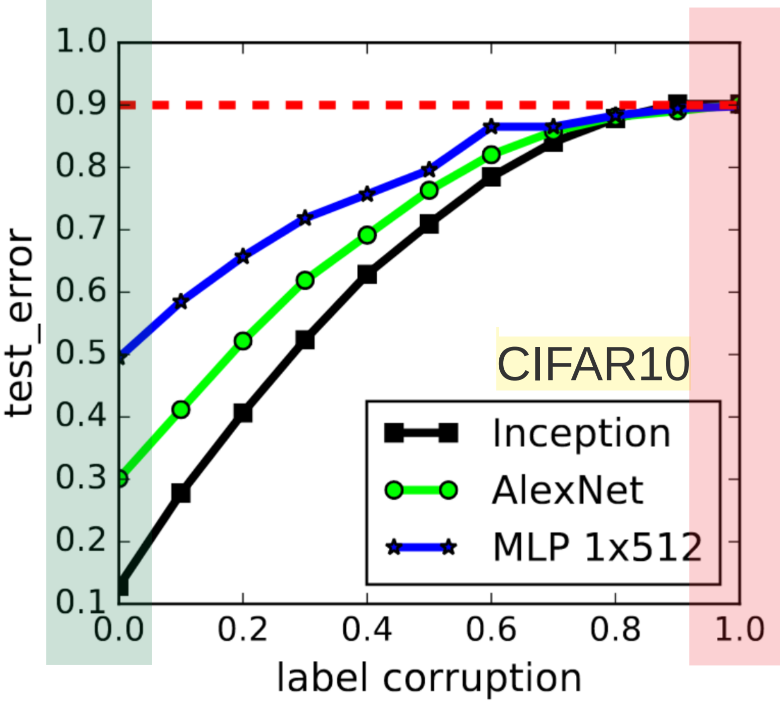


New Complexity Measures Required!

Steady increase in generalisation error by label corruption.

<u>Model capacity</u> & <u>*N*</u> are **NOT** changed **BUT** generalisation error dramatically changed!

$$P_{gen}\Big|_{E_{train}=0} \leq O(\frac{VCdim}{N})$$



Regularisation

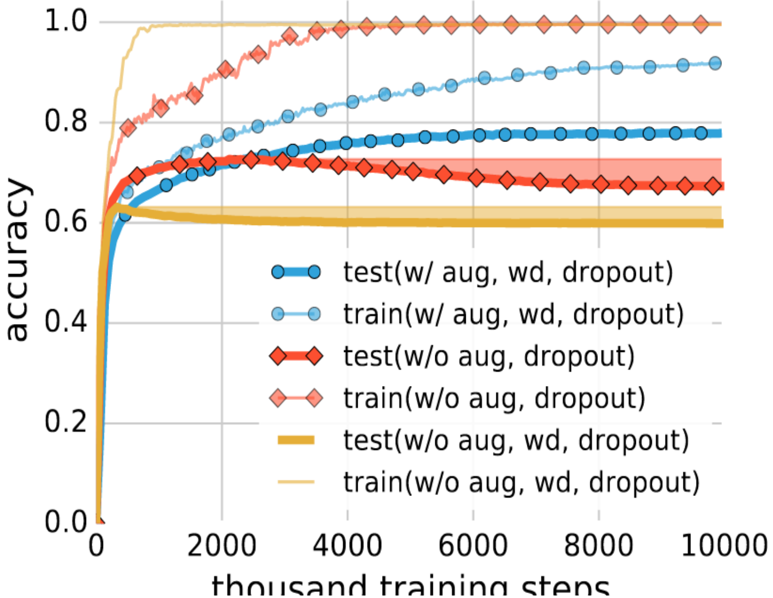
Regularisation

- Definition: A mechanism that constraints the model (hypothesis space) or empowers the data
- GOAL: Avoids fitting noise
- Effect: decreases variance, may increase the bias
- Types:
  - Explicit: Data augmentation, weight decay, drop out
  - Implicit: Early stop, batch normalisation

Explicit Regularisation Effect

Dropout
Dropout+WD
Dropout+WD+DAug

ImageNet – Inception V3



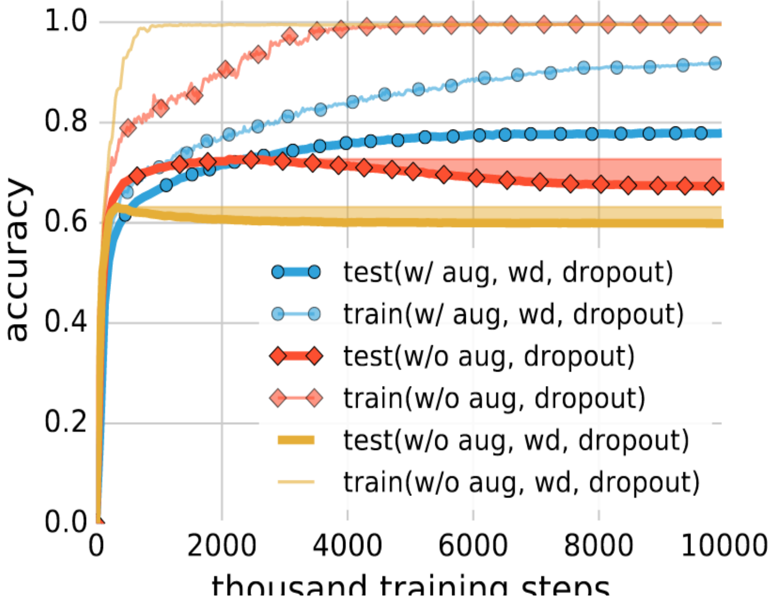
Explicit Regularisation Effect

Dropout
Dropout+WD
Dropout+WD+DAug

No remarkable generalisation improvement

– It helps but is not a game-changer

ImageNet – Inception V3

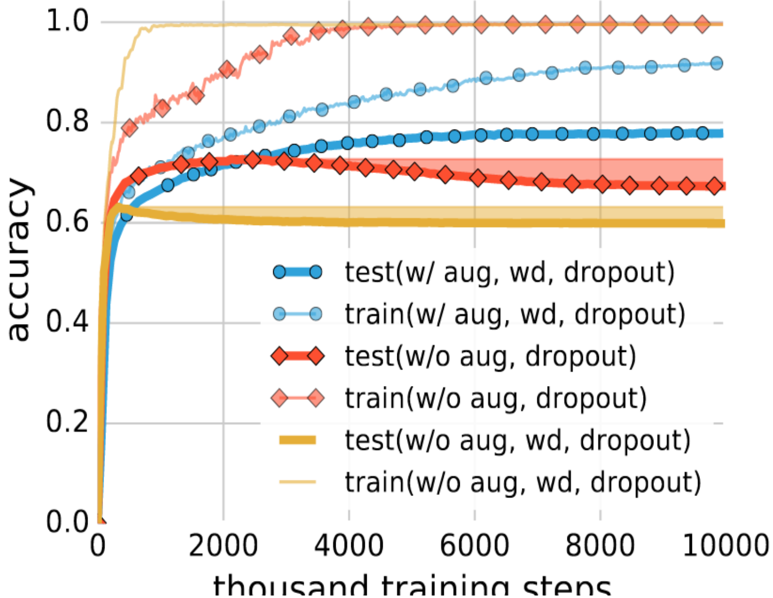


Explicit Regularisation Effect

Dropout
Dropout+WD
Dropout+WD+DAug

Dropout (alone)
- shatters the training data
- benefits from early stopping

ImageNet – Inception V3

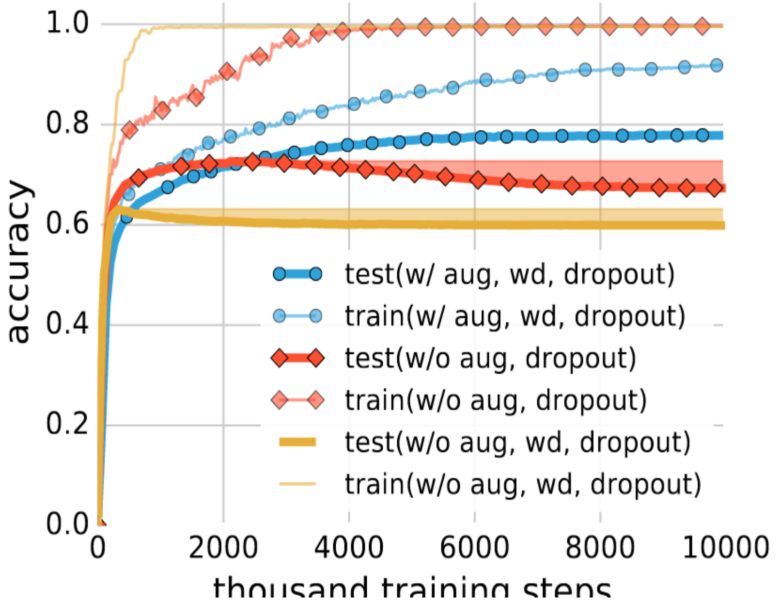


Explicit Regularisation Effect

Dropout
Dropout+WD
Dropout+WD+DAug

Dropout+WD
- shatters the training data
- benefits from early stopping
- **WD** is not necessarily useful!
  - * **Dropout+WD** worse than **Dropout**

