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SCHOOL OF ENGINEERING

Regularization

**A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle,
K. Packhäuser, M. Zinnen**

Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

April 24, 2023



Outline

Introduction to Regularization

Classical Techniques

Regularization in the Loss Function

Normalization

Dropout

Initialization

Transfer Learning

Multi-Task Learning (MTL)



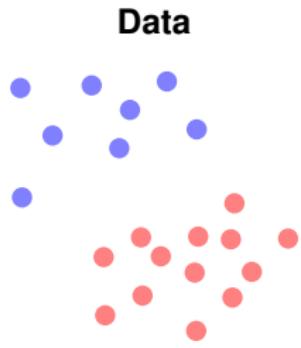
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Introduction to Regularization

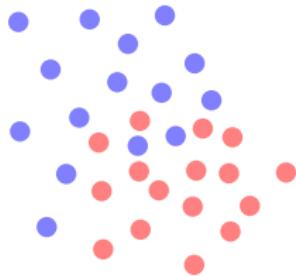


Fitting appropriately



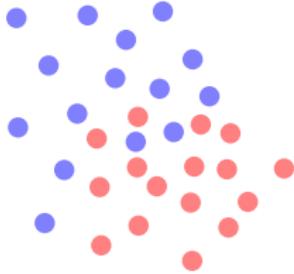
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Data

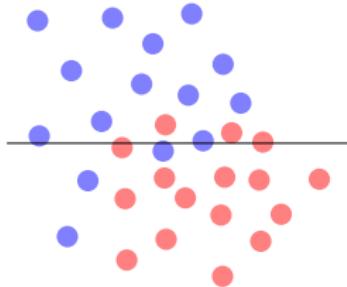


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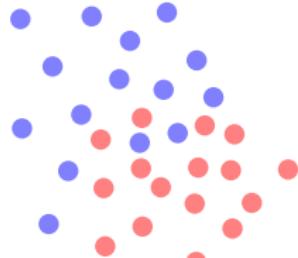


Underfitting

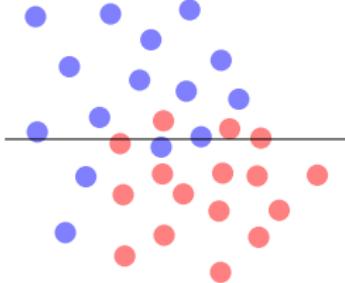


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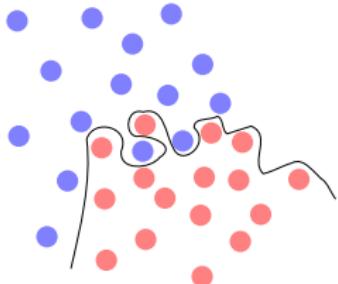
Data



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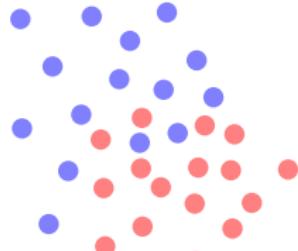


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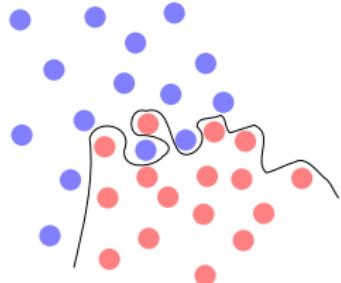


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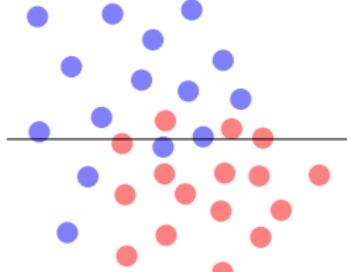
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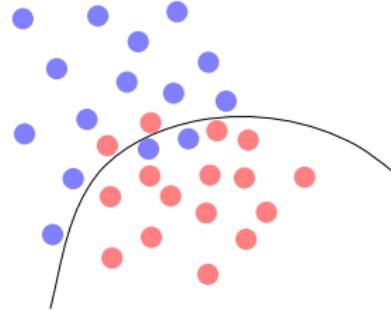
Overfitting



Underfitting



Sensible boundary



Bias Variance Decomposition

- Regression **problem** [3] with **h , ideal** value from the true distribution:

$$\mathbf{h} = h(\mathbf{x}) + \epsilon, \quad \epsilon = \mathcal{N}(0, \sigma_\epsilon).$$

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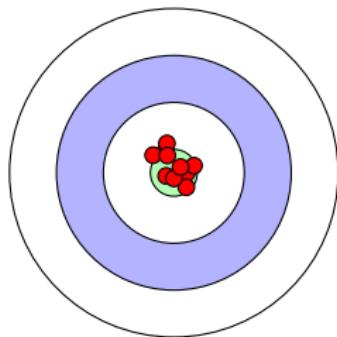
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- Integrating this over every datapoint \mathbf{x} we get $L_D(\mathbf{X})$ from the $\ell_D(\mathbf{x})$.
- A similar decomposition exists for classification using the zero-one loss [9, pp. 468-471].

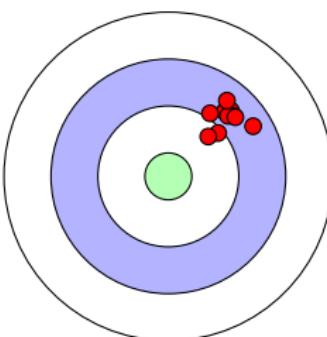
Bias Variance Tradeoff

Low variance

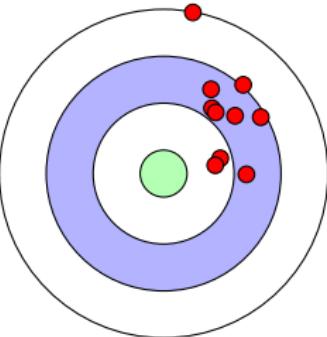
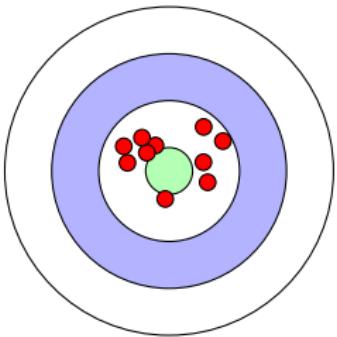
Low bias



High bias



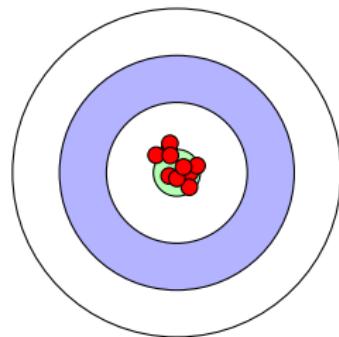
High variance



- We'd like to **minimize** bias and variance

Bias Variance Tradeoff

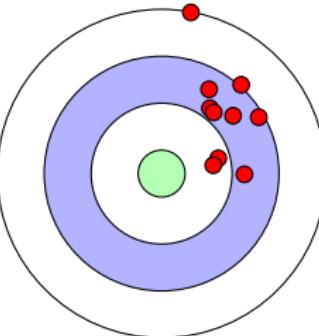
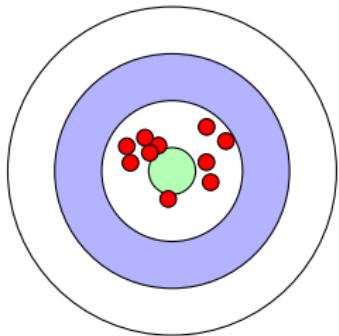
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Low bias

High bias

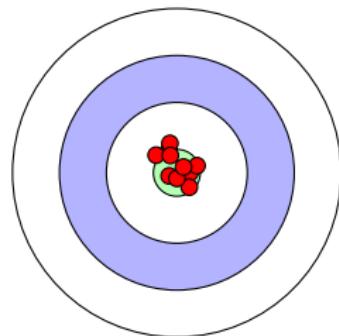
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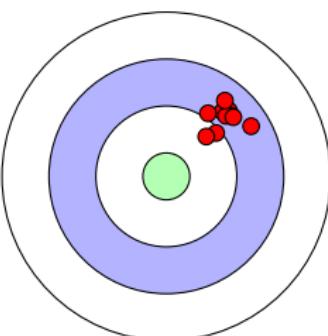
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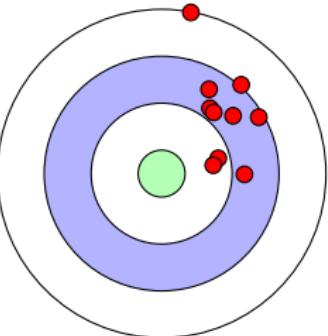
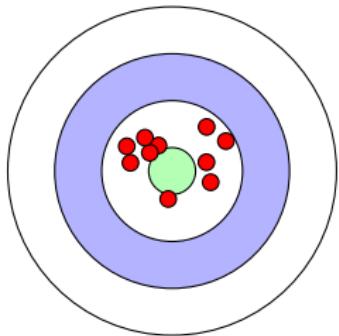


Low bias



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- We'd like to **minimize bias and variance**
- However, if we choose a type of model for a given dataset:
 - Simultaneously optimizing **bias** and **variance** is **impossible** in general
- Bias and variance can be studied together as **model capacity**

