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SCHOOL OF ENGINEERING

Regularization

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M. Hoffmann**

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

November 13, 2018



Outline

Introduction to Regularization

Classical Techniques

Regularization in the Loss Function

Normalization

Dropout

Initialization

Transfer Learning

Multi-Task Learning (MTL)



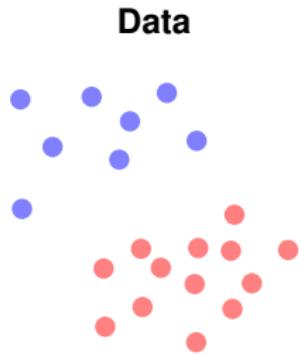
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Introduction to Regularization

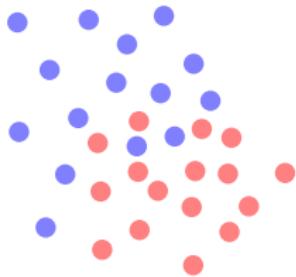


Fitting appropriately



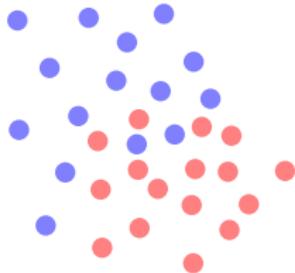
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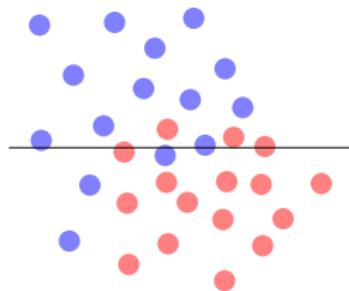


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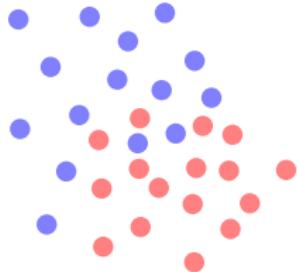


Underfitting

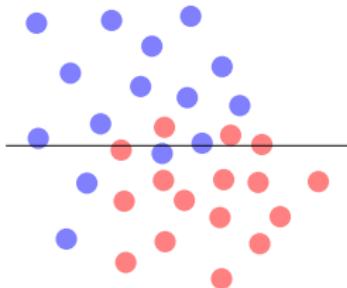


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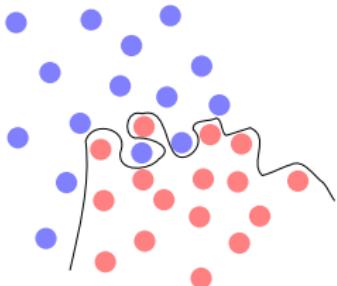
Data



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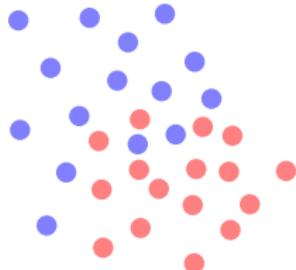


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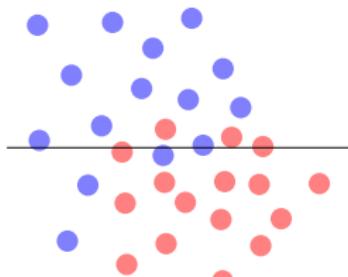


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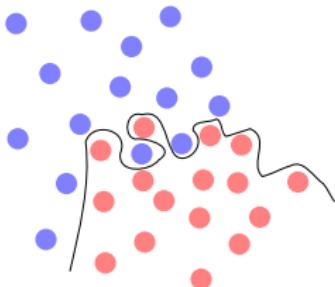
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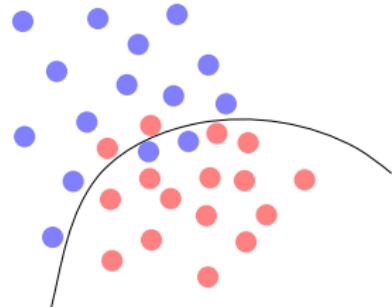
Underfitting



Overfitting



Sensible boundary



Bias Variance Decomposition

- Regression **problem** [5] 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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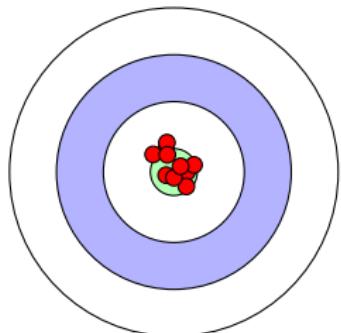
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- Integrating this over every datapoint \mathbf{x} we get $L_D(\mathbf{X})$ from the $\ell_D(\mathbf{x})$.
- A similar decomposition exists for classification using the zero-one loss [6, pp. 468-471].

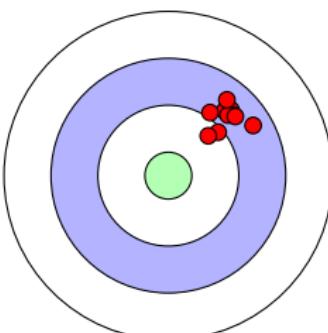
Bias Variance Tradeoff

Low variance

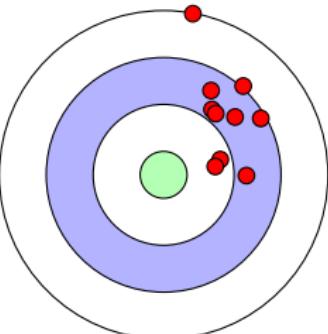
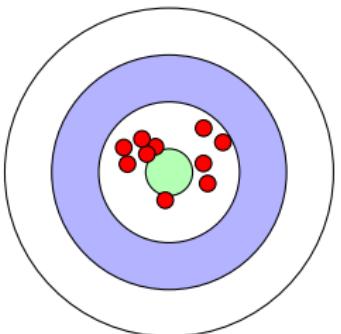
Low bias



High bias



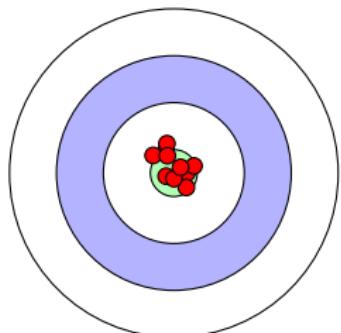
High variance



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

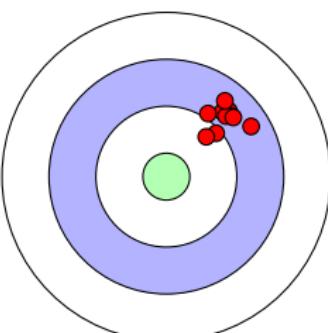
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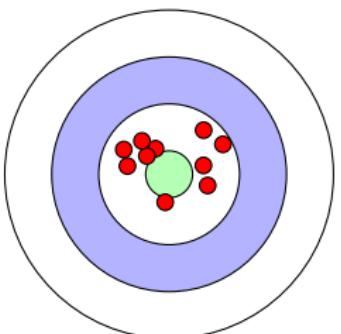