ImageNet – Inception V3

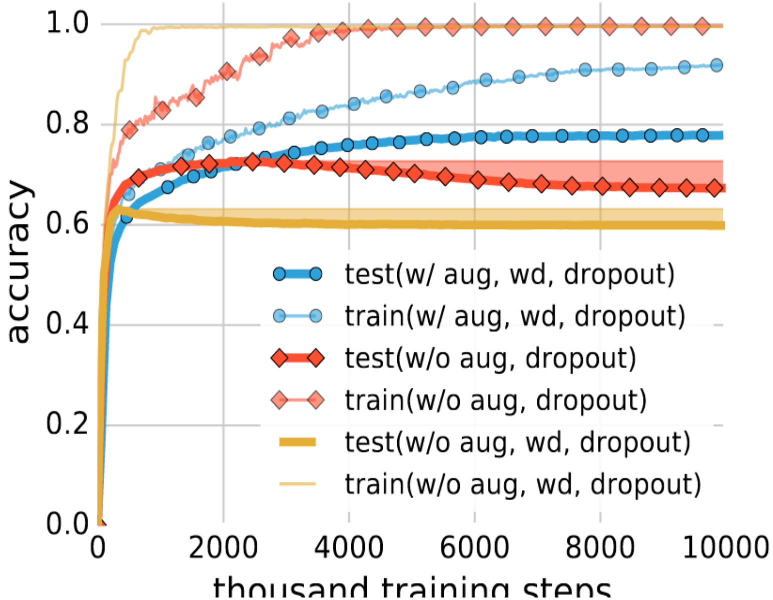


Explicit Regularisation Effect

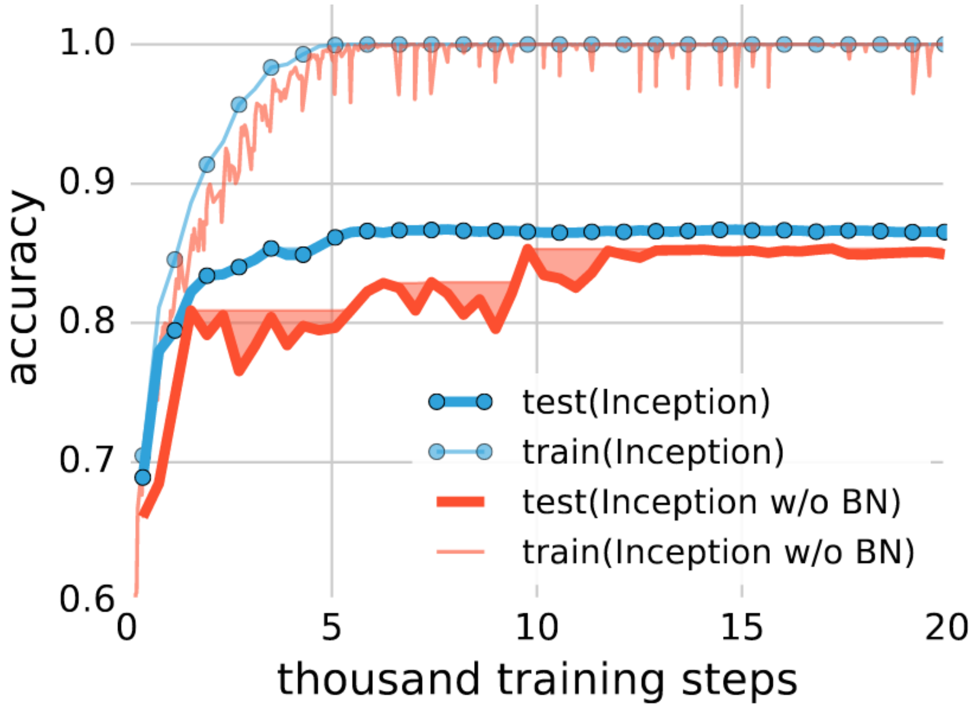
Dropout
Dropout+WD
Dropout+WD+DAug

Dropout+WD+DAug
- does not shatter training data
- early stopping is not useful
- is the best after enough iterations

ImageNet – Inception V3



Batch Normalisation (BN) Effect

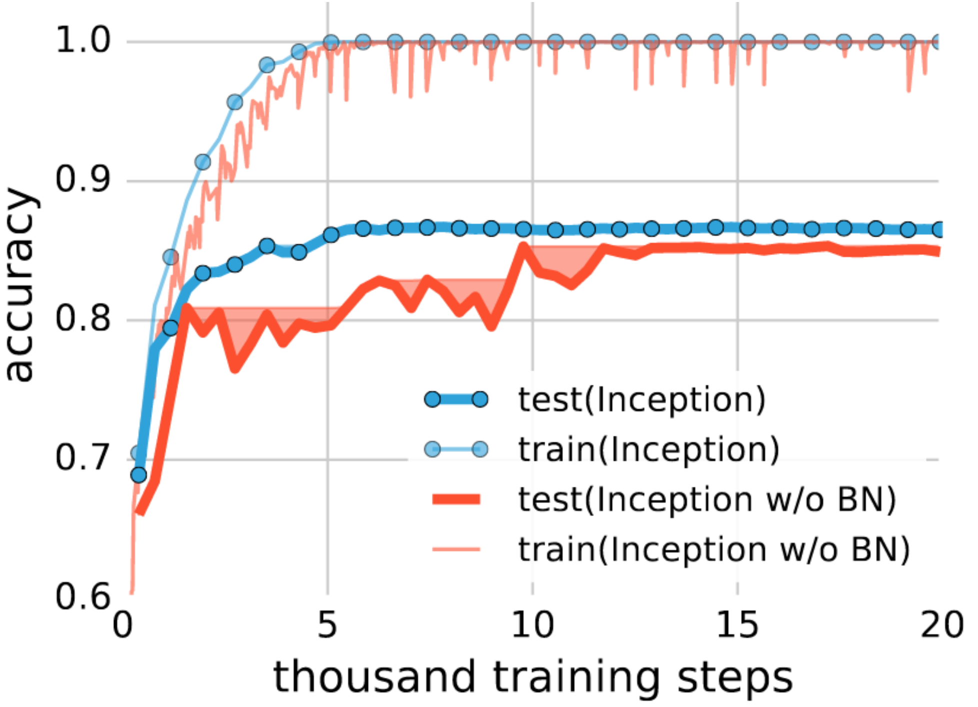


(b) Inception on CIFAR10

Batch Normalisation (BN) Effect

Makes training dynamic smoother

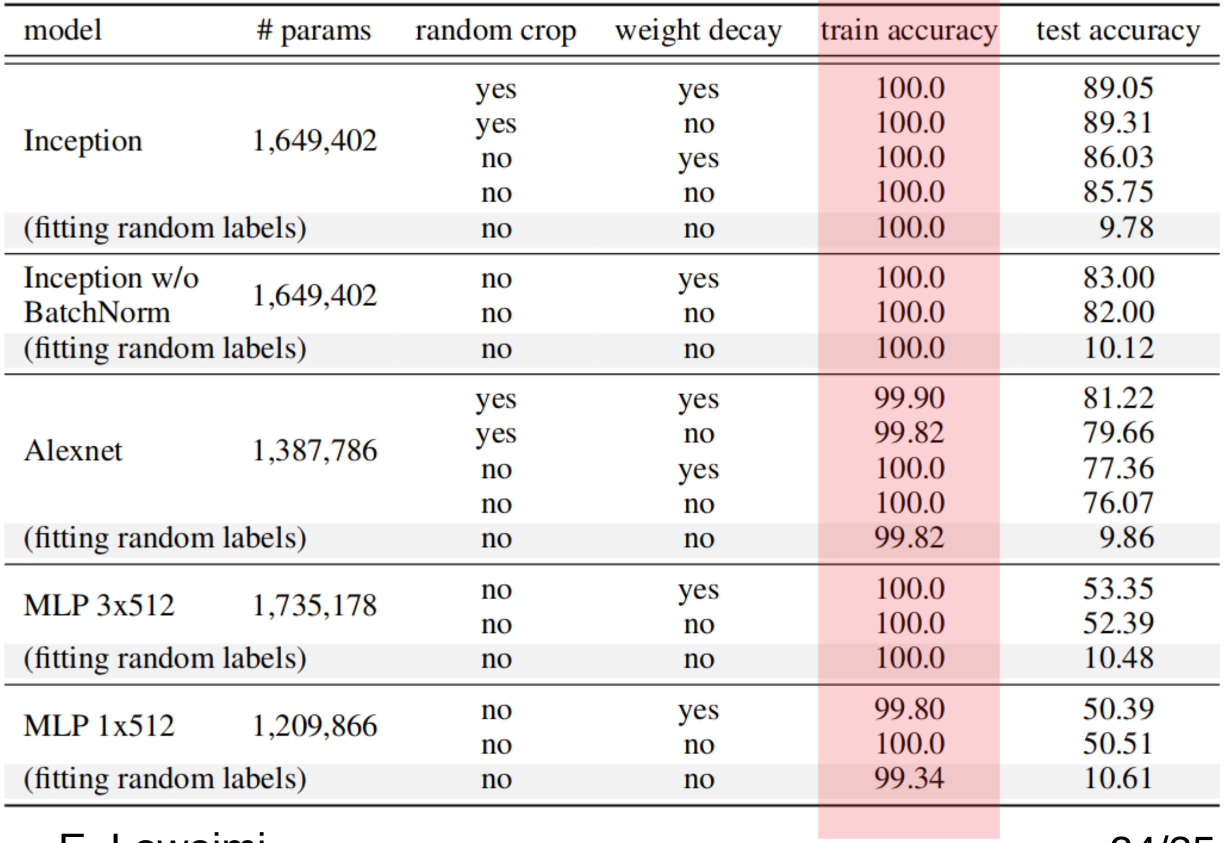
Upto 4% generalisation error reduction
[not much, after enough iterations]