Model Capacity

- **Capacity** of a model \mapsto **variety of functions** it can approximate
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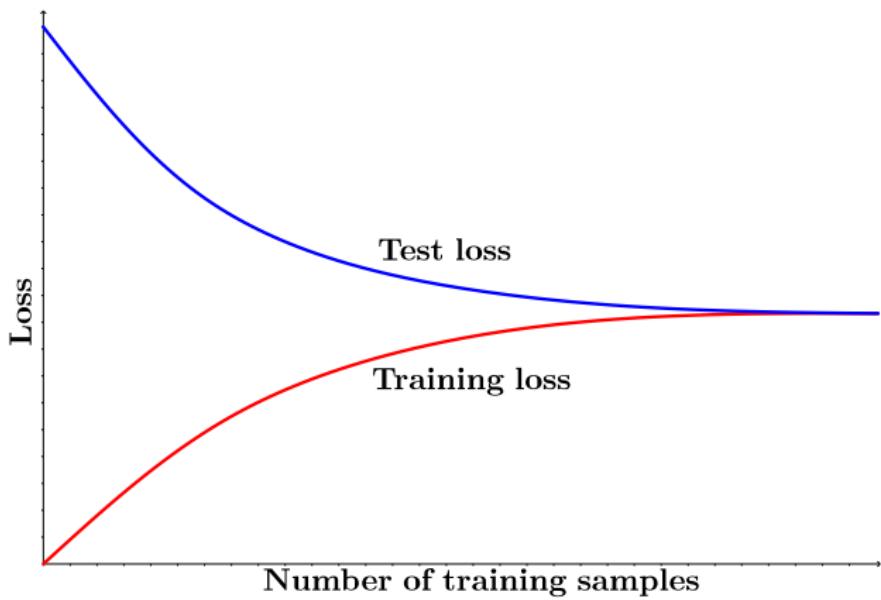
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 - VC dimension of neural networks is usually **extremely high** compared to classical methods
 - Remember the paper learning ImageNet with random labels? [18]

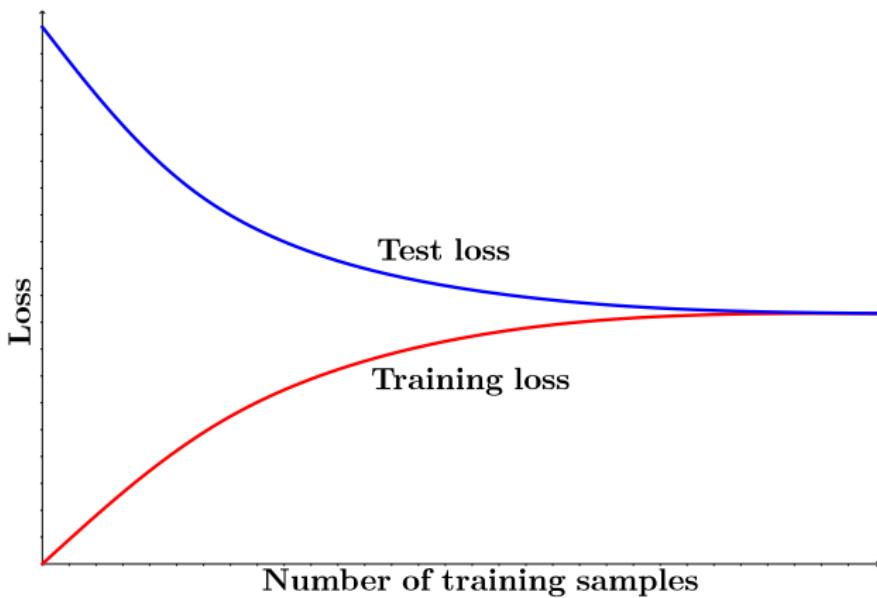
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 - Remember the paper learning ImageNet with random labels? [18]
 - VC dimension is **ineffective** in judging the **real capacity** of neural networks
- We can always reduce the **bias** by \uparrow the **model capacity**

The Role of Data

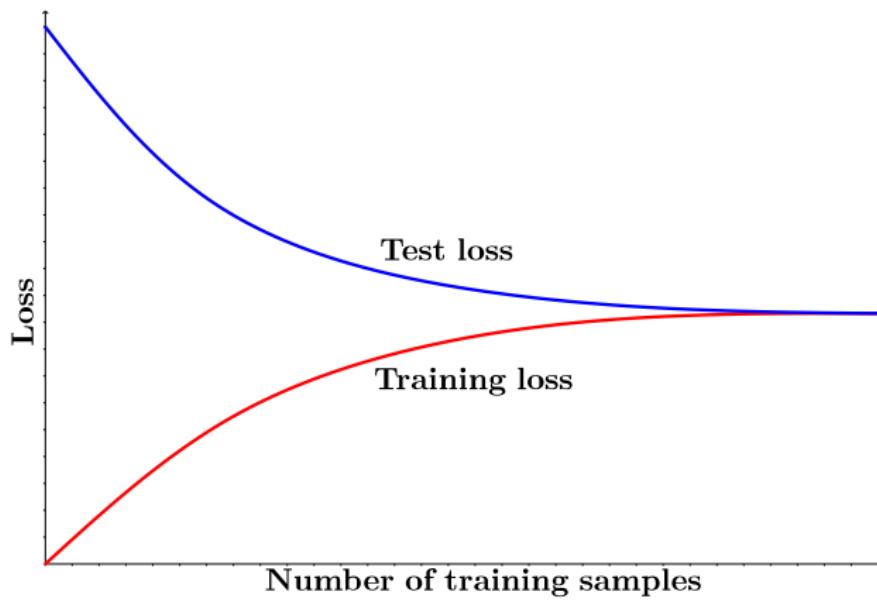


The Role of Data



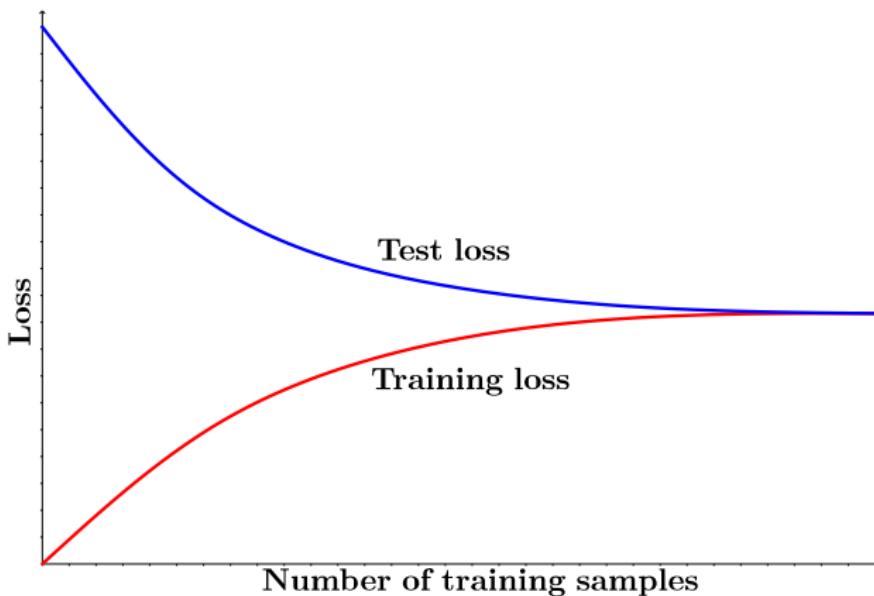
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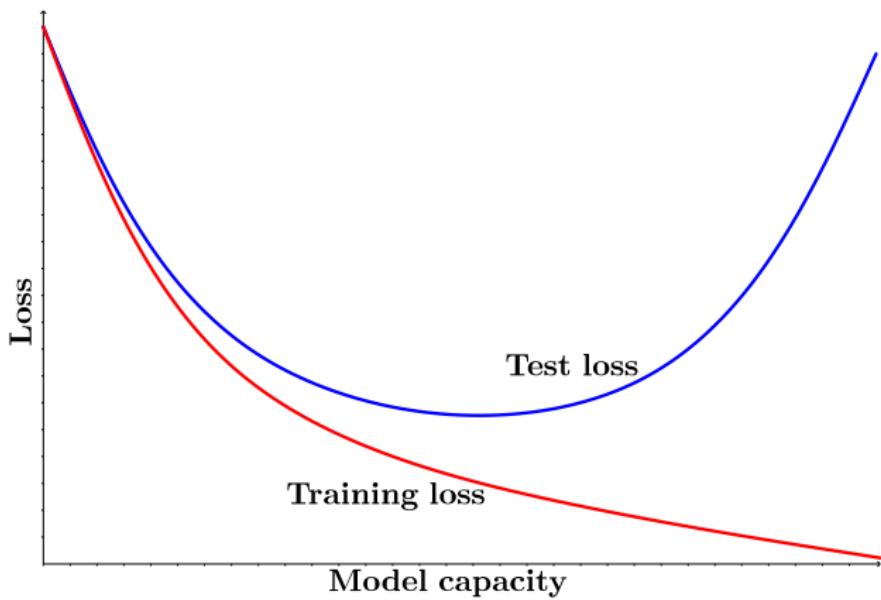
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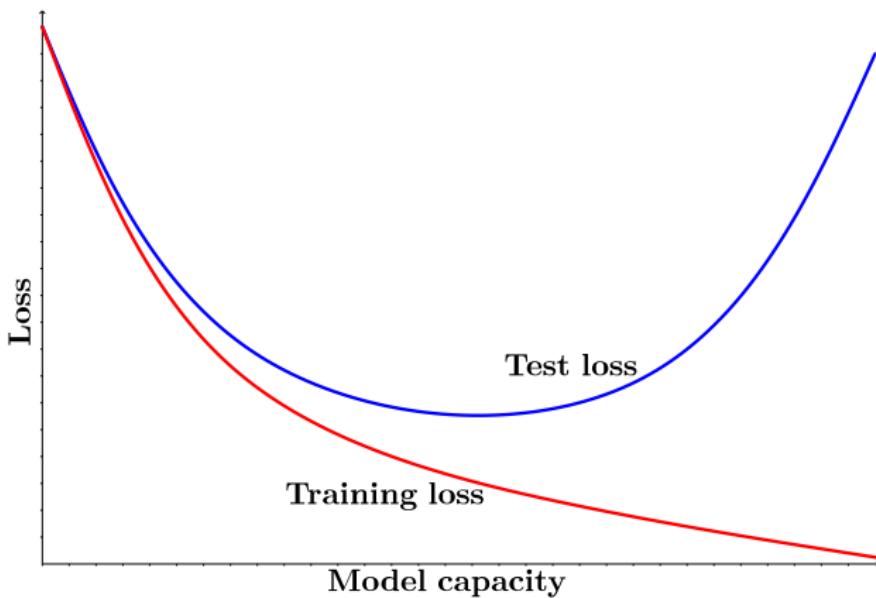