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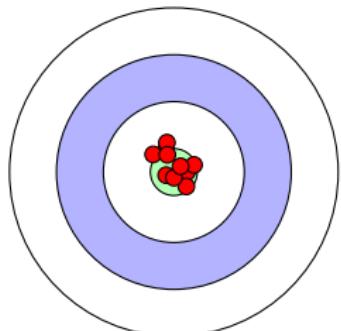
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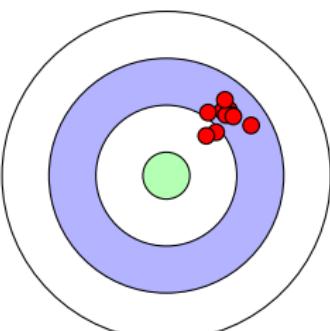
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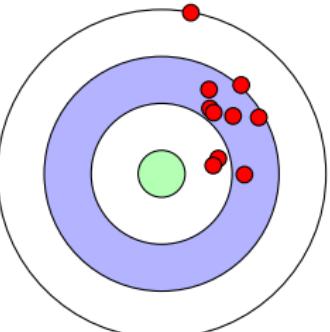
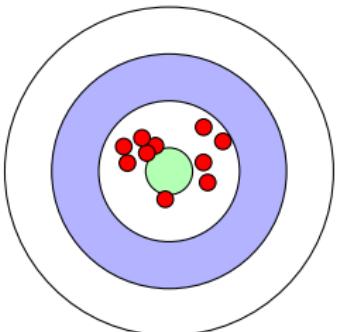


Low bias



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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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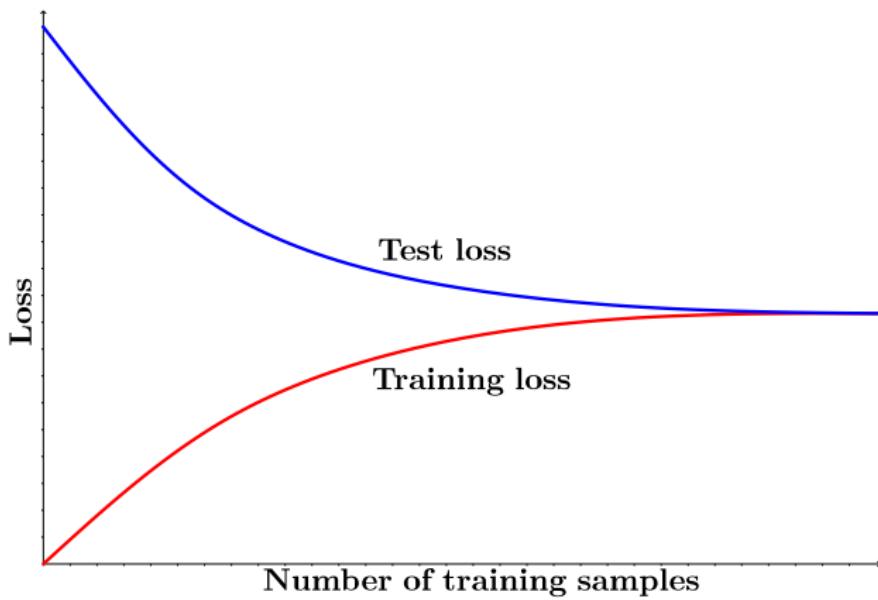
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 - VC dimension of neural networks is usually **extremely high** compared to classical methods
 - Remember the paper learning ImageNet with random labels? [14]

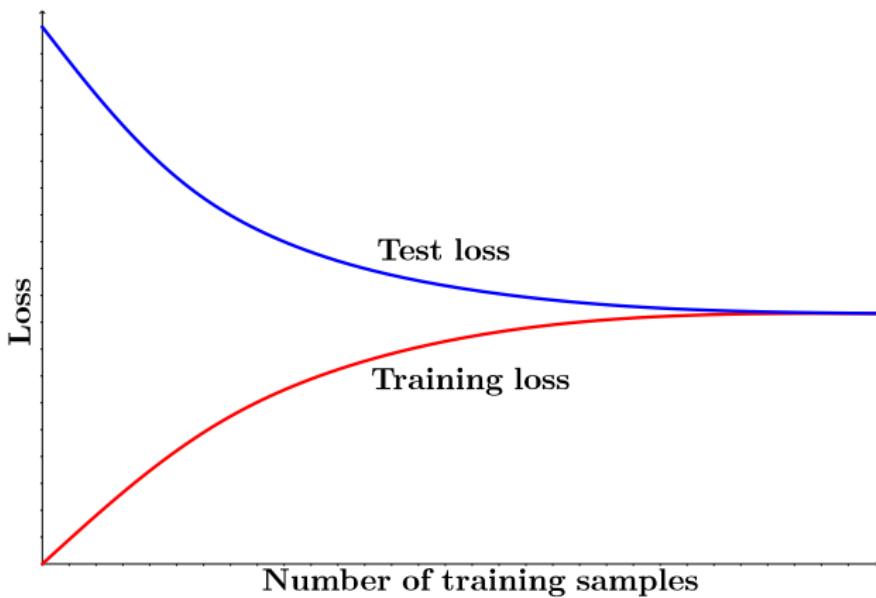
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 - Remember the paper learning ImageNet with random labels? [14]
 - VC dimension is **ineffective** in judging the **real capacity** of neural networks
- We can always reduce the **bias** by \uparrow the **model capacity**