(b) Inception on CIFAR10

Regularisation Effect on Accuracy

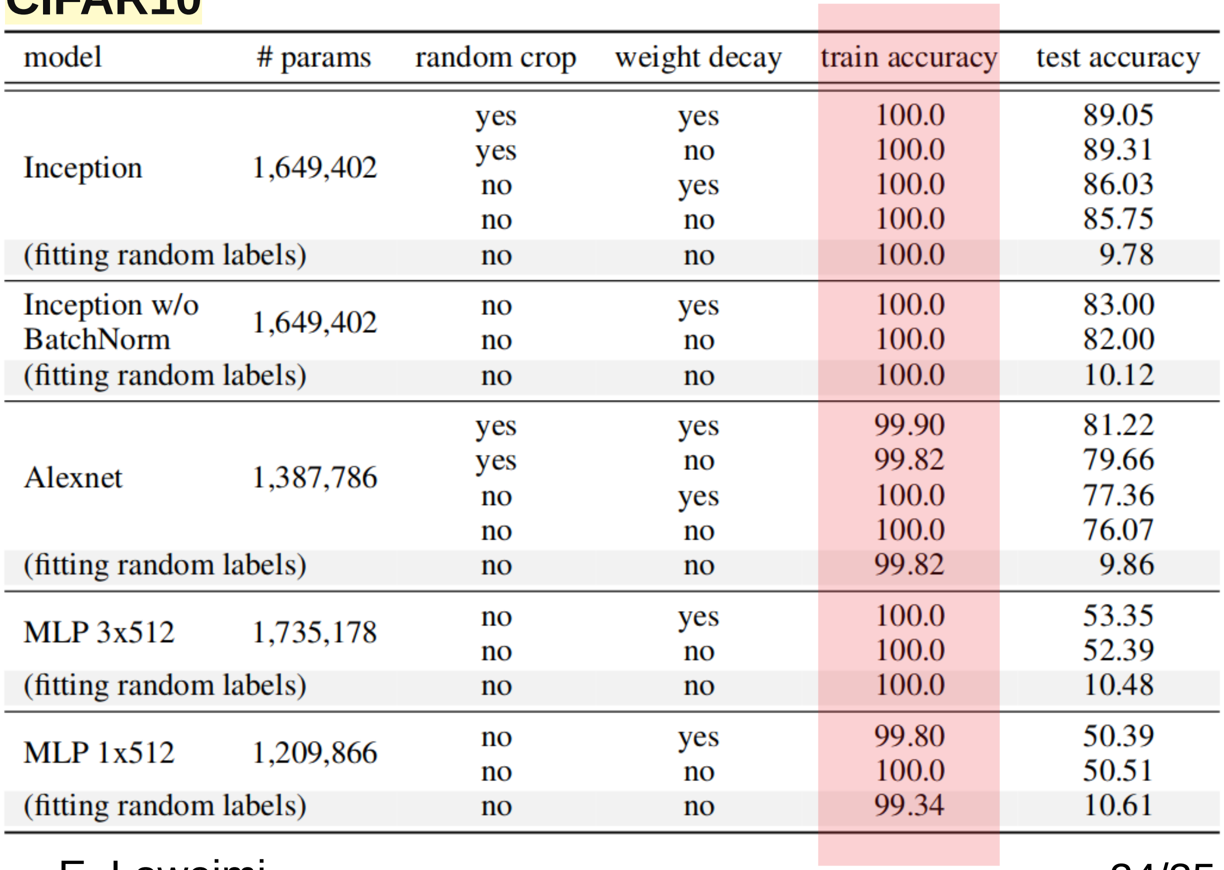
CIFAR10



model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Regularisation Effect on Accuracy

CIFAR10



model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

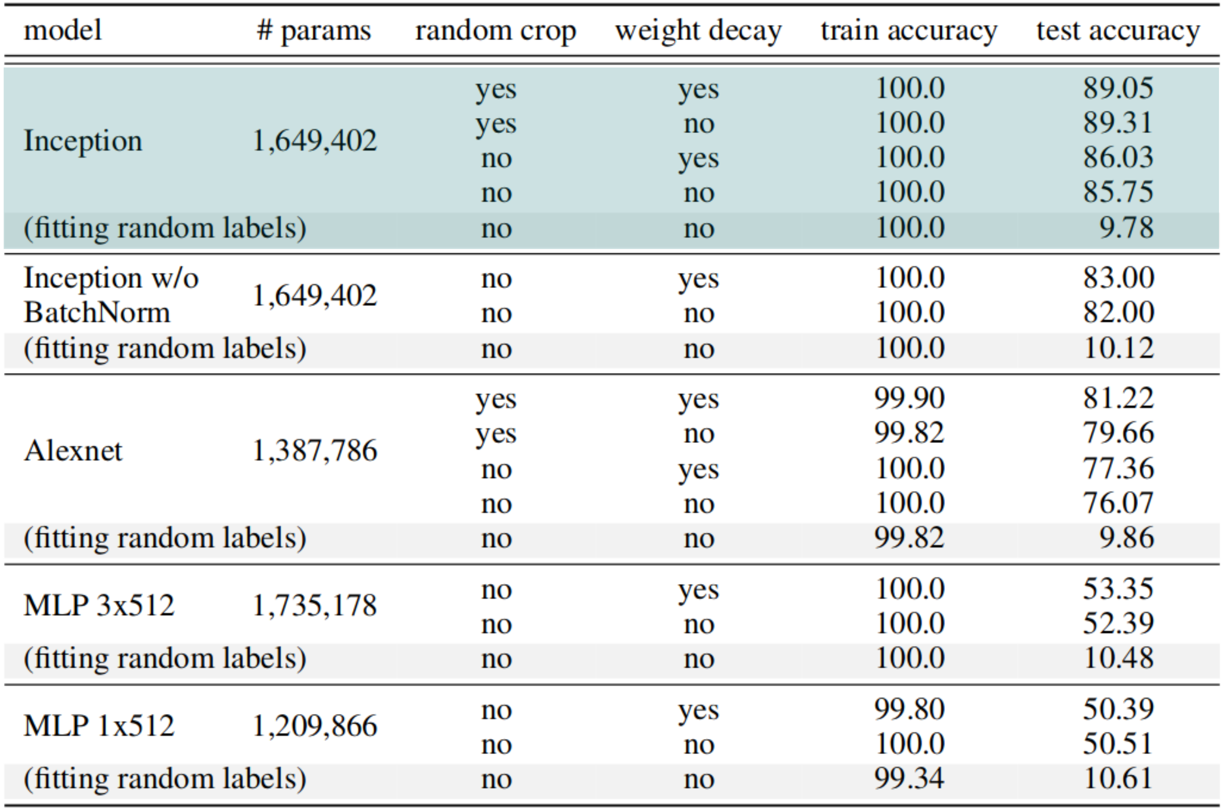
Almost all architectures **shatter** the training set (~ 100% Accuracy).