- The **variance** can be optimized by using **more training data**
- The model capacity has to **match** the **size** of the **training set**
- What if we can't acquire more data?

Finite Dataset

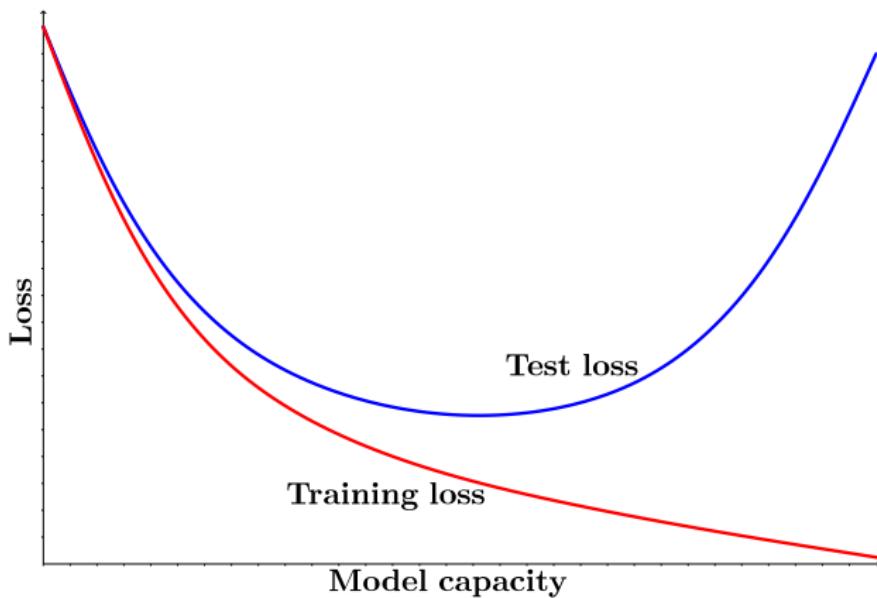


Finite Dataset



- We can trade an \uparrow in **bias** for \downarrow in **variance**

Finite Dataset



- We can trade an \uparrow in **bias** for \downarrow in **variance**
- For a **specific problem** there might be favorable tradeoffs!

Regularization reduces Overfitting

How can we find such a favorable tradeoff?

- By enforcing prior knowledge

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Model prior knowledge

- Augment data
- Adapt architecture
- Adapt training process
- Preprocessing

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Actual regularizers

- Equality constraints
- Inequality constraints

**NEXT TIME
ON DEEP LEARNING**



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Regularization - Part 2

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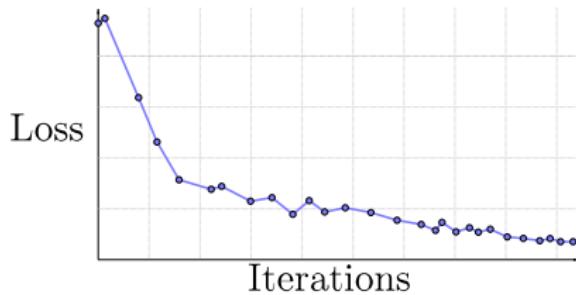
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Classical Techniques



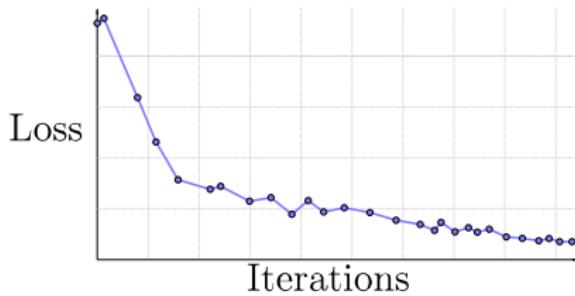
Overfitting on Learning Curve

Training set

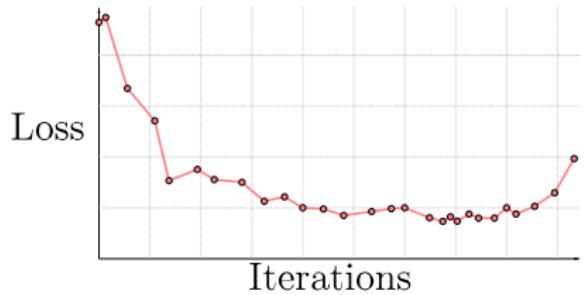


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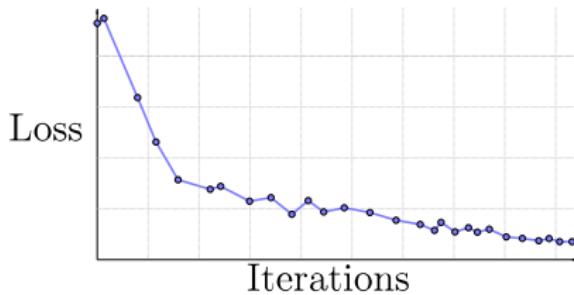


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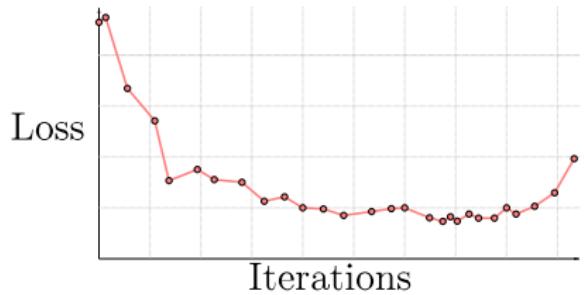


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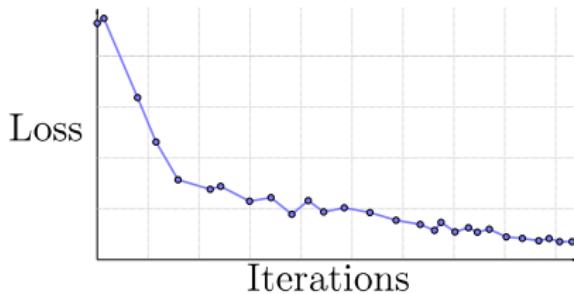
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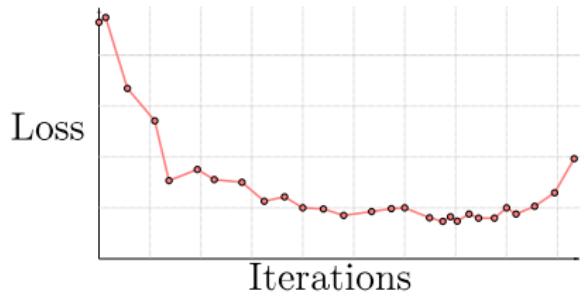
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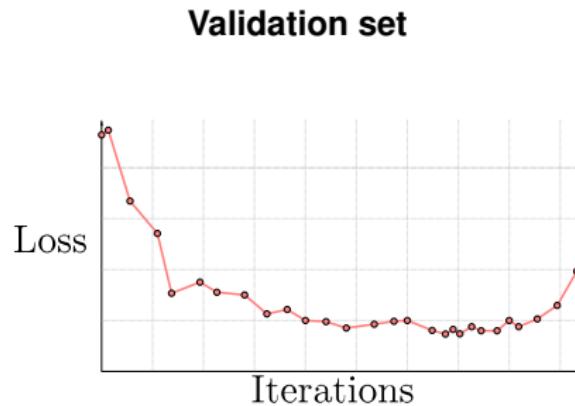


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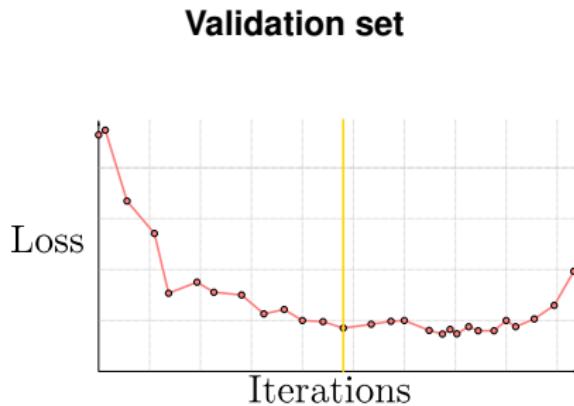


- Test set **must not** be used for training!
 - Split of **validation set** from training data

Early Stopping

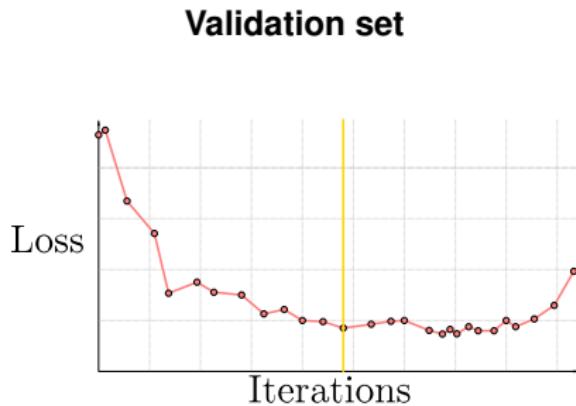


Early Stopping



- Define stopping criterion

Early Stopping



- Define stopping criterion
- Use parameters with **minimum validation loss**

Data Augmentation

→ Artificially enlarge dataset

Data Augmentation

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 - But how?