The Role of Data

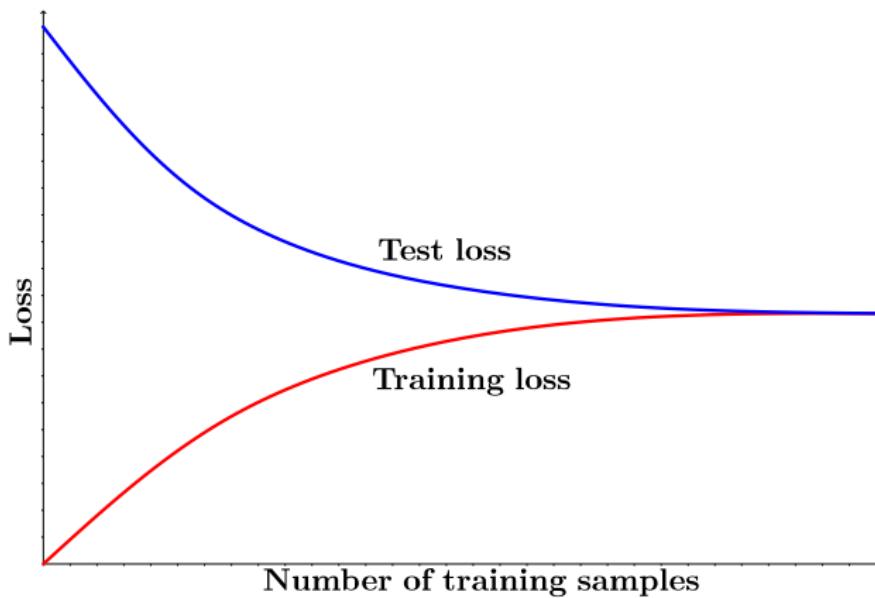


The Role of Data



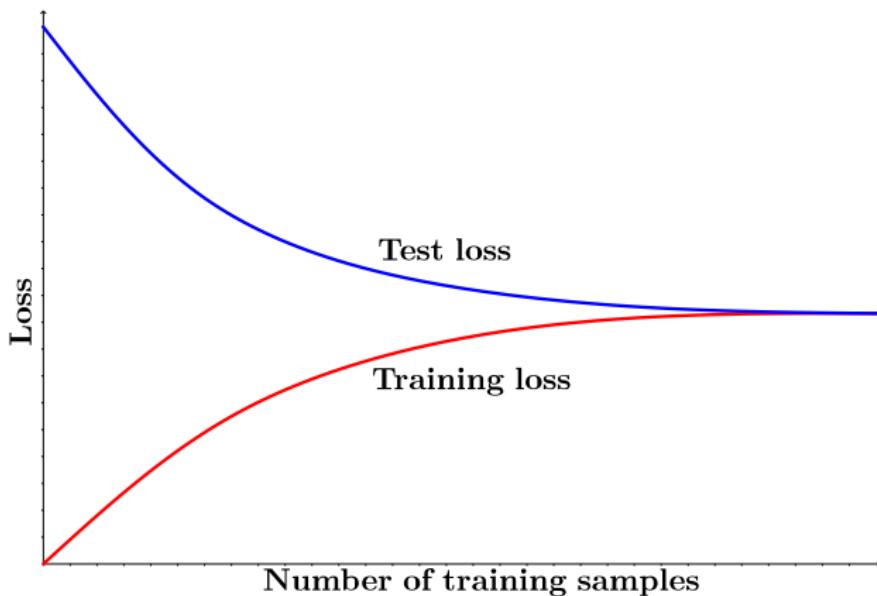
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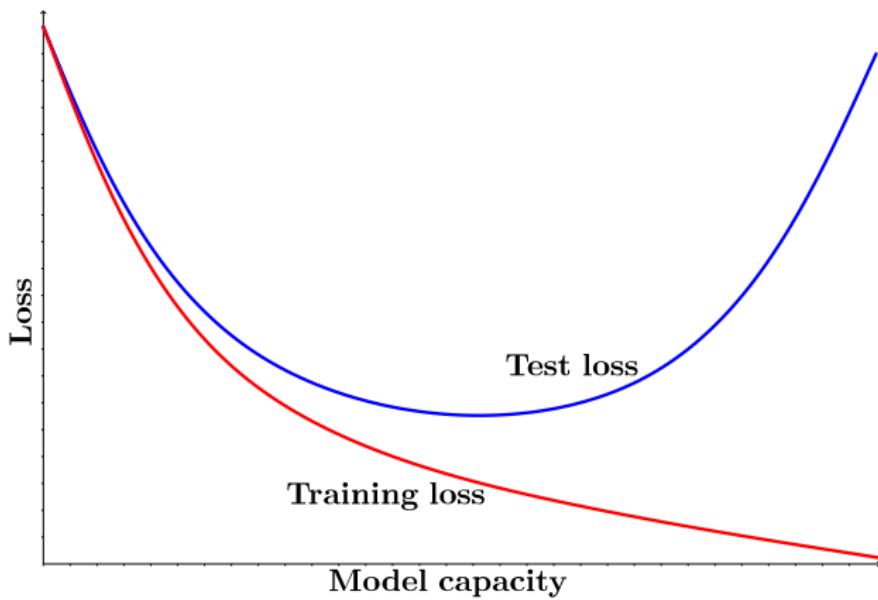
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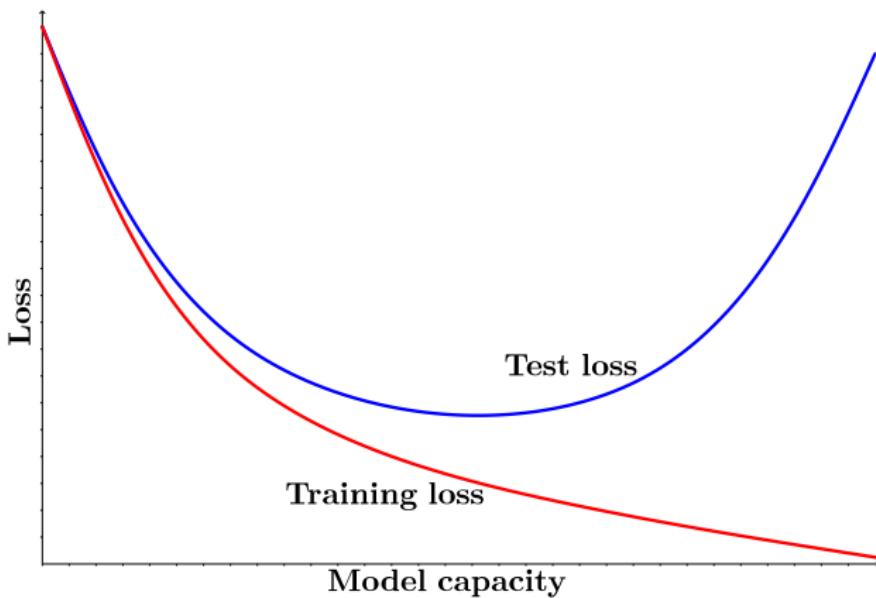


- The **variance** can be optimized by using **more training data**
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- What if we can't acquire more data?

Finite Dataset

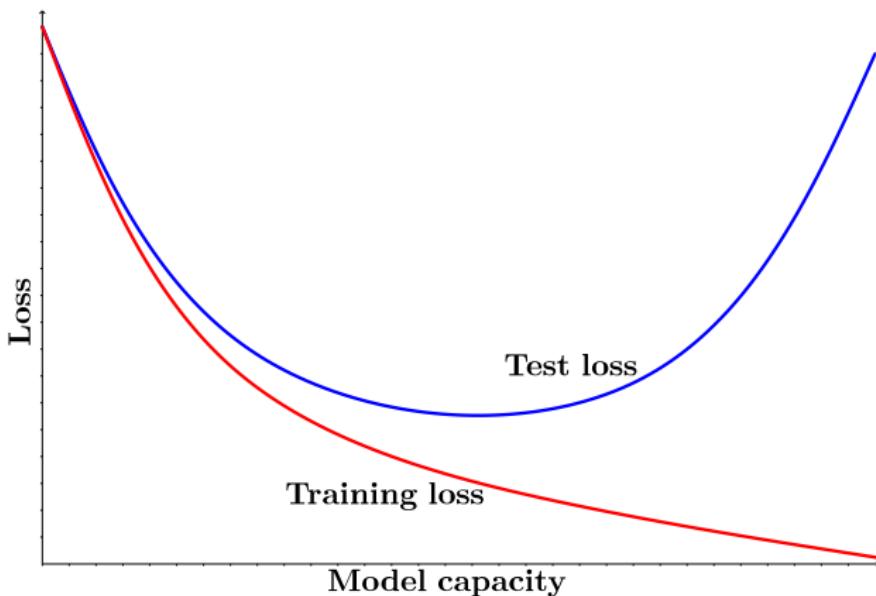


Finite Dataset



- 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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- Augment data
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Actual regularizers

- Equality constraints
- Inequality constraints



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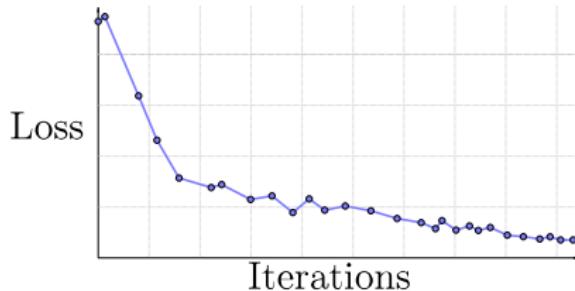
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Classical Techniques