Regularisation Effect on Accuracy

Inception with BN

- No Reg. → 85.75%
- WD → +0.28
- DA → +3.56
- WD+DA → +3.30

CIFAR10



model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Regularisation Effect on Accuracy

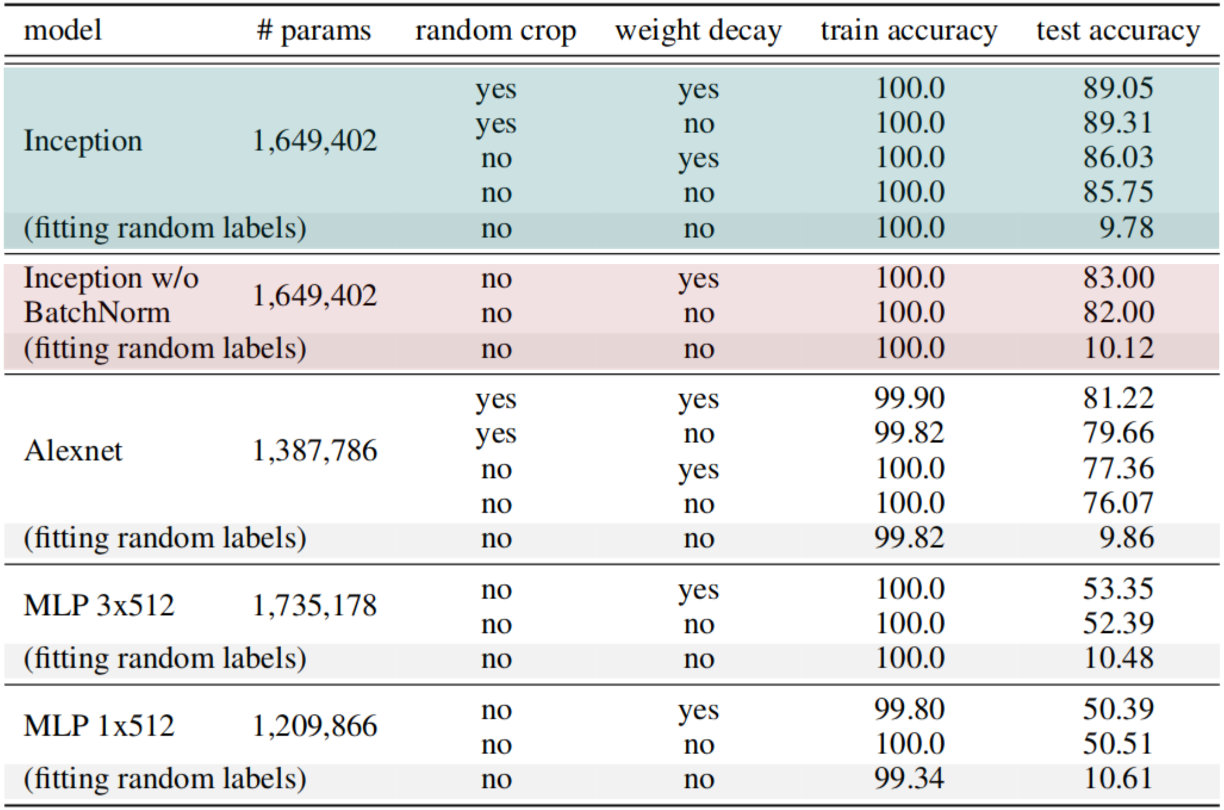
Inception with BN

- – No Reg. → 85.75%
- – WD → +0.28
- – DA → +3.56
- – WD+DA → +3.30

Inception withOUT BN

- – No Reg. → 82.0
- – WD → +1.0

CIFAR10



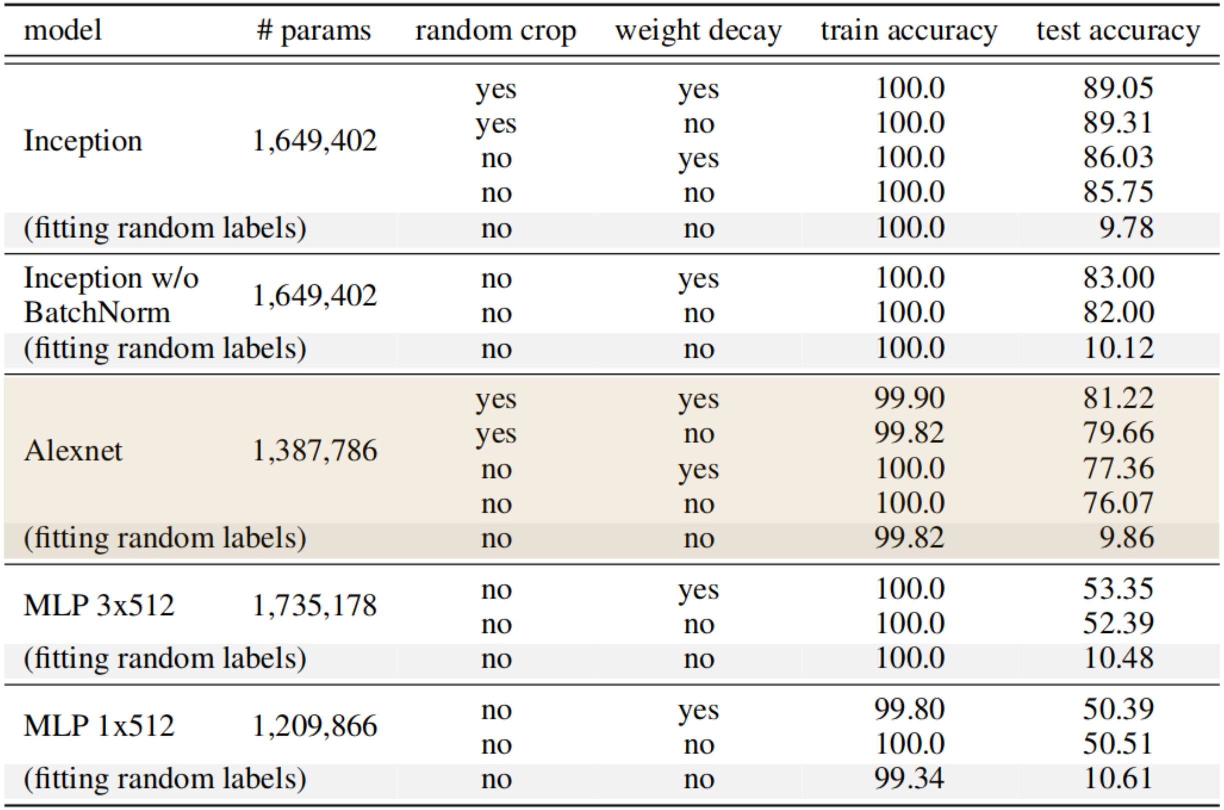
model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Regularisation Effect on Accuracy

Alexnet

- No Reg. → 76.07%
- WD → +1.29
- DA → +2.96
- WD+DA → +5.15

CIFAR10



model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Regularisation Effect on Accuracy