Data Augmentation

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- Every **transformation** which the **label** should be **invariant** to:

Probably the same class:



Data Augmentation

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Still you have to be careful!



Data Augmentation

Common transformations:

Data Augmentation

Common transformations:

1. random spatial transformations:
 - affine transformations
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 - ...

Data Augmentation

Common transformations:

1. random spatial transformations:
 - affine transformations
 - elastic transformations
 - ...
2. pixel transformations
 - changing resolution
 - random noise
 - changing pixel distribution
 - ...

Regularization in the Loss Function

Maximum A Posteriori Estimation

- **Bayesian** approach considering the weights uncertain: $\mathbf{w} \mapsto p(\mathbf{w})$
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- Because $p(\mathbf{Y}|\mathbf{X})$ does not depend on \mathbf{w} , and \mathbf{X} and \mathbf{w} are independent, we can obtain an estimate as:

$$\text{MAP}(\mathbf{w}) := \underset{\mathbf{w}}{\text{maximize}} \quad \{ p(\mathbf{Y}|\mathbf{X}, \mathbf{w}) p(\mathbf{w}) \}$$

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Augmenting the Loss Function

Enforce

Augmenting the Loss Function

Enforce ...small norm:

$$\tilde{L}(\mathbf{w}, \mathbf{X}, \mathbf{Y}) = L(\mathbf{w}, \mathbf{X}, \mathbf{Y}) + \lambda \|\mathbf{w}\|_2^2$$

Augmenting the Loss Function

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When λ is positive, we can identify this as the Lagrangian function of:

$$\underset{\mathbf{w}}{\text{minimize}} \quad \{L(\mathbf{w}, \mathbf{X}, \mathbf{Y})\} \quad \text{s.t. : } \|\mathbf{w}\|_2^2 \leq \alpha$$

with an unknown data-dependent α .

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Backpropagation of the augmented loss:

$$\mathbf{w}^{(k+1)} = \underbrace{(1 - \eta \lambda) \mathbf{w}^{(k)}}_{\text{Shrinkage}} - \eta \frac{\partial L}{\partial \mathbf{w}^{(k)}}$$

- Often called “weight decay”

Augmenting the Loss Function

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$$\mathbf{w}^{(k+1)} = \underbrace{(1 - \eta \lambda) \mathbf{w}^{(k)}}_{\text{Shrinkage}} - \eta \frac{\partial L}{\partial \mathbf{w}^{(k)}}$$

- Often called “weight decay”
- If we optimize the **training-loss** for λ we will usually receive $\lambda = 0$.

Augmenting the Loss Function

Enforce ...small norm:

$$\tilde{L}(\mathbf{w}, \mathbf{X}, \mathbf{Y}) = L(\mathbf{w}, \mathbf{X}, \mathbf{Y}) + \lambda \|\mathbf{w}\|_2^2$$

When λ is positive, we can identify this as the Lagrangian function of:

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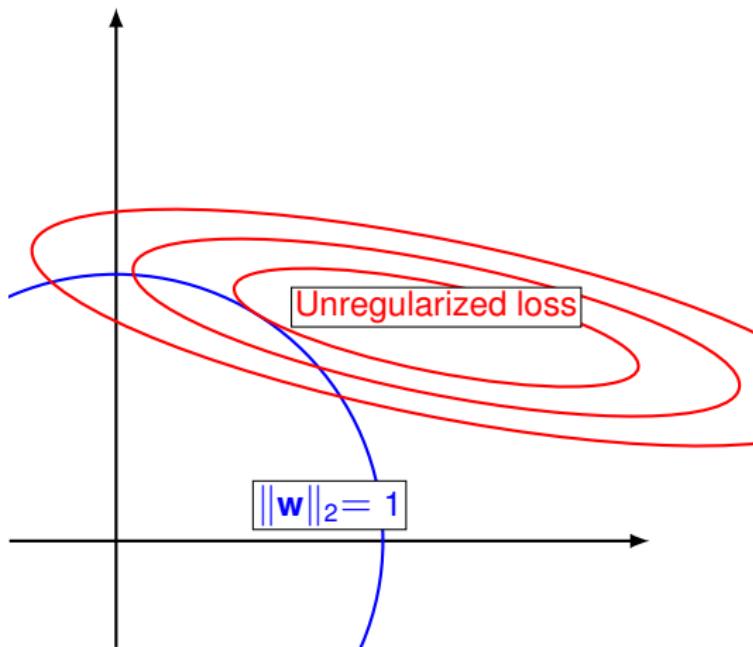
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- We trade increased **bias** for reduced **variance**

Graphical Effect of L₂ Regularization



Augmenting the Loss Function (cont.)

Enforce

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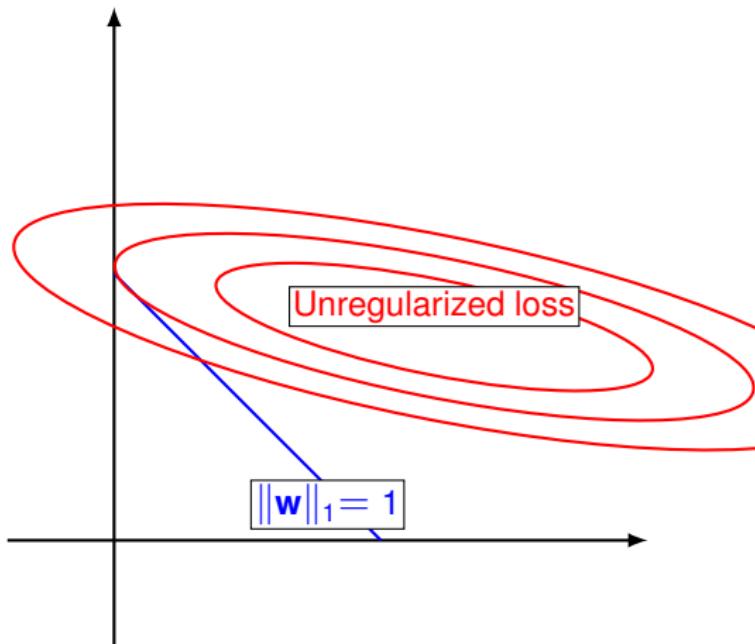
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Backpropagation of the augmented loss with the corresponding **subgradient**:

$$\mathbf{w}^{(k+1)} = \underbrace{\mathbf{w}^{(k)} - \eta \lambda \text{sign}(\mathbf{w}^{(k)})}_{\text{Other shrinkage}} - \eta \frac{\partial L}{\partial \mathbf{w}^{(k)}}$$

→ Same as before

Graphical Effect (cont.)



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- Perform parameter update, then project to unit-“ball”
- Still a kind of shrinkage
- Prohibits **exploding gradients** but also hides it

Other Variants of Changing the Loss

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- Different variants have been used for **sparse autoencoders**
- We will cover this when we talk about unsupervised learning

**NEXT TIME
ON DEEP LEARNING**



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Regularization - Part 3

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle,
K. Packhäuser, M. Zinnen

Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

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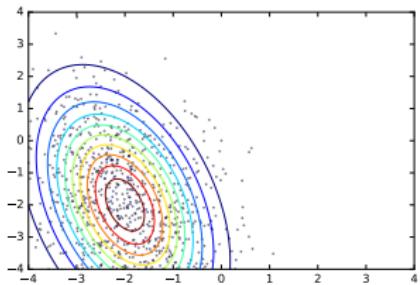
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Normalization



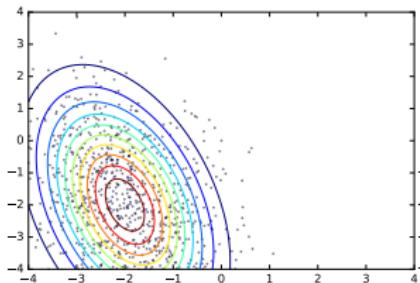
Data Normalization

Original data

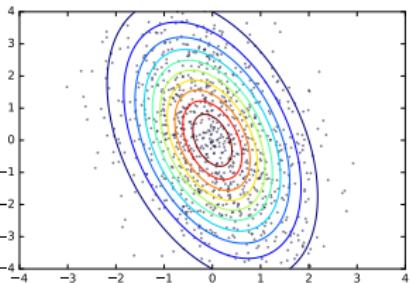


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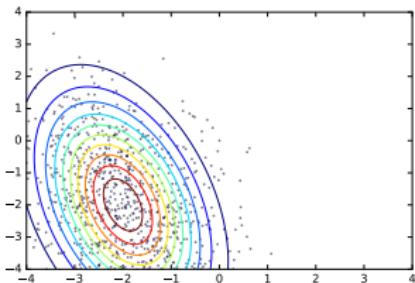