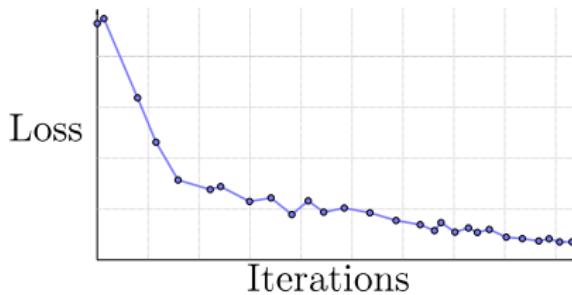
Overfitting on Learning Curve

Training set

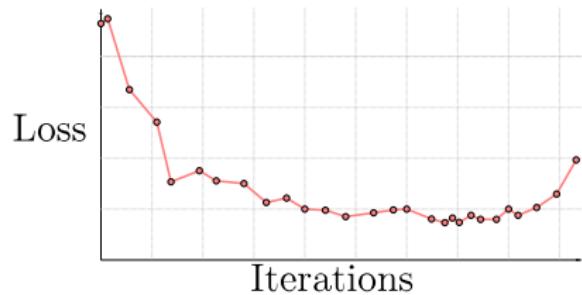


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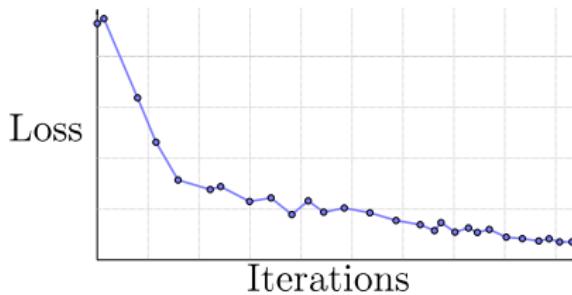


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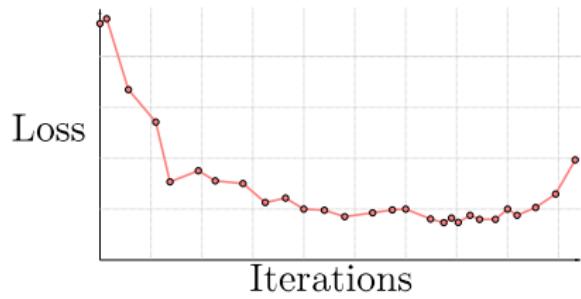


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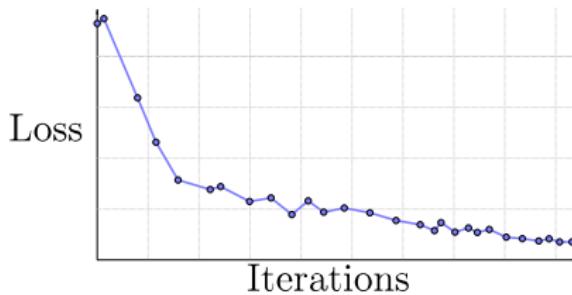
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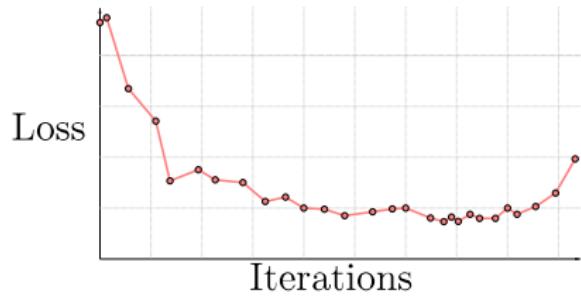
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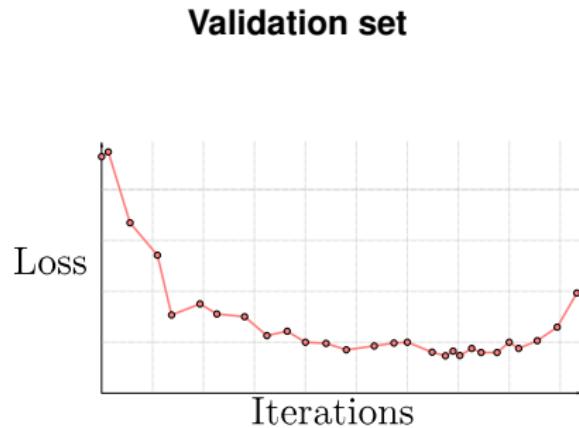


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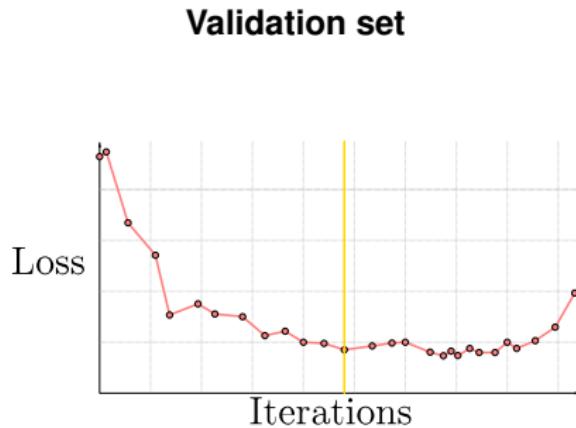


- Test set **must not** be used for training!
 - Split of **validation set** from training data

Early Stopping

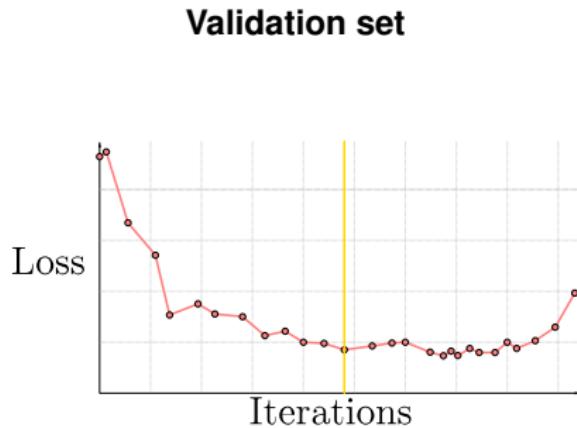


Early Stopping



- 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

→ Artificially enlarge dataset

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

Probably the same class:

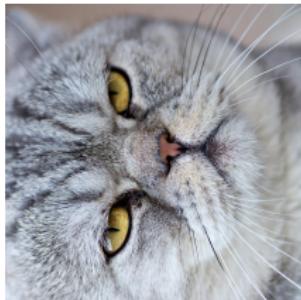


Data Augmentation

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Still you have to be careful!



Data Augmentation

Common transformations:

Data Augmentation

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1. random spatial transformations:
 - affine transformations
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Data Augmentation

Common transformations:

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

Regularization in the Loss Function

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

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MLE estimator Prior

Augmenting the Loss Function

Enforce

Augmenting the Loss Function

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with an unknown data-dependent α .