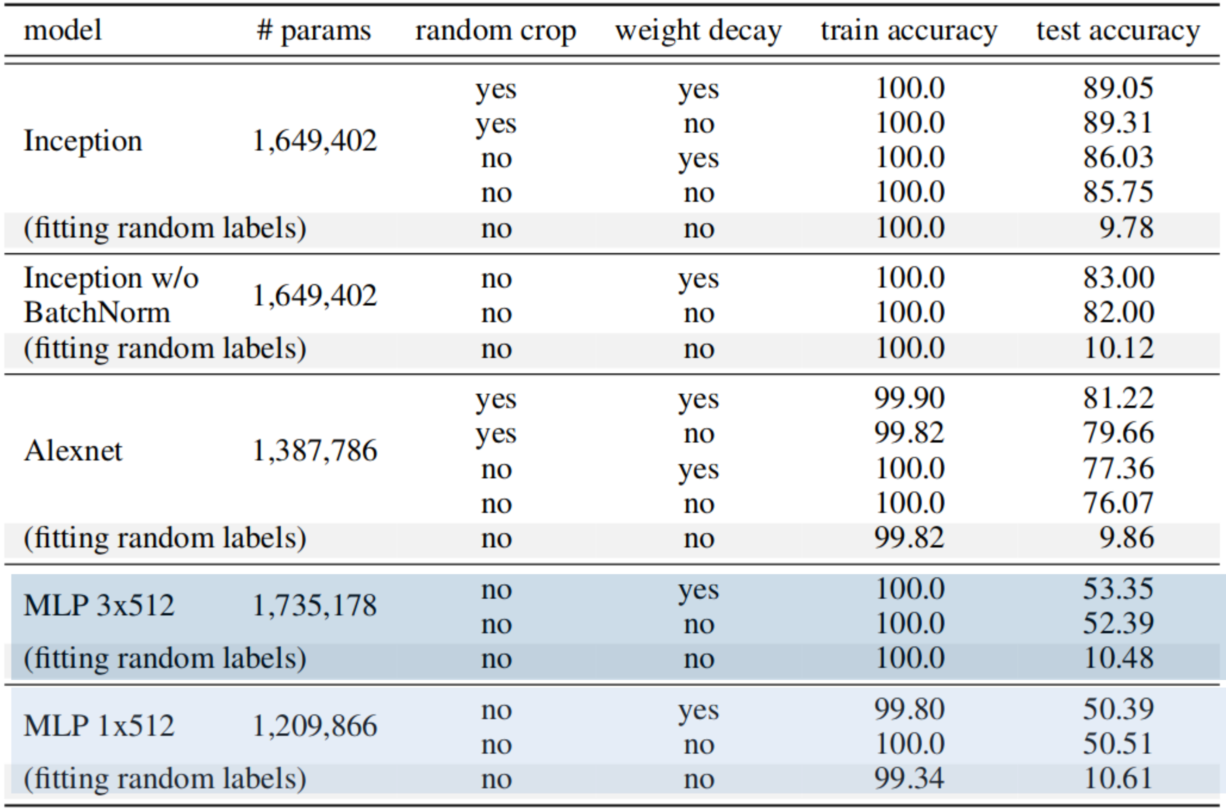
MLP 3x512

- No Reg. → 52.39%
- WD → +0.96

MLP 1x512

- No Reg. → 50.51
- WD → -0.12

CIFAR10



model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Architecture Effect

Inception with BN → 85.75

Inception withOUT BN → 82.0

Alexnet → 76.07

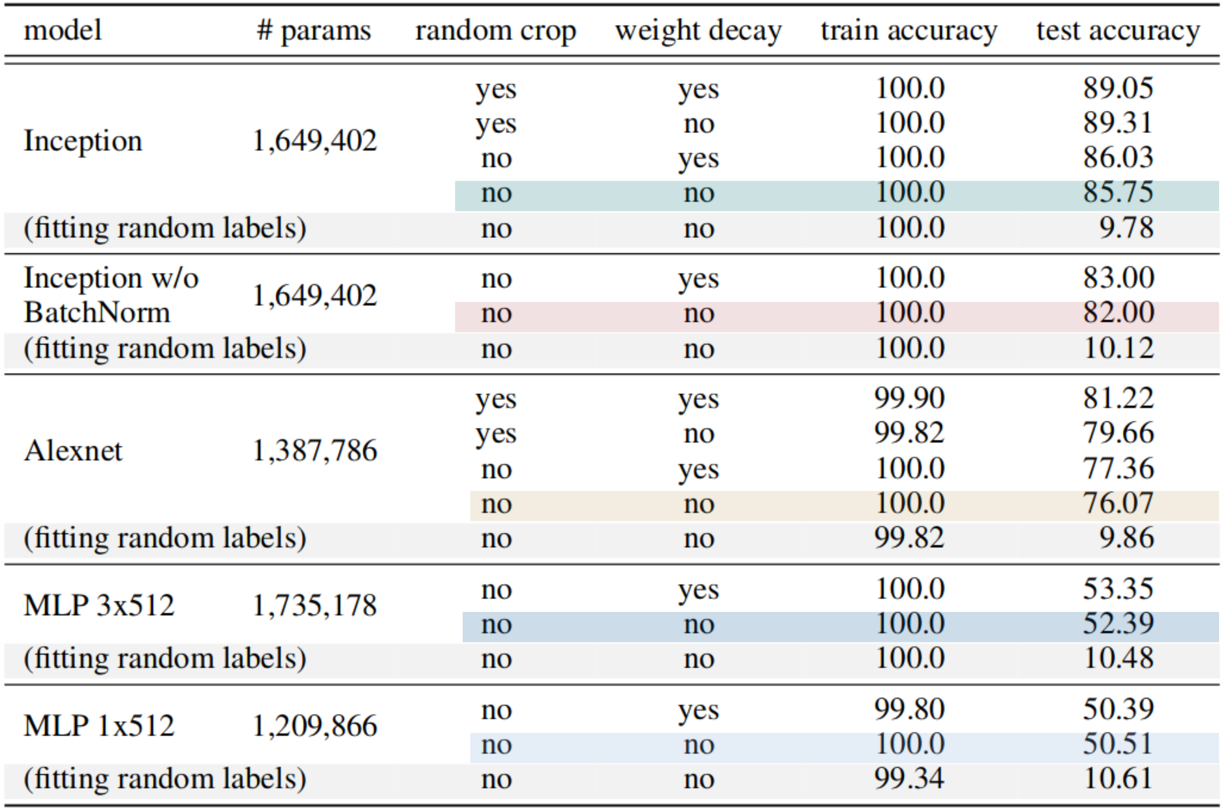
MLP 3x512 → 52.39

MLP 1x512 → 50.51

Max Performance Improvement

- By **Reg.: +3.56** (85.75 → 89.31)
- By **Arch.: +35.24** (50.51 → 85.75)

CIFAR10



model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61

Architecture Effect

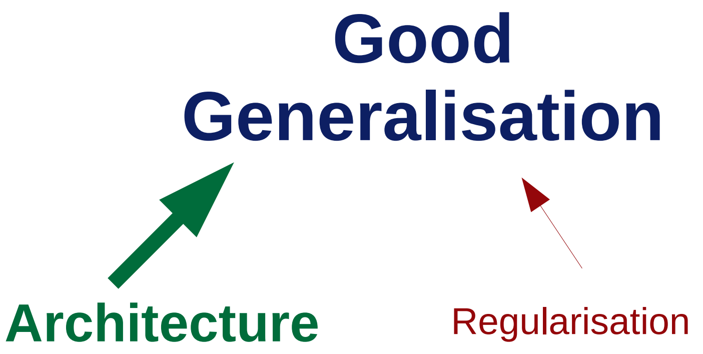
Inception with BN → 85.75

Inception withOUT BN → 82.0

Alexnet → 76.07

MLP 3x512 → 52.39

MLP 1x512 → 50.51



Good Generalisation

Architecture

Regularisation

Max Performance Improvement

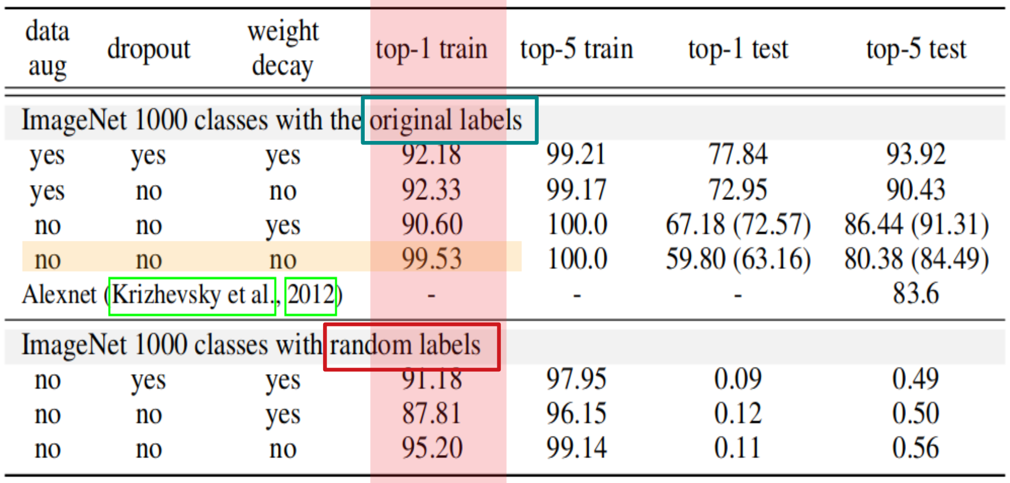
- By **Reg.: +3.56** (85.75 → 89.31)
- By **Arch.: +35.24** (50.51 → 85.75)

"… *while regularization is important, bigger gains can be achieved by simply changing the model architecture.*"

Regularisation Effect on Accuracy

Inception V3 **shatters** ImageNet when … True labels R used & regularises R off

ImageNet – Inception V3



data aug	dropout	weight decay	top-1 train	top-5 train	top-1 test	top-5 test
ImageNet 1000 classes with the original labels						
yes	yes	yes	92.18	99.21	77.84	93.92
yes	no	no	92.33	99.17	72.95	90.43
no	no	yes	90.60	100.0	67.18 (72.57)	86.44 (91.31)
no	no	no	99.53	100.0	59.80 (63.16)	80.38 (84.49)
Alexnet (Krizhevsky et al., 2012)			-	-	-	83.6
ImageNet 1000 classes with random labels						
no	yes	yes	91.18	97.95	0.09	0.49
no	no	yes	87.81	96.15	0.12	0.50
no	no	no	95.20	99.14	0.11	0.56