Mean subtracted

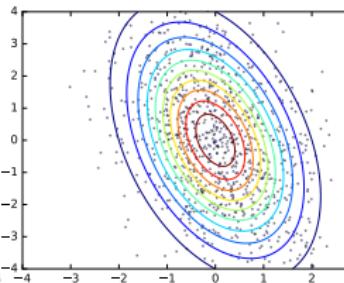


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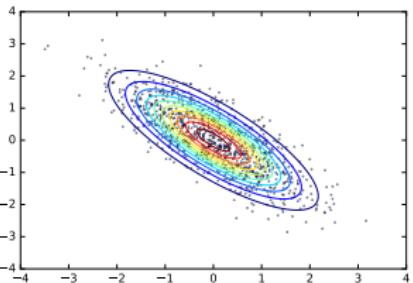
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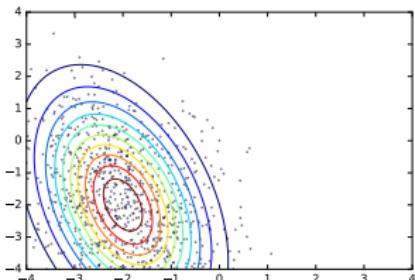


Normalized variance

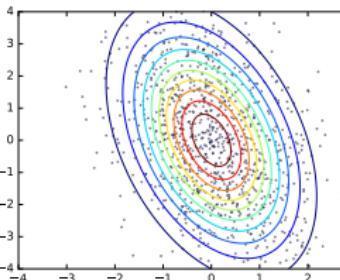


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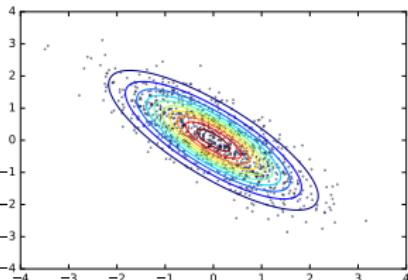
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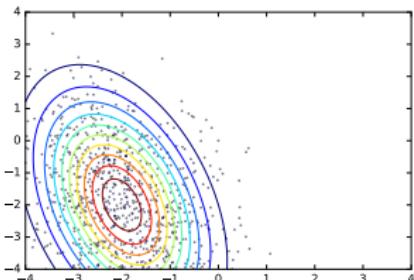
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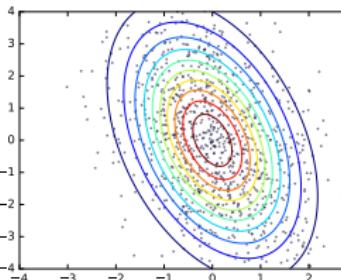
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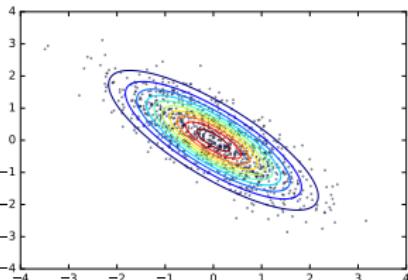
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- Normalization of input data
- Normalization **within** the network

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- Normalization as a new layer with 2 parameters, γ and β

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- So the μ and σ are **vectors, of the same dimension** as the **activation vector**.
- Paired with **convolutional** layers batch normalization is **different** by computing a **scalar** μ and σ for every **channel**.

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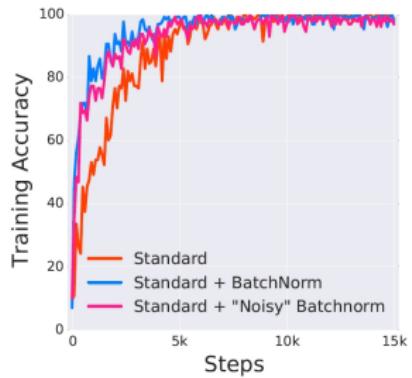
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- **But:** Little concrete evidence to support this theory

Why does batch normalization help? (cont.)

NeurIPS 2018: How Does Batch Normalization Help Optimization? [19]:

- BN helps **even** if internal covariate shift is introduced again afterwards

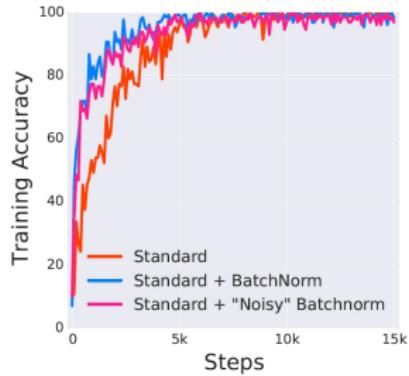


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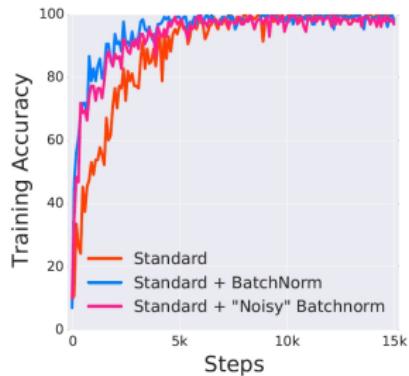


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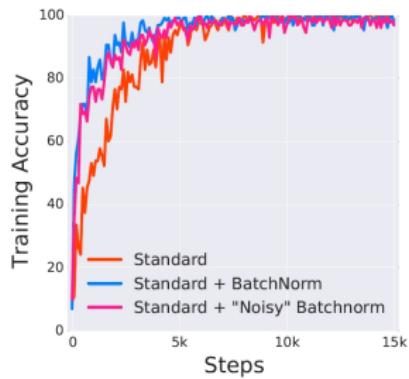


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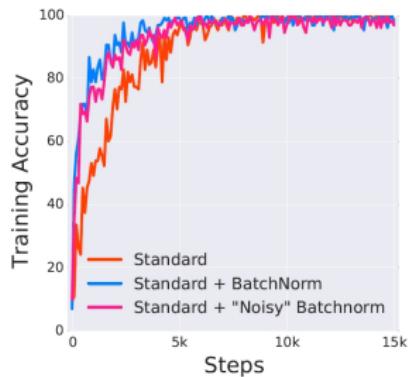


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- BN improves stability e.g. with respect to hyperparameters, initialization, convergence
- Similar properties also observed for l_p -normalization



Source: [19]

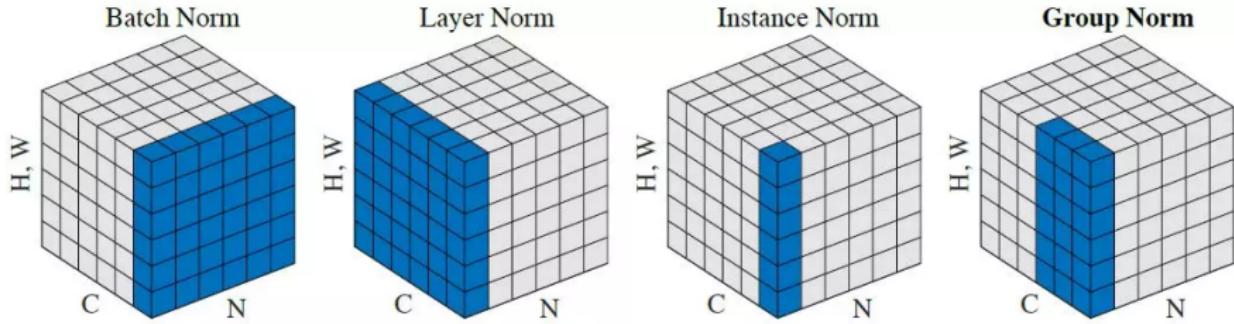
Generalizations

$$\hat{y} = f\left(g \frac{x - \mu}{\sigma} + b\right)$$

y : output
 f : activation function
 x : input
 g, b : adaptive gain and bias
 μ, σ : mean and std dev.