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Backpropagation of the augmented loss:

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- 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:

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

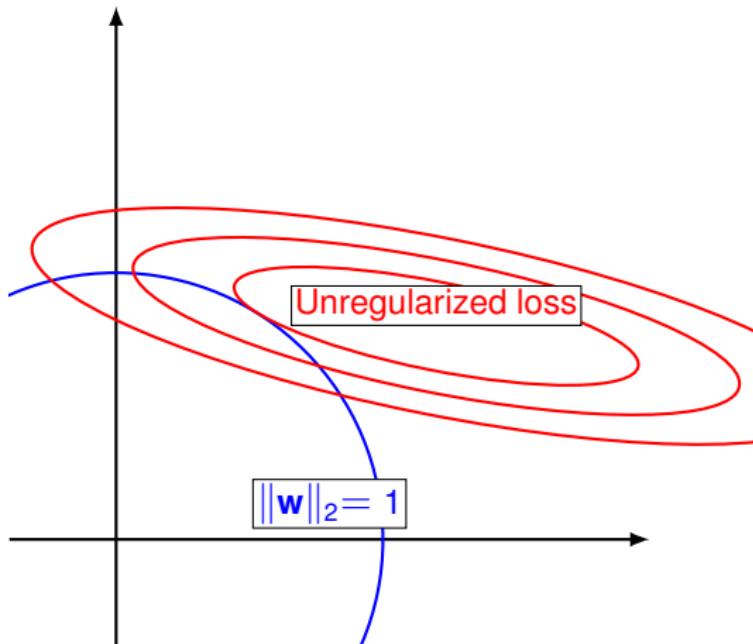
with an unknown data-dependent α .

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”
- If we optimize the **training-loss** for λ we will usually receive $\lambda = 0$.
- We trade increased **bias** for reduced **variance**

Graphical Effect of L₂ Regularization



Augmenting the Loss Function (cont.)

Enforce

Augmenting the Loss Function (cont.)

Enforce ...sparsity:

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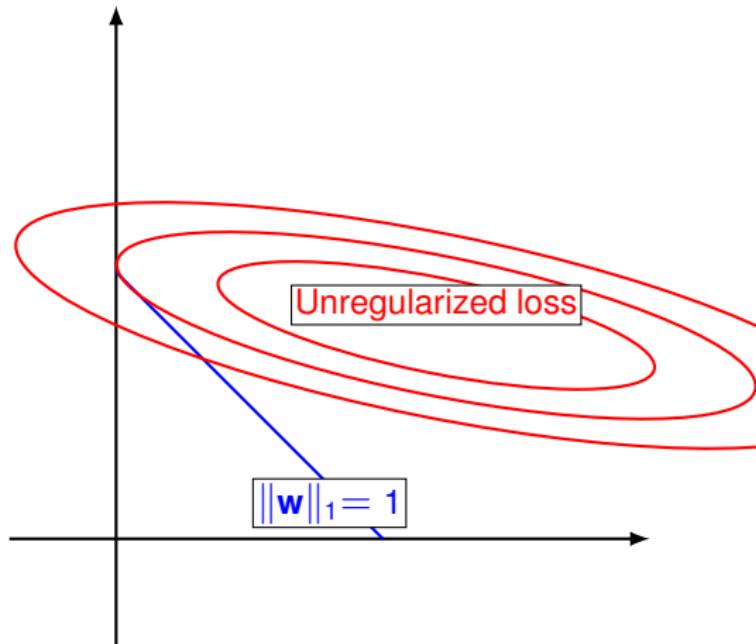
with an unknown data-dependent α .

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.)



Norm constraints

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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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- We can have a **constraint** and a λ **individual** for every layer
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- Instead of the weights, **activations** can be **constrained**
- Different variants have been used for **sparse autoencoders**
- We will cover this when we talk about unsupervised learning



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Normalization



Internal Covariate Shift

- ReLU is not **zero-centered**
- Initialization and input distribution might not be normalized
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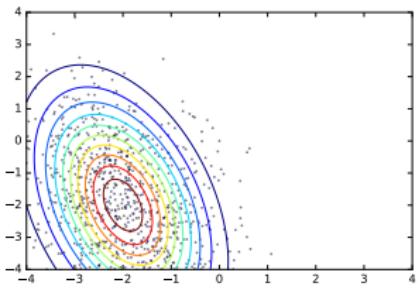
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 - **Slow learning**

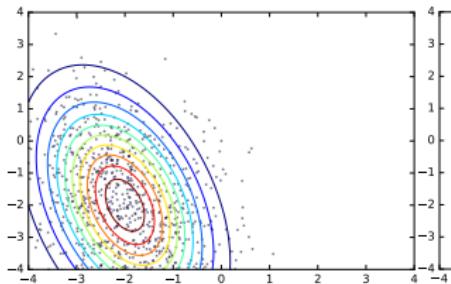
Data Normalization

Original data

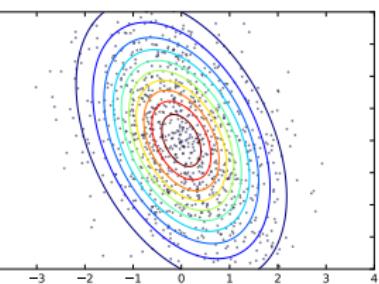


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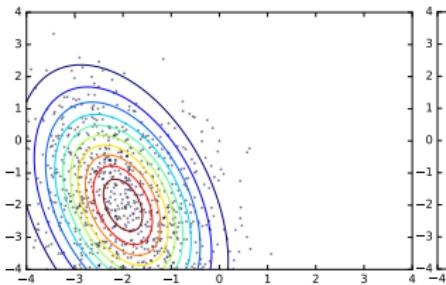


Mean subtracted

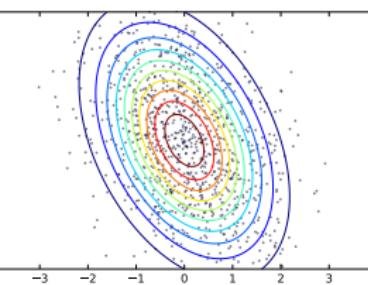


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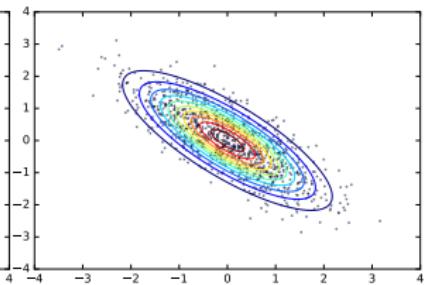
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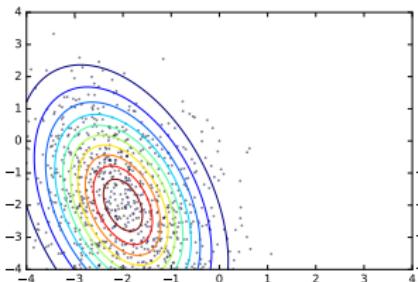