Accuracy – ImageNet – Inception V3

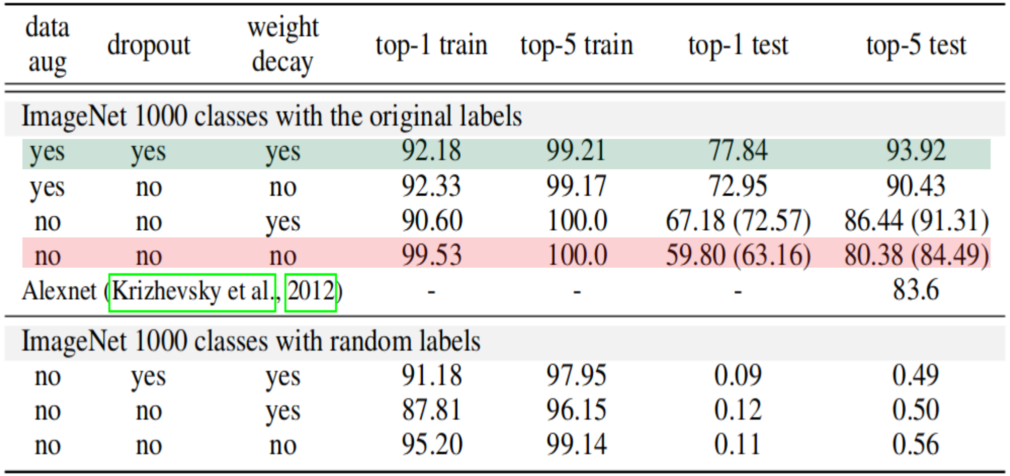
Top-1

- – No Reg → 59.80
- – No Reg & ES → +3.36 (63.16)

- – WD →+7.38
- – WD & ES → +12.77(ES→+5.39)

- – DA→+12.15

- – DA+WD+DO→+18.04%



data aug	dropout	weight decay	top-1 train	top-5 train	top-1 test	top-5 test
ImageNet 1000 classes with the original labels						
yes	yes	yes	92.18	99.21	77.84	93.92
yes	no	no	92.33	99.17	72.95	90.43
no	no	yes	90.60	100.0	67.18 (72.57)	86.44 (91.31)
no	no	no	99.53	100.0	59.80 (63.16)	80.38 (84.49)
Alexnet (Krizhevsky et al., 2012)			-	-	-	83.6
ImageNet 1000 classes with random labels						
no	yes	yes	91.18	97.95	0.09	0.49
no	no	yes	87.81	96.15	0.12	0.50
no	no	no	95.20	99.14	0.11	0.56

Accuracy – ImageNet – Inception V3

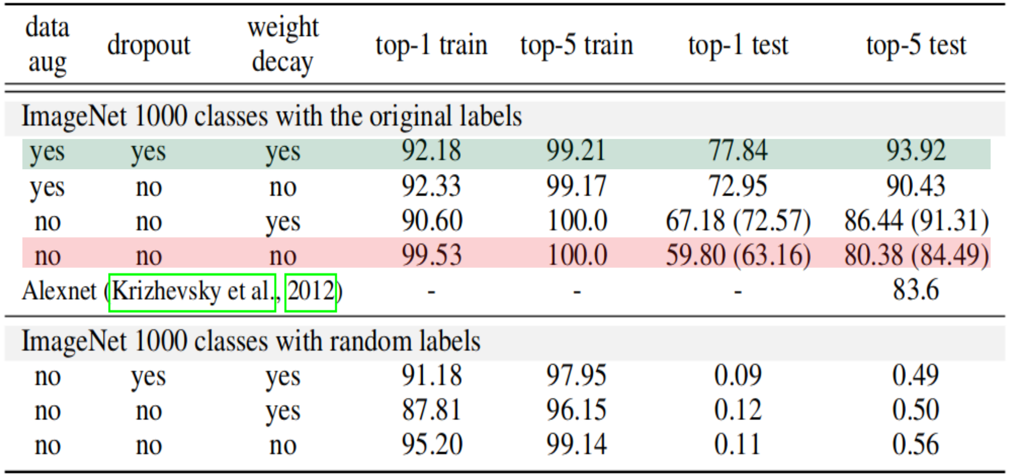
Top-5

– No Reg → 80.38
– No Reg & ES → +4.11 (84.49)

– WD →+6.06
– WD & ES → +10.93(ES→+4.87)

– DA→+10.05

– DA+WD+DO→+13.54%

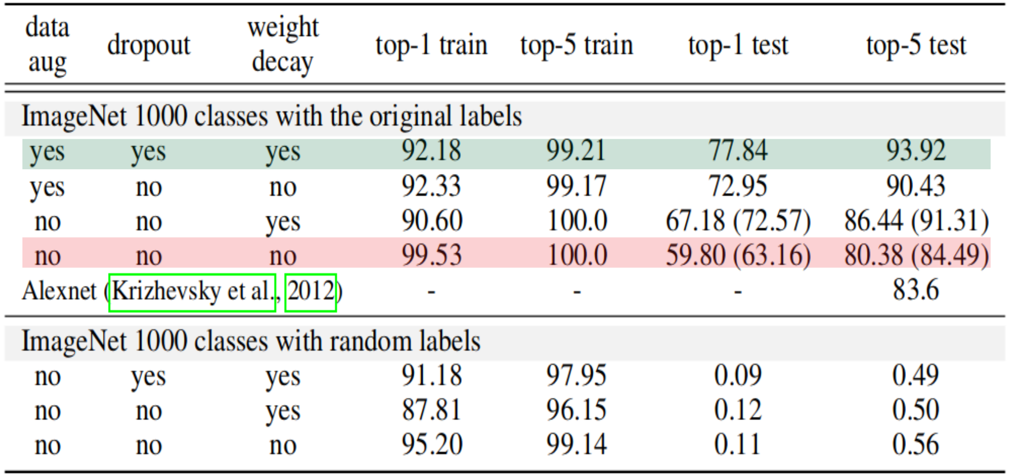


data aug	dropout	weight decay	top-1 train	top-5 train	top-1 test	top-5 test
ImageNet 1000 classes with the original labels						
yes	yes	yes	92.18	99.21	77.84	93.92
yes	no	no	92.33	99.17	72.95	90.43
no	no	yes	90.60	100.0	67.18 (72.57)	86.44 (91.31)
no	no	no	99.53	100.0	59.80 (63.16)	80.38 (84.49)
Alexnet (Krizhevsky et al., 2012)			-	-	-	83.6
ImageNet 1000 classes with random labels						
no	yes	yes	91.18	97.95	0.09	0.49
no	no	yes	87.81	96.15	0.12	0.50
no	no	no	95.20	99.14	0.11	0.56

Accuracy – ImageNet – Inception V3

Top-5

- Alexnet (Challenge Winner) → 83.6
- Inception V3
  - No Reg. → 80.38
  - ES → 84.49
  - WD → 86.44
  - WD & ES → 91.31
  - DA → 90.43
  - DA+DO+WD → 93.2



data aug	dropout	weight decay	top-1 train	top-5 train	top-1 test	top-5 test
ImageNet 1000 classes with the original labels						
yes	yes	yes	92.18	99.21	77.84	93.92
yes	no	no	92.33	99.17	72.95	90.43
no	no	yes	90.60	100.0	67.18 (72.57)	86.44 (91.31)
no	no	no	99.53	100.0	59.80 (63.16)	80.38 (84.49)
Alexnet (Krizhevsky et al., 2012)			-	-	-	83.6
ImageNet 1000 classes with random labels						
no	yes	yes	91.18	97.95	0.09	0.49
no	no	yes	87.81	96.15	0.12	0.50
no	no	no	95.20	99.14	0.11	0.56

Accuracy – ImageNet – Inception V3

Top-5

– Alexnet (Challenge Winner) → 83.6

– Inception V3
  – No Reg. → 80.38
  – ES → 84.49
  – WD → 86.44
  – WD & ES → 91.31
  – DA → 90.43
  – DA+DO+WD → 93.2

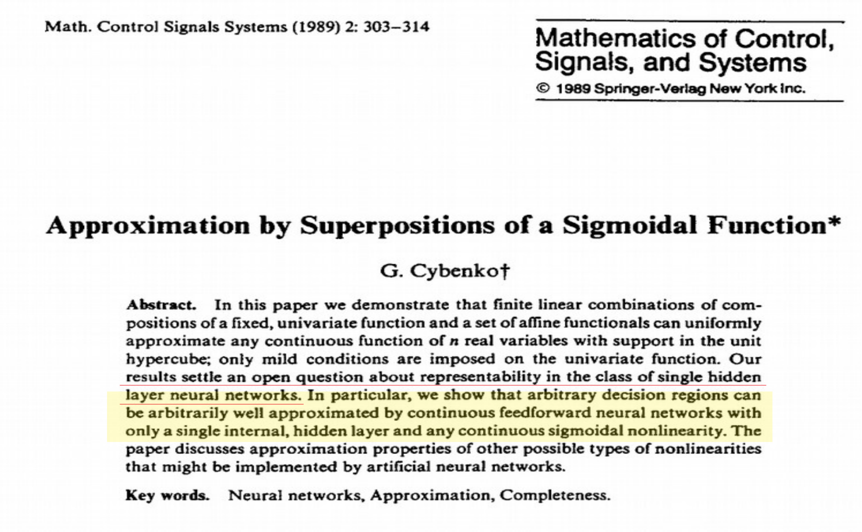
Win the challenges by spending time on ...