Calculating μ, σ over

- ... activations of a batch [1], a layer [15], spatial dims [13], a group [11]
- ... weights of a layer [20]



Source: Wu et al. [11]

Self Normalizing Neural Networks

- Method that **addresses** the **stability problem** of SGD [14]

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With $\lambda_{01} = 1.0507$ and $\alpha_{01} = 1.6733$ for $\mu = 0$ and $\sigma = 1$

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- The **SNN** concept resembles **batch normalization**



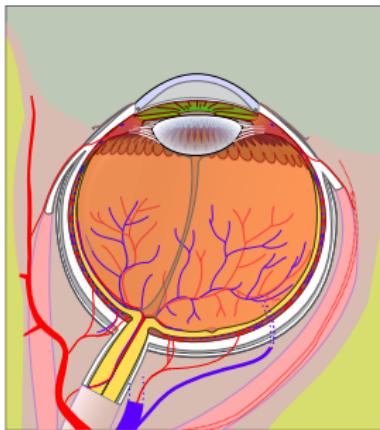
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Dropout



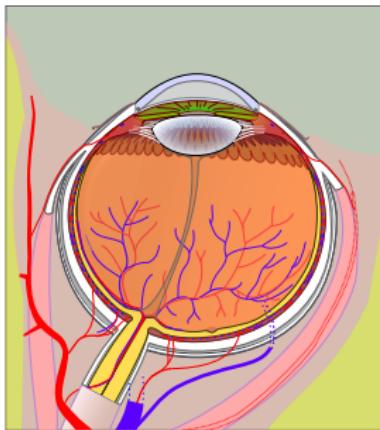
Co-adaptation



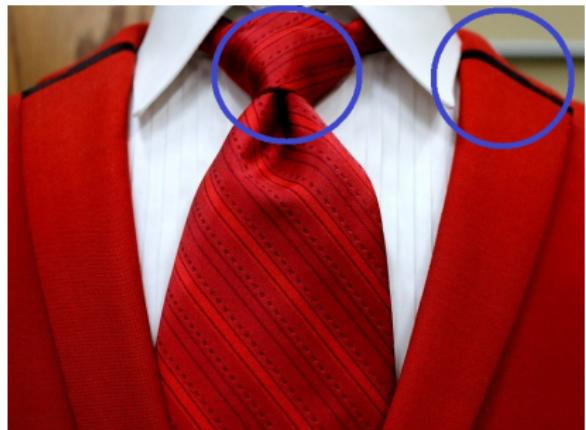
All elements **depend** on each other

Source: Jordi March / CC-BY-SA-3.0

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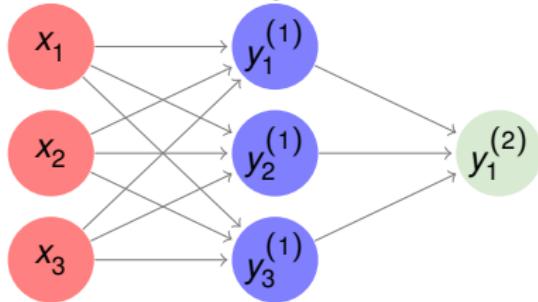
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→Contrary to **independent** features

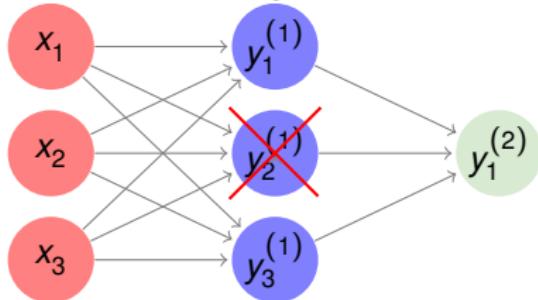
Dropout and Dropconnect

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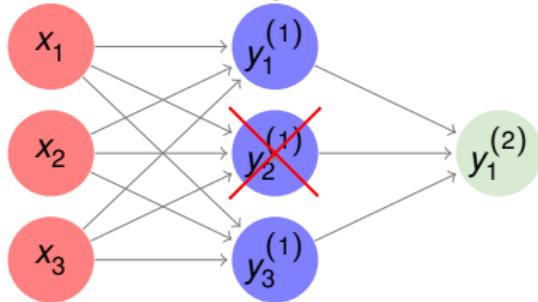
Dropout



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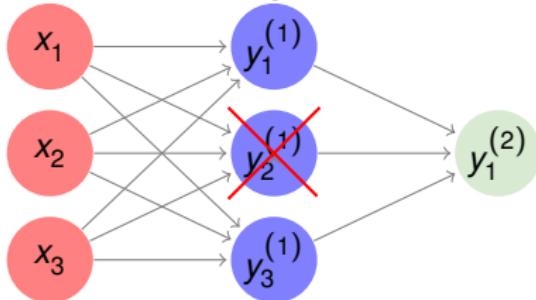
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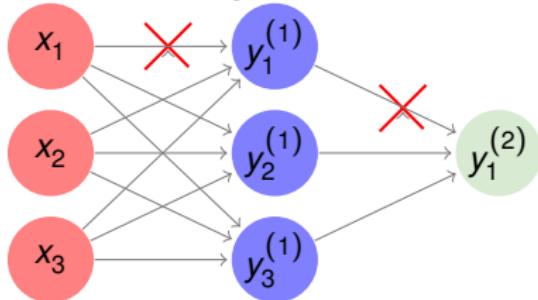
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- Generalizes Dropout
- Less efficient implementation (masking)

**NEXT TIME
ON DEEP LEARNING**



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Regularization - Part 4

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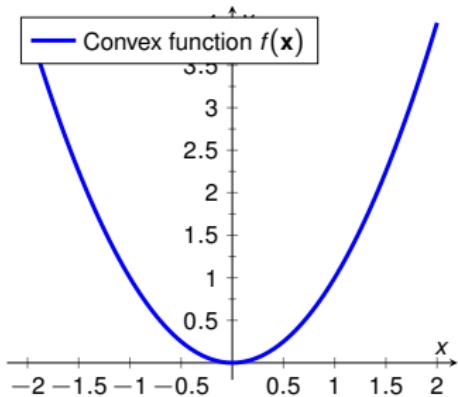
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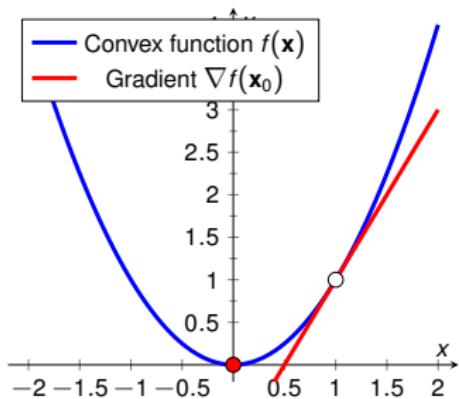
Initialization



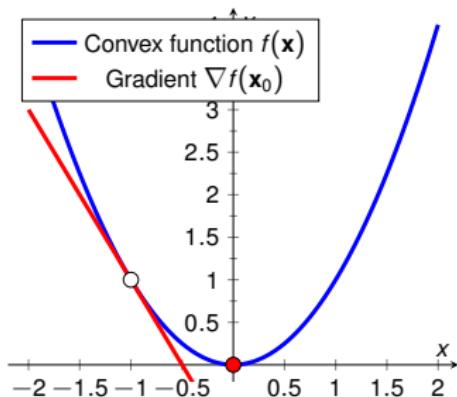
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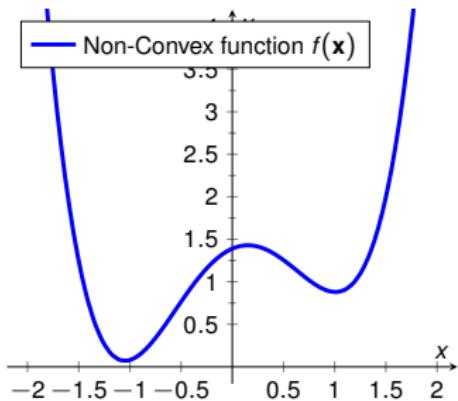


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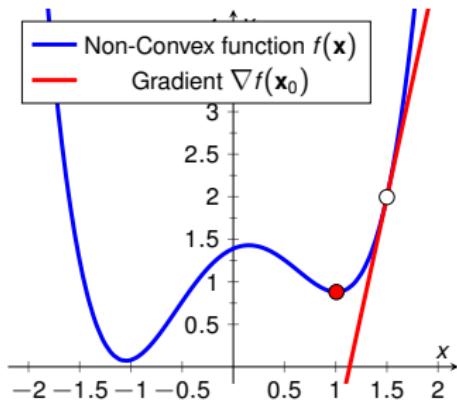
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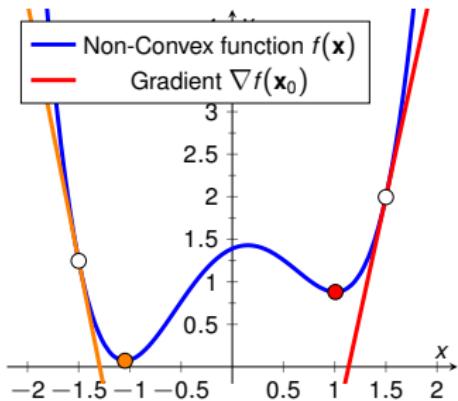
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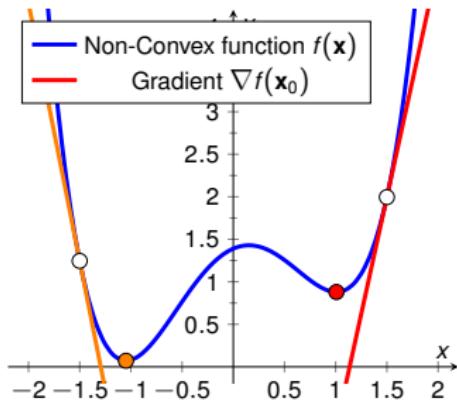
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- Neural Networks with a non-linearity are in general **non-convex**

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- **Bias** units can simply be **initialized to zero**

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- Similar to the learning rate their **variance** influences the **stability** of learning
- **Small** uniform/Gaussian values work

Calibrating the variances

- Suppose we have a single **linear** neuron with weights **W** and an input **X**
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- Output is:

$$\hat{Y} = \mathbf{WX} = \left(\sum_{n=1}^N W_n X_n \right) + b$$

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- If W_n and X_n have zero-mean: $\text{Var}(W_n X_n) = \text{Var}(W_n) \text{Var}(X_n)$
- Now we assume the X_n and W_n to be **Independent and Identically Distributed**:

$$\text{Var}(\hat{Y}) = \underbrace{N \text{Var}(W_n)}_{\text{scales Var}} \text{Var}(X_n)$$