Normalized variance

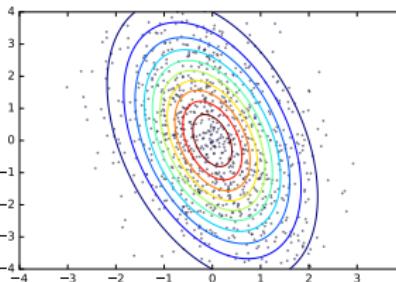


Data Normalization

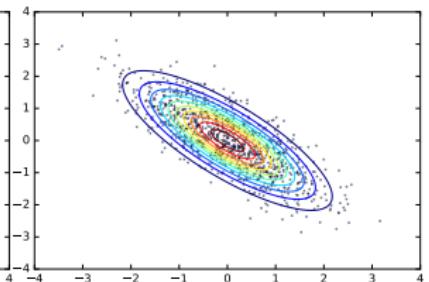
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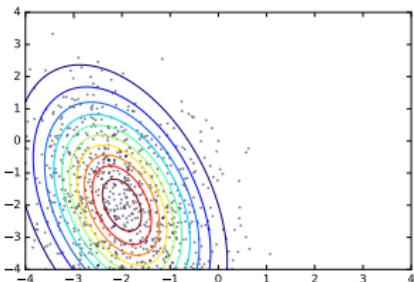
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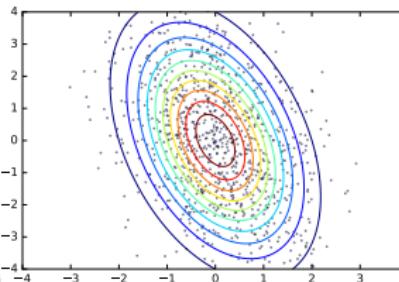
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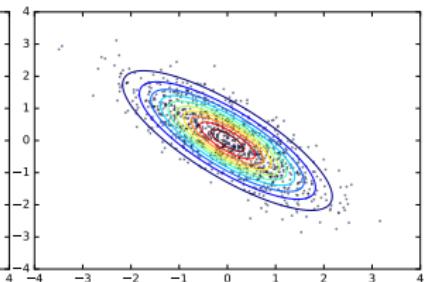
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- Normalization: min/max or **variance**
- Only use **training data** to calculate normalization!

Batch normalization

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$$\tilde{x}_i = \frac{x_i - \mu_{B,i}}{\sqrt{\sigma_{B,i}^2 + \epsilon}}$$

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- Paired with **convolutional** layers batch normalization is **different** by computing a **scalar** μ and σ for every **channel**.

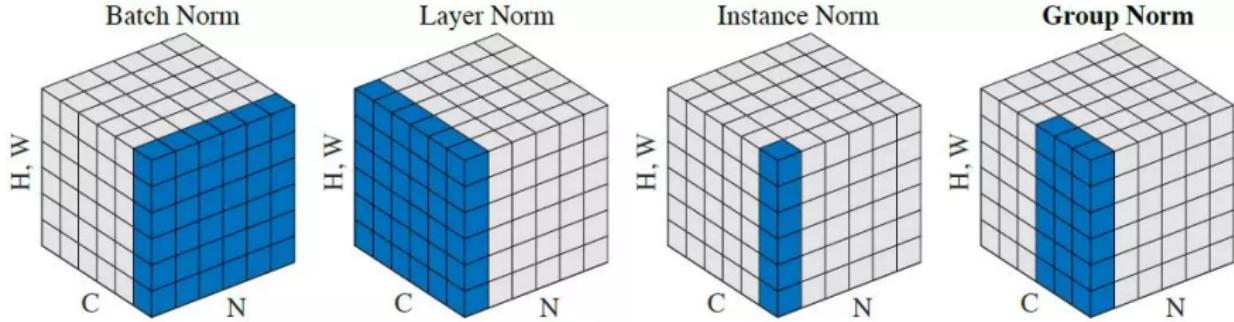
Generalizations

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

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 → [13], a layer → [3], spatial dims → [1], a group → [2]
- ... weights of a layer → [11]



Source: Wu et al. [2]

Self Normalizing Neural Networks

- Method that **addresses** the **stability problem** of SGD [19]

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

- Guarantee that μ and the σ of the activations stays near 0 and 1 through the network
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- The **SNN** concept resembles **batch normalization**



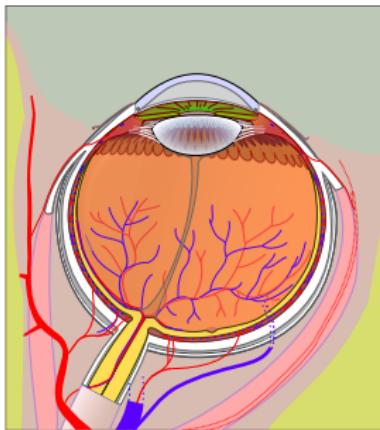
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Dropout



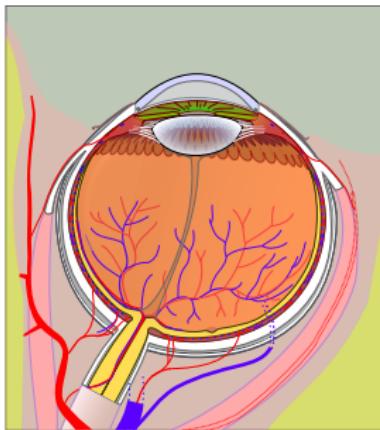
Co-adaptation



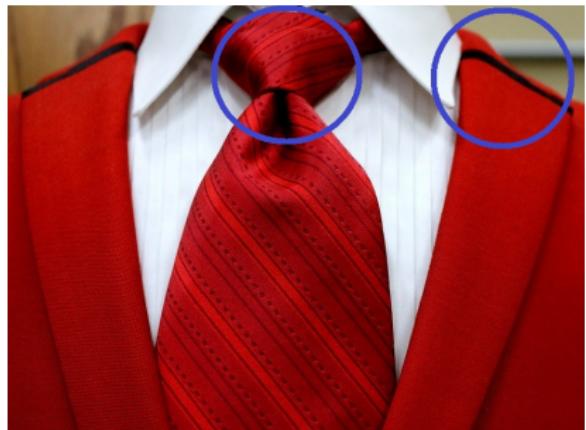
All elements **depend** on each other

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

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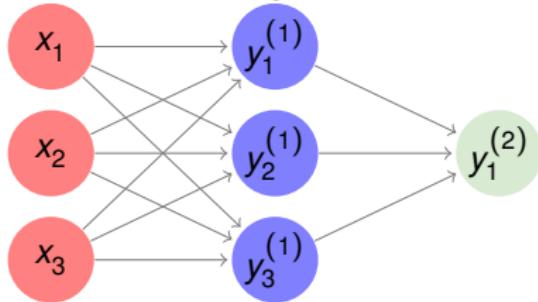


→Contrary to **independent** features

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

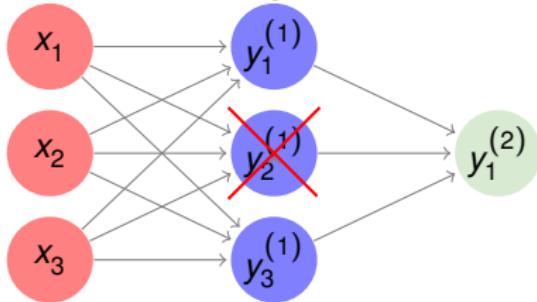
Dropout and Dropconnect

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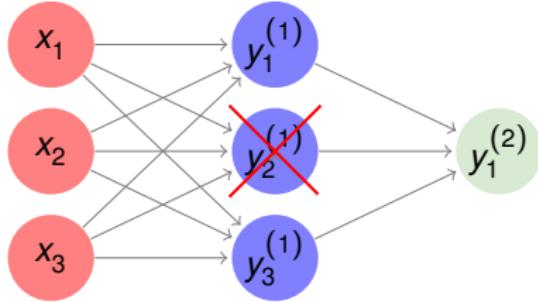
Dropout