1. ARCHITECTURE, rather than REGULARISATION!
2. Data augmentation

Finite Sample Expressivity

Universal Approximation Theorem (UAT)

- *A MLP with one hidden layer can approximate any continuous function up to an arbitrary constant*
  - Proved by *Cybenko* for Sigmoidal Activation in 1989



Math. Control Signals Systems (1989) 2: 303–314

Mathematics of Control, Signals, and Systems
© 1989 Springer-Verlag New York Inc.

Approximation by Superpositions of a Sigmoidal Function*

G. Cybenko†

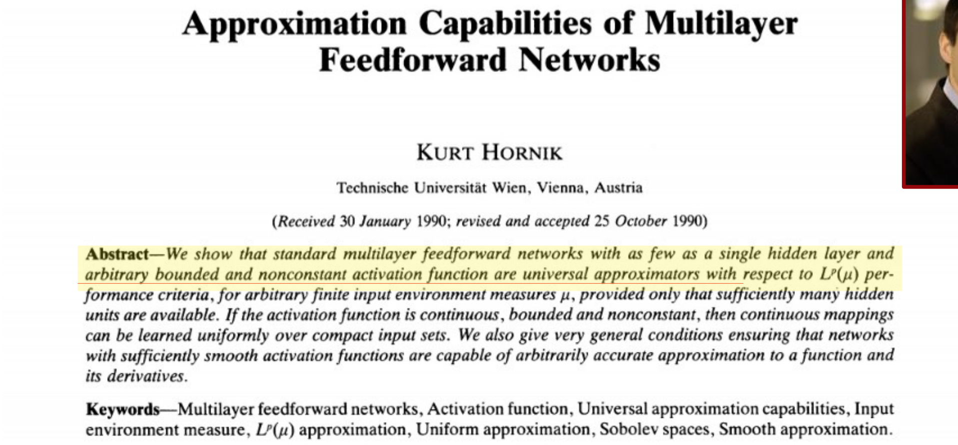
Abstract. In this paper we demonstrate that finite linear combinations of compositions of a fixed, univariate function and a set of affine functionals can uniformly approximate any continuous function of *n* real variables with support in the unit hypercube; only mild conditions are imposed on the univariate function. Our results settle an open question about representability in the class of single hidden layer neural networks. In particular, we show that arbitrary decision regions can be arbitrarily well approximated by continuous feedforward neural networks with only a single internal, hidden layer and any continuous sigmoidal nonlinearity. The paper discusses approximation properties of other possible types of nonlinearities that might be implemented by artificial neural networks.

Key words. Neural networks, Approximation, Completeness.

Universal Approximation Theorem (UAT)

- *A MLP with one hidden layer can approximate any continuous function up to an arbitrary constant*
    - Proved by *Hornik* for any bounded & non-constant function in 1991

Neural Networks, 4(2), 251–257, 1991



Approximation Capabilities of Multilayer Feedforward Networks

Kurt Hornik

Technische Universität Wien, Vienna, Austria

(*Received* 30 *January* 1990; *revised and accepted* 25 *October* 1990)

Abstract—*We show that standard multilayer feedforward networks with as few as a single hidden layer and arbitrary bounded and nonconstant activation function are universal approximators with respect to $L^p(\mu)$ performance criteria, for arbitrary finite input environment measures μ, provided only that sufficiently many hidden units are available. If the activation function is continuous, bounded and nonconstant, then continuous mappings can be learned uniformly over compact input sets. We also give very general conditions ensuring that networks with sufficiently smooth activation functions are capable of arbitrarily accurate approximation to a function and its derivatives.*

Keywords—Multilayer feedforward networks, Activation function, Universal approximation capabilities, Input environment measure, $L^p(\mu)$ approximation, Uniform approximation, Sobolev spaces, Smooth approximation.

Universal Approximation Theorem (UAT)

"… *It is not the specific choice of the activation function, but rather the MLP architectures which give the NNs the potential of being universal function approximator*."

wikipedia

UAT – Some Points

- Approximation ≡ Fitting
  - No distinction between learning or memorising

UAT – Some Points

- Approximation ≡ Fitting
  - No distinction between learning or memorising
- Silent about algorithmic learnability of the weights
  - It’s about existence, NOT how to learn

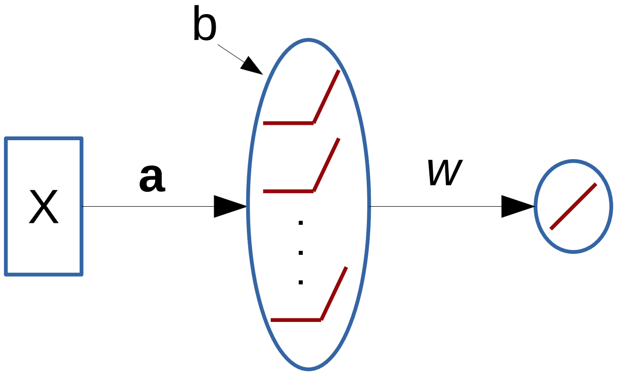
UAT – Some Points

- Approximation ≡ Fitting
  - No distinction between learning or memorising
- Silent about algorithmic learnability of the weights
  - It’s about existence, NOT how to learn
- Defined on the *population* level
  - What about the “sample” level?

UAT@Finite-Sample Level

- **Theorem.** *There exists a two-layer NN with ReLU activation and 2n+d weights that can represent any function on a sample of size n in d dimensions.*

$$C(x) = \sum_{i=1}^{n} w_i \phi(x; a, b) = \sum_{i=1}^{n} w_i \ ReLU\{a^T x - b_i\}$$



UAT@Finite-Sample Level

- **Theorem.** *There exists a two-layer NN with ReLU activation and 2n+d weights that can represent any function on a sample of size n in d dimensions.*

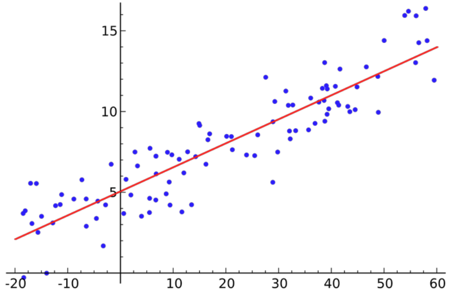
Too flexible → overfitting
Any reason to generalise well?

Appeal to Linear Systems

Overdetermined Linear Systems

$$y = Xw, \quad X \in \mathbb{R}^{n\times d}$$

- Known > Unknown, n > d≡#parameters
  - No solution
  - Least Square Error (LSE)

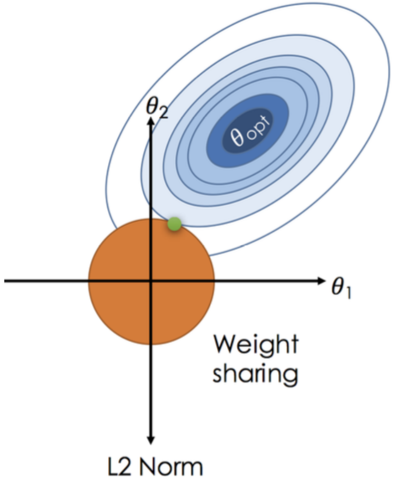


$$\min_{w} \|Xw - y\|_2^2 \longrightarrow w = (\overset{\text{Correlation matrix}}{\underset{\text{d x d}}{\boxed{X^T X}}})^{-1} X^T y$$

Underdetermined Linear Systems

$$y = Xw, \quad X \in \mathbb{R}^{n \times d}$$

- Over-parametrised, n < d≡#parameters
  - Infinite solutions when X is full-rank
  - Minimum L$_2$-norm solution



$$\min_{w} \quad \|w\|_2^2 \qquad s.t. \quad y = Xw \quad \longrightarrow \quad w = X^T(\underbrace{\boxed{XX^T}}_{\text{n x n}})^{-1}y$$

Gram (Kernel) matrix

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n\times d} \qquad\qquad E = e^T e = \|Xw - y\|_2^2$$

$$w_d^{(t+1)} = w_d^{(t)} - \eta \nabla_{w_d} E = w_d^{(t)} - \eta e^{(t)} x_d^{(t)}$$