Xavier initialization

- We can “calibrate” the variances for the forward-pass by initializing with a zero-mean Gaussian: $\mathcal{N}(0, \sigma)$ with $\sigma^2 = \frac{1}{\text{fan_in}}$ where “fan_in” is the **input** dimension of the weights

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 - However the backward-pass
needs $\sigma^2 = \frac{1}{\text{fan_out}}$
where “fan_out” is the **output** dimension of the weights
 - So we average those two:
- $$\sigma = \sqrt{\frac{2}{\text{fan_out} + \text{fan_in}}}$$
- Named “**Xavier**” initialization after the first author [21]

He initialization

- the assumption of **linear** neurons is a problem
- He et al. [12] showed, for ReLUs it's better to use:

$$\sigma = \sqrt{\frac{2}{\text{fan_in}}}$$

Conventional Initial Choices

- L₂ regularization
- Dropout using $p = 0.5$ for FCN, use selectively in CNNs
- Mean subtraction
- Batch normalization
- He initialization



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Transfer Learning



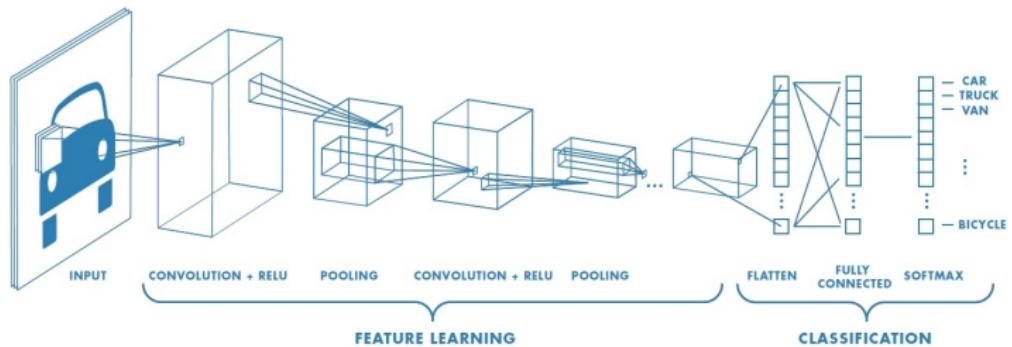
Transfer Learning

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Transfer Learning

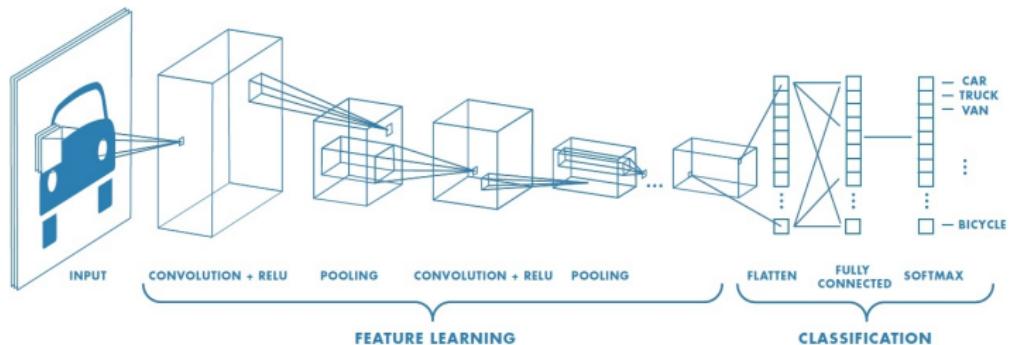
- Most **medical datasets** are prohibitively **small**
- **Reuse models** trained on e.g. ImageNet
 - for a **different task** on the **same data**
 - on **different data** for the **same task**
 - on **different data** for a **different task**

Weight Transfer



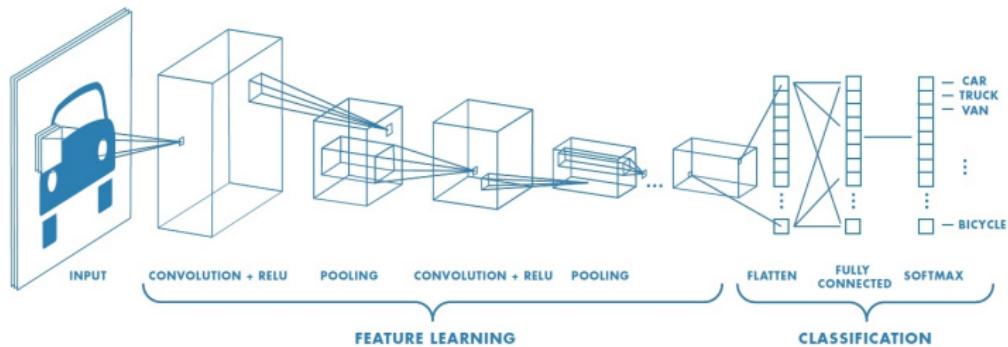
- What should we transfer?

Weight Transfer



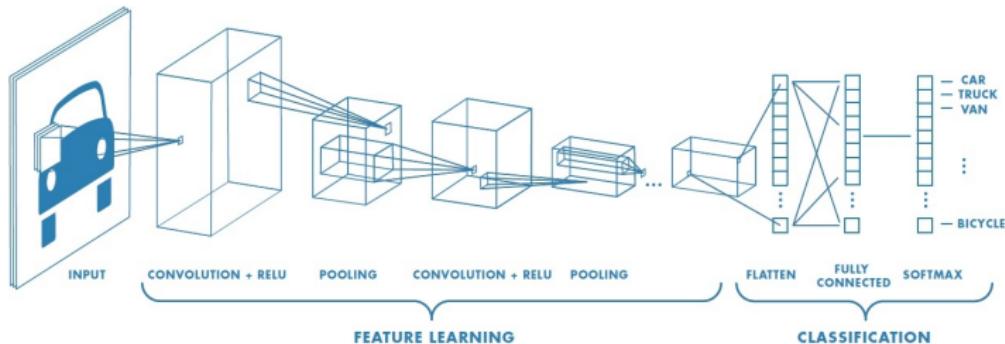
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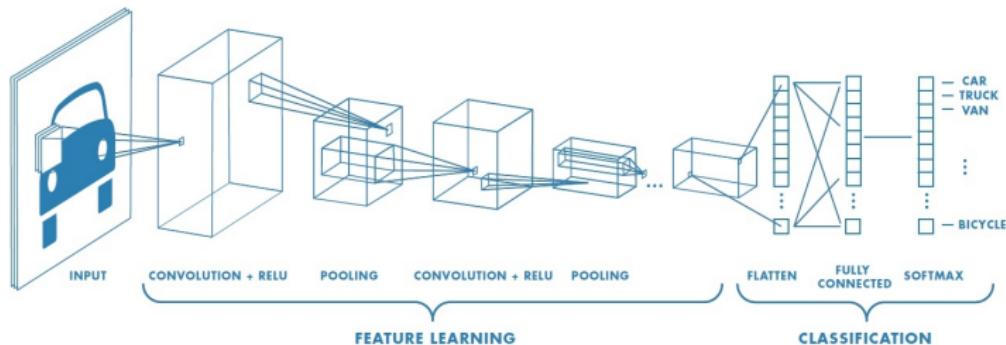
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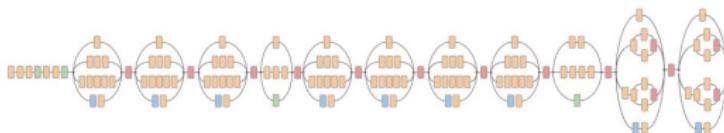
- What should we transfer?
 - Convolutional layers extract features
 - Expectation: Less task-specific in earlier layers
- We cut the network at some depth in the feature extraction part
- The extracted parts can be
 1. fixed by setting $\eta = 0$
 2. **fine-tuned**

Example: Skin Cancer classification

Skin lesion image

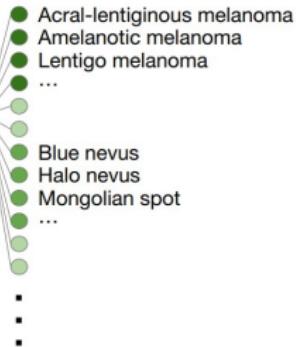


Deep convolutional neural network (Inception v3)



- Convolution
- AvgPool
- MaxPool
- Concat
- Dropout
- Fully connected
- Softmax

Training classes (757)



- State-of-the-art architecture, pre-trained on ImageNet
- Fine-tuned on skin cancer data [5]

Source: <https://www.nature.com/articles/nature21056>

Transfer between modalities

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- Alternative: Use feature representations of other network as a loss function
 - Perceptual loss
- Always use transfer learning!

NEXT TIME
ON DEEP LEARNING



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Regularization - Part 5

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle,
K. Packhäuser, M. Zinnen

Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

April 24, 2023





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Multi-Task Learning (MTL)



Concept

- So far: One network for one task
- Transfer learning: **Reuse** a network
- Can we do more?

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 - Learning to play the piano and the violin
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Source: <https://commons.wikimedia.org/wiki/File:Klavierquintett.JPG>

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Even better than reusing: Learning them **simultaneously** can provide a better understanding of the **shared underlying concepts**.

Source: <https://commons.wikimedia.org/wiki/File:Klavierquintett.JPG>

Concept (cont.)