- Randomly set activations to zero with probability $1 - p$

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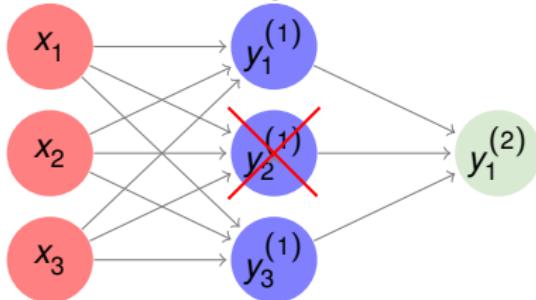
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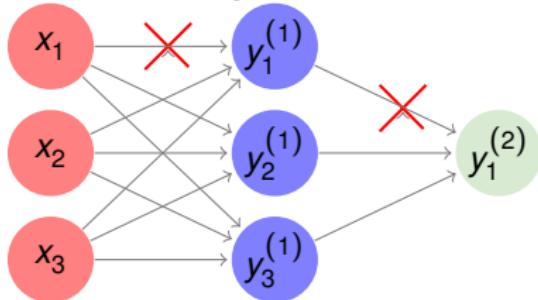
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- Generalizes Dropout
- Less efficient implementation (masking)



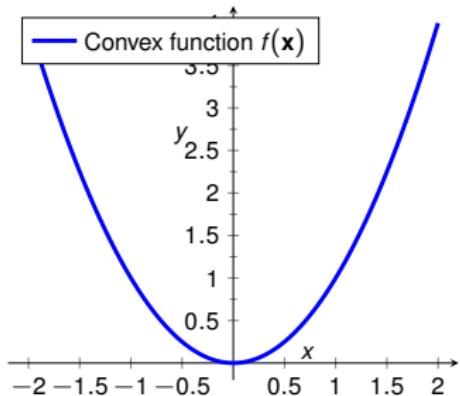
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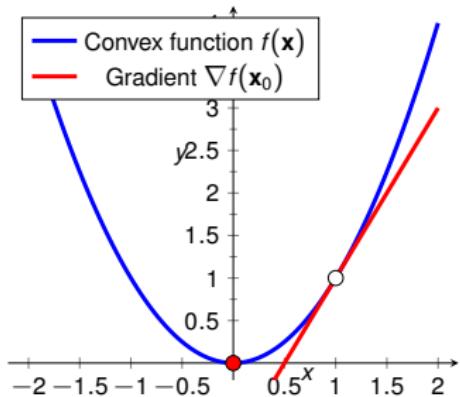
Initialization



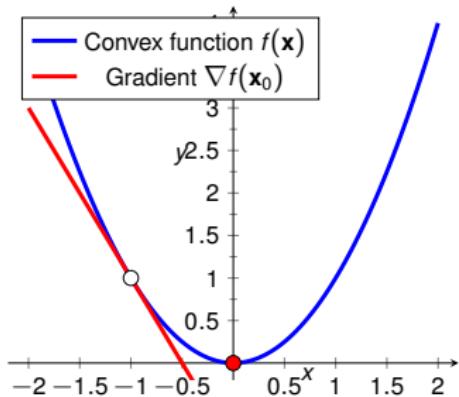
Does initialization matter?



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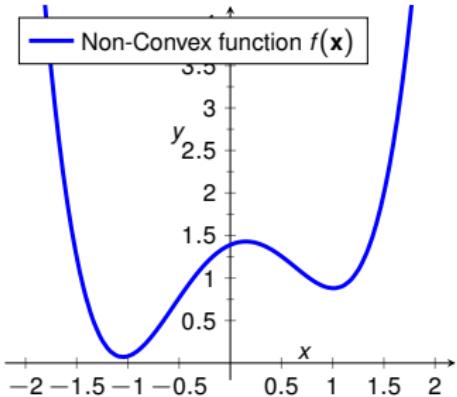


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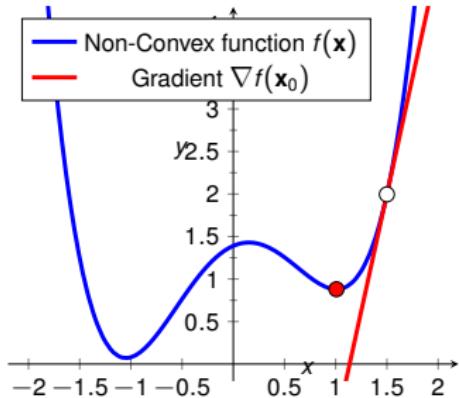
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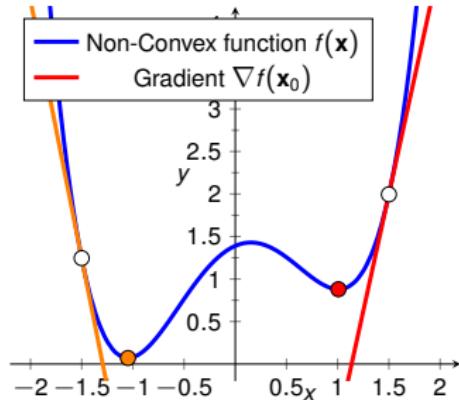
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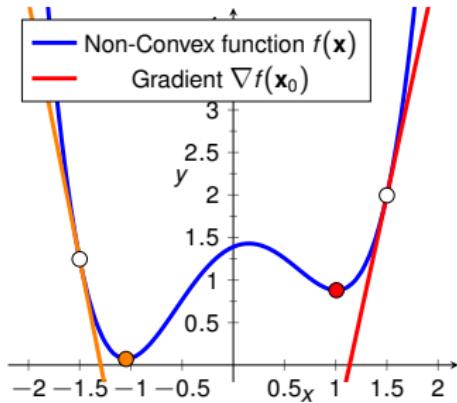
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- But it **does** for every **non-convex** problem
- Neural Networks with a non-linearity are in general **non-convex**

Simple Initialization

Bias

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

Weights

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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**
- Capital letters here mark them as **random variables!**

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- Now we assume the X_n and W_n to be **Independent and Identically Distributed**:

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

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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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 [17]

He initialization

- the assumption of **linear** neurons is a problem
- He et al. [18] 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