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n \times d} \qquad\qquad E = e^T e = \|Xw - y\|_2^2$$

$$w_d^{(t+1)} = w_d^{(t)} - \eta \nabla_{w_d} E = w_d^{(t)} - \eta e^{(t)} x_d^{(t)}$$

$$w^{(t+1)} \Big|_{w^{(0)}=0} = X^T \alpha$$

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n\times d}$$

$$E = e^T e = \|Xw - y\|_2^2$$

$$w_d^{(t+1)} = w_d^{(t)} - \eta \nabla_{w_d} E = w_d^{(t)} - \eta e^{(t)} x_d^{(t)}$$

$$w^{(t+1)}\Big|_{w^{(0)}=0} = X^T \alpha \longleftarrow$$

Weights lie in the span of data points

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n\times d}$$

$$E = e^T e = \|Xw - y\|_2^2$$

$$w^{(t+1)}\Big|_{w^{(0)}=0} = X^T\alpha \quad \longrightarrow \quad \begin{aligned} y &= Xw^{(t)} \\ &= XX^T\alpha \end{aligned}$$

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n\times d}$$

$$E = e^T e = \|Xw - y\|_2^2$$

when t → ∞ equality holds!

$$w^{(t+1)}\Big|_{w^{(0)}=0} = X^T\alpha \longrightarrow \begin{aligned} y &= Xw^{(t\to\infty)} \\ &= XX^T\alpha \end{aligned}$$

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n \times d} \qquad\qquad E = e^T e = \|Xw - y\|_2^2$$

$$y = \overset{\text{square}}{\boxed{XX^T}}\alpha \longrightarrow \alpha = (XX^T)^{-1}y \longrightarrow w \overset{t\to\infty}{=} X^T(XX^T)^{-1}y$$

Unique solution
for α

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n \times d}$$

$$E = e^T e = \|Xw - y\|_2^2$$

$$y = \boxed{XX^T}\alpha \longrightarrow \alpha = (XX^T)^{-1}y \longrightarrow \boxed{w \overset{t \to \infty}{=} X^T(XX^T)^{-1}y}$$

Unique solution for *α*

– SGD solution ≡ min L_2-norm solution for underdetermined linear system

SGD Solution for a Linear System

$$y = Xw, \quad X \in \mathbb{R}^{n \times d} \qquad\qquad E = e^T e = \|Xw - y\|_2^2$$

$$y = \boxed{XX^T}\alpha \longrightarrow \alpha = (XX^T)^{-1}y \longrightarrow \boxed{w \overset{t\to\infty}{=} X^T(XX^T)^{-1}y}$$

Unique solution
for *α*

– SGD solution ≡ min L$_2$-norm solution for underdetermined linear system
===>>> SGD *implicitly* does some regularisation

SGD Implicit Regularisation

$$w_t \xrightarrow{t\to\infty} X^T(\boxed{XX^T})^{-1}y$$

Fairly good generalisation, corroborates SGD performs some implicit regularisation.

Dataset	Preprocessing (Kernelise)	Test Error
MNIST	None	**1.2%**
	Gabor filters	**0.6%**
CIFAR-10	None	46%
	Random ConvNet	17%

SGD Implicit Regularisation – Caveat

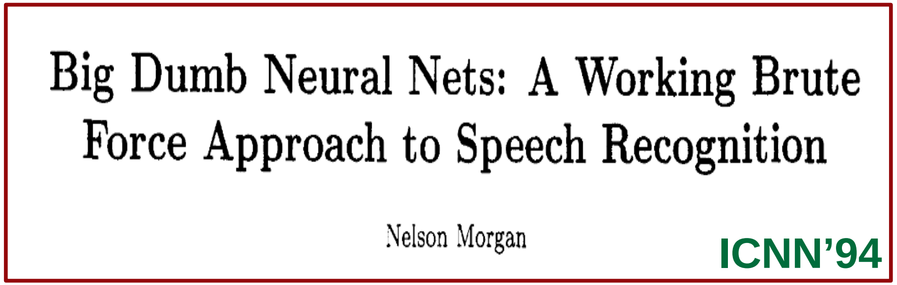
$$w_t \xrightarrow{t\to\infty} X^T(XX^T)^{-1}y$$

Dataset	Preprocessing (Kernelise)	Test Error	L_2-norm
MNIST	None	**1.2%**	**220**
	Gabor filters	**0.6%**	**390**
CIFAR-10	None	46%	-
	Random ConvNet	17%	-

UNFORTUNATELY,
Minimum L_2-norm is not predictive of generalisation performance.

Do we need the global optimum for a better generalisation?

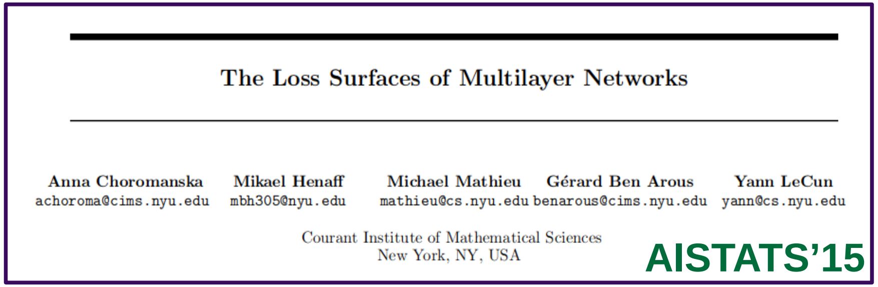
Do we need the global optimum for a better generalisation?



Big Dumb Neural Nets: A Working Brute Force Approach to Speech Recognition

Nelson Morgan

ICNN’94



The Loss Surfaces of Multilayer Networks

Anna Choromanska achoroma@cims.nyu.edu

Mikael Henaff mbh305@nyu.edu

Michael Mathieu mathieu@cs.nyu.edu

Gérard Ben Arous benarous@cims.nyu.edu

Yann LeCun yann@cs.nyu.edu

Courant Institute of Mathematical Sciences
New York, NY, USA

AISTATS’15

“… we essentially never reach the global minimum. In fact it is not even clear that we would want to reach the global minimum for the training data, since we wish to generalise to the best possible minimum for previously unseen data, which is what we will be using the net for.”

“Struggling to find the global minimum on training (as opposed to one of the many good local ones) is not useful in practice and may lead to overfitting.”

Wrap-up – Paper Contributions

Understanding Deep Learning Requires Rethinking Generalization

ICLR 2017

- Optimisation is easy, even when learning is impossible
- Investigating the role of regularisation
- Finite-sample expressivity of NNs
- SGD’s implicit regularisation in linear models

Wrap-up – Conclusions

- Conventional wisdom about generalisation fails to explain why DNNs generalise well in practice
- #parameters does not necessarily mean model complexity
- [Large enough] DNNs easily fit (learn/memorise) [any, even random] labels
- Explicit regularisation may improve generalisation performance BUT is neither necessary nor sufficient for controlling generalisation error
- DNN optimisation continues to remain easy even when learning is hard or generalisation is poor
- SGD MAY act as an implicit regulariser
- Finding global optimum is not important for having a good generalisation

That’s it!

- Thanks for Your Attention!
- Appendices

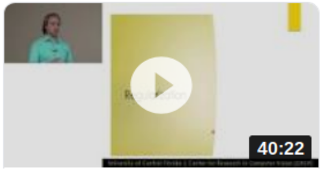
  A1. References

  A2. VC-dimension

  A3. SGD Solution for a Linear System

References

- Paper
- Slides
- Poster
- Codes
- Presentations

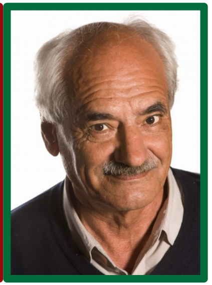


This Week in Machine Learning & AI
TWiML Online Meetup #4
Understanding Deep Learning Requires Rethinking Generalization
Presented by Bruno Gonçalves
Wednesday, 13 December 2017
1:05:04
TWiML&AI

- Comments in OpenReview.net

VC Dimension

Vapnik



Chervonenkis

- A measure of hypothesis class *capacity*
- *Cardinality* of the largest set of points algorithm can *shatter*
  - Shatter: 0 error for any label assignment on training data
- Goal: Gives an upper bound for the generalisation error
- Criticism: too loose
- Valid when #Parameters << #TrainingData (*N*), with prob 1-*η*

$$E_{test}\Big|_{E_{train}>0} \leq E_{train} + O^*(\sqrt{\frac{VC_{dim} - \ln \eta}{N}}) \qquad E_{test}\Big|_{E_{train}=0} \leq O^*(\frac{VC_{dim} - \ln \eta}{N})$$