- Idea: Train a network **simultaneously** on **multiple related** tasks

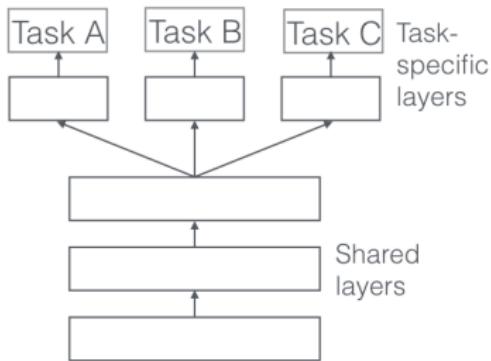
Concept (cont.)

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- Adapt loss function to assess performance for multiple tasks

Concept (cont.)

- Idea: Train a network **simultaneously** on **multiple related** tasks
- Adapt loss function to assess performance for multiple tasks
- Multi task learning introduces an **inductive bias**: We prefer a model that can explain more than one task
- Reduces risk of **overfitting** on one particular task [2]
→ model generalizes better

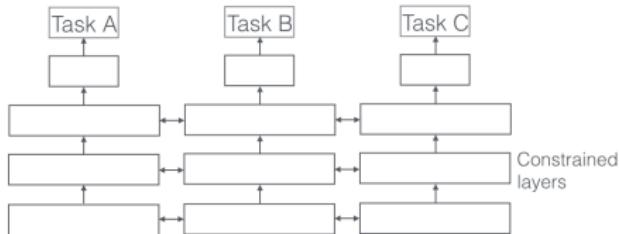
Hard parameter sharing



- Several hidden layers shared between all tasks
- Additional task-specific output layers
- Baxter '97 [2]: Multi-task learning of N tasks reduces chance of overfitting by an order of N

Source: <http://ruder.io/multi-task/>

Soft parameter sharing



- Each model has its own parameters
- Instead of forcing equality, distance between parameters is regularized as part of the loss function
- Options e.g. l_2 -norm, trace-norm, ...

Source: <http://ruder.io/multi-task/>

Auxiliary tasks

- Additional tasks have own purpose or are just **auxiliary** to the original task

Auxiliary tasks

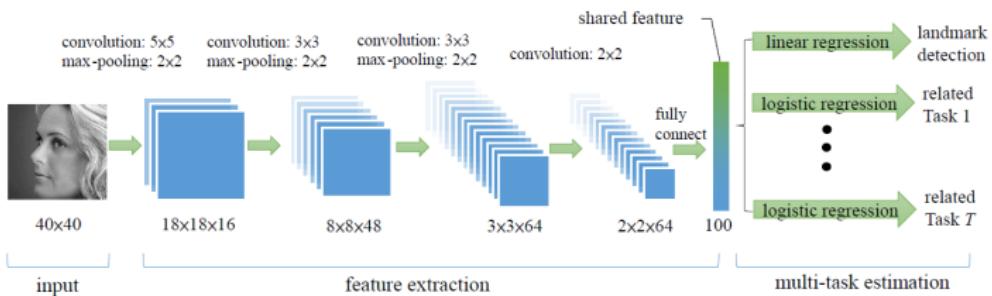
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Auxiliary tasks

- Additional tasks have own purpose or are just **auxiliary** to the original task
- Example: **Facial Landmark Detection** by Zhang et al. 2014 [22]
- Facial landmark detection impeded by occlusion and pose variances
- Simultaneously learn to estimate landmarks **and** “subtly” related task:
 - Face pose
 - Smiling/not smiling
 - Glasses/no glasses (occlusion)
 - Gender



Source: [22]

Auxiliary tasks (cont.)

Auxiliary Tasks

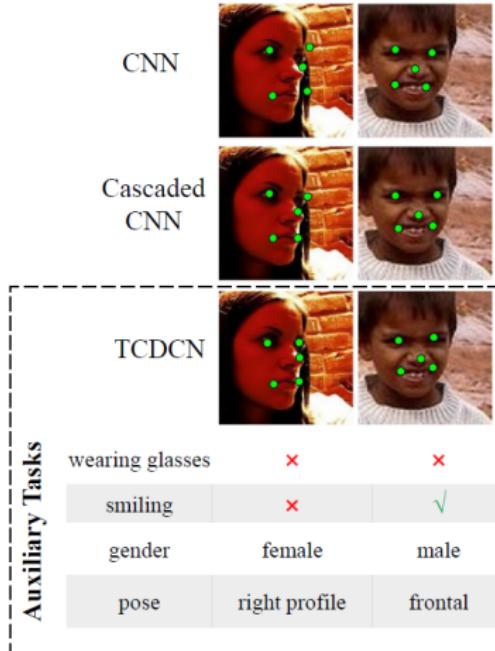
	CNN	Cascaded CNN	TCDCN	wearing glasses	smiling	gender	pose
				✗	✗	✓	✗
				✗	✓	✗	✗
				✗	✗	female	right profile
				✓	✗	male	frontal
				✗	✗	female	left
				✓	✗	male	frontal
				✗	✗	male	frontal
				✗	✗	female	right profile

Landmark detection

Source: [22]

Auxiliary tasks (cont.)

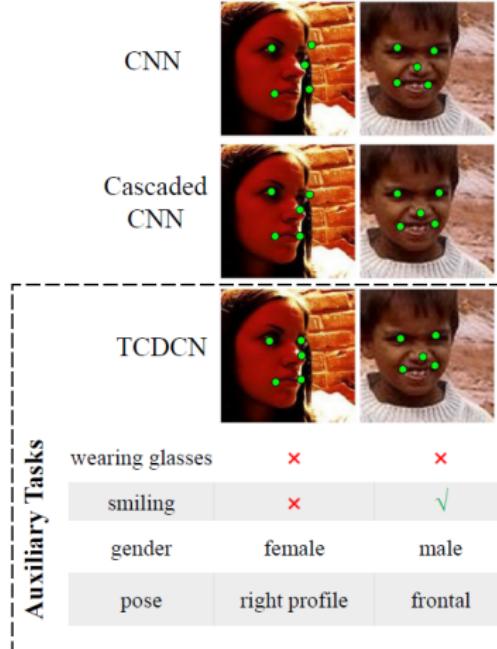
- Certain features difficult to learn for one task but easy for a related one [4]



Source: [22]

Auxiliary tasks (cont.)

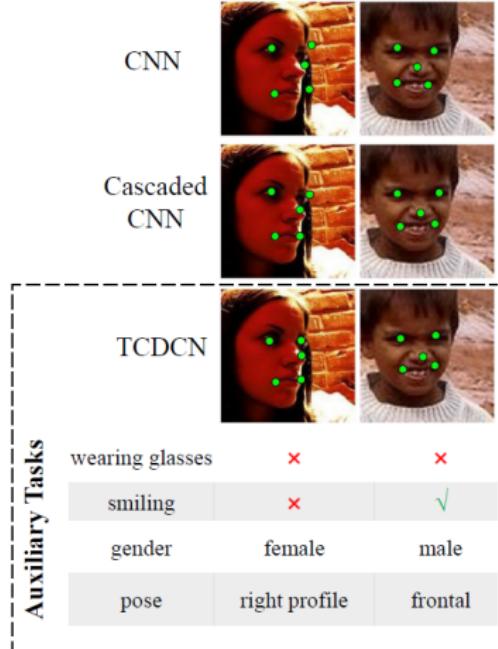
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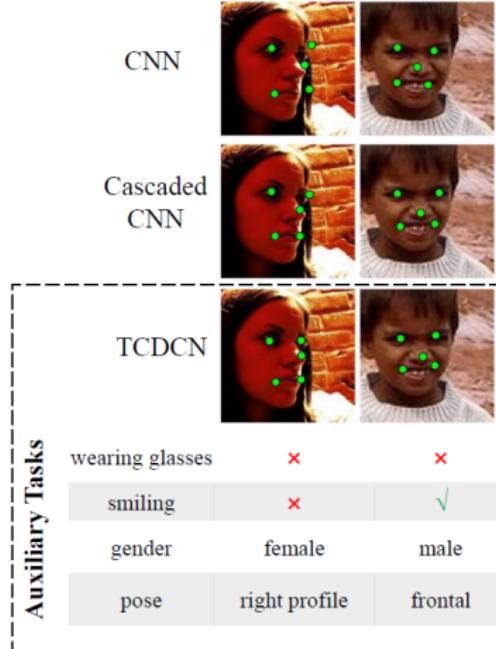
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Auxiliary tasks (cont.)

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- Auxiliary tasks can help to “steer” training in a specific direction
- Include prior knowledge by choosing appropriate auxiliary tasks
- Tasks can have different convergence rates
→ Task-based early-stopping
- Open research question: **What are appropriate auxiliary tasks?**



Source: [22]

**NEXT TIME
ON DEEP LEARNING**

Coming Up

- Practical recommendations to make training work
- Evaluation of performance
- Methods to deal with common problems
- Concrete case studies using all the pieces you now learned

Comprehensive Questions

- What is the bias-variance tradeoff?
- What is model capacity?
- Describe three techniques to address overfitting in a neural network.
- Why do we often need a validation set?
- Can we optimize the hyperparameter λ by gradient descend on the training set?
- What connects the covariate shift problem and the ReLU?
- How can we address the covariate shift problem?
- Which problem do current initialization schemes try to address?
- What is transfer learning?

Further Reading

- [Link](#) - for details on Maximum A Posteriori estimation and the bias-variance decomposition
- [Link](#) - for a comprehensive text about practical recommendations for regularization
- [Link](#) - the paper about calibrating the variances



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