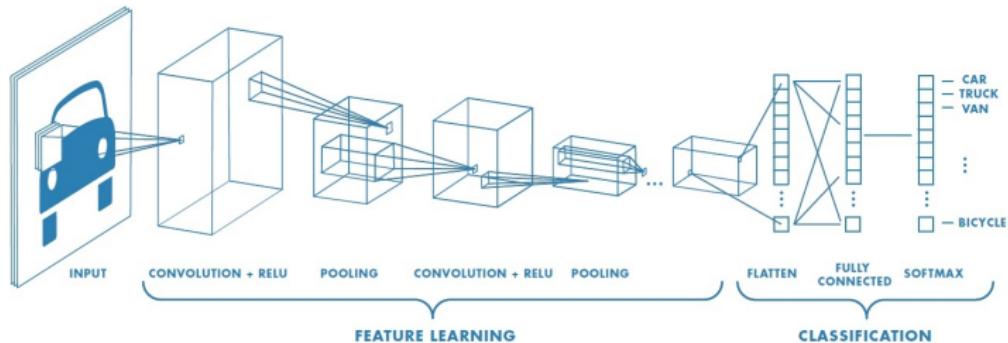
Transfer Learning

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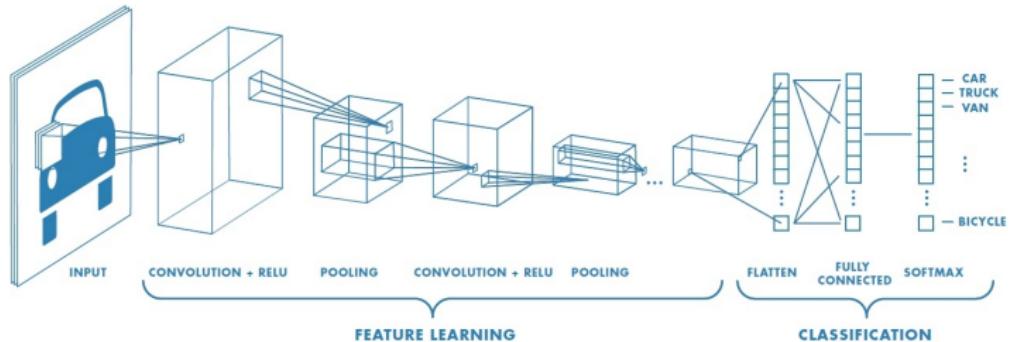
- Most **medical datasets** are prohibitively **small**
- **Reuse models** trained on e.g. ImageNet
 - for a **different task** on the **same data**
 - on **different data** for the **same task**
 - on **different data** for a **different task**

Weight Transfer



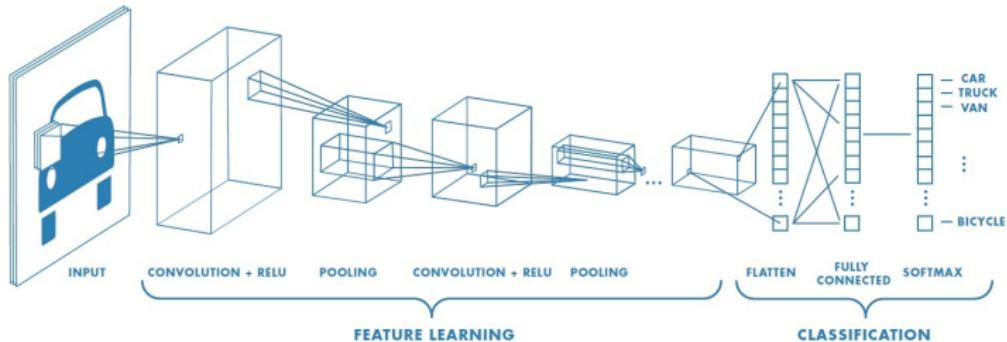
- What should we transfer?

Weight Transfer



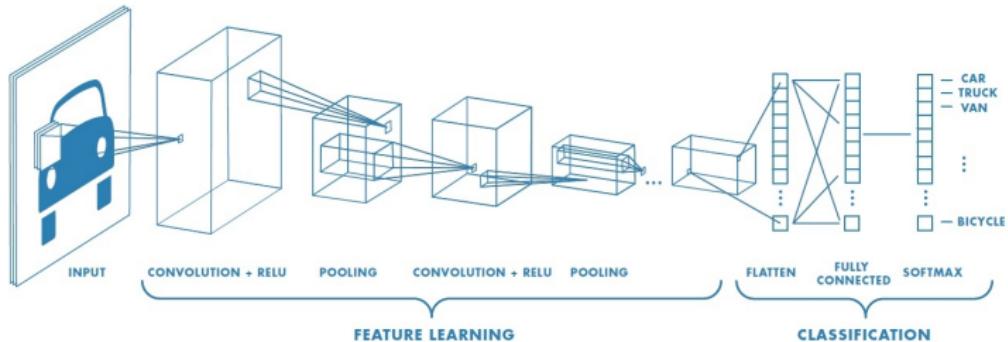
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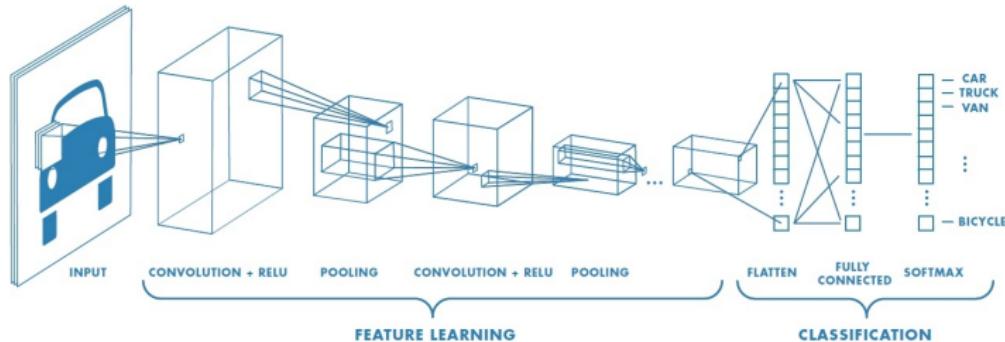
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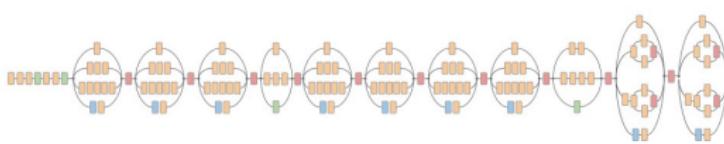
- What should we transfer?
 - Convolutional layers extract features
 - Expectation: Less task-specific in earlier layers
- We cut the network at some depth in the feature extraction part
- The extracted parts can be
 1. fixed by setting $\eta = 0$
 2. **fine-tuned**

Example: Skin Cancer classification

Skin lesion image



Deep convolutional neural network (Inception v3)



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

Training classes (757)

- Acral-lentiginous melanoma
- Amelanotic melanoma
- Lentigo melanoma
- ...
- Blue nevus
- Halo nevus
- Mongolian spot
- ...
- ...

- State-of-the-art architecture, pre-trained on ImageNet
- Fine-tuned on skin cancer data [21]

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

Transfer between modalities

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- Always use transfer learning!



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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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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**

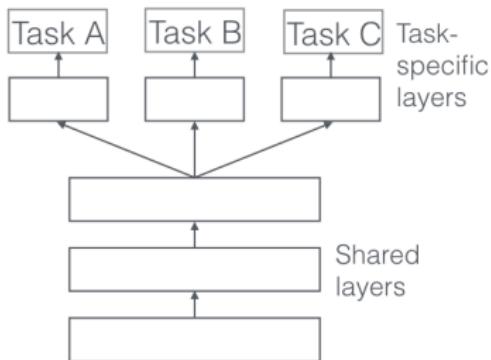
Concept (cont.)

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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 [4]
→ model generalizes better

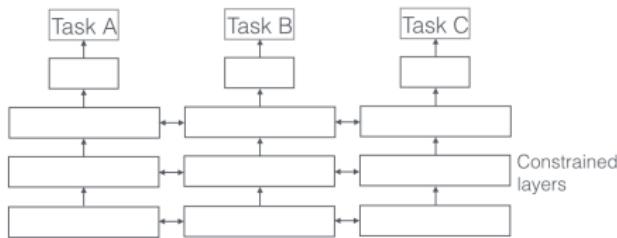
Hard parameter sharing



- Several hidden layers shared between all tasks
- Additional task-specific output layers
- Baxter '97 [4]: 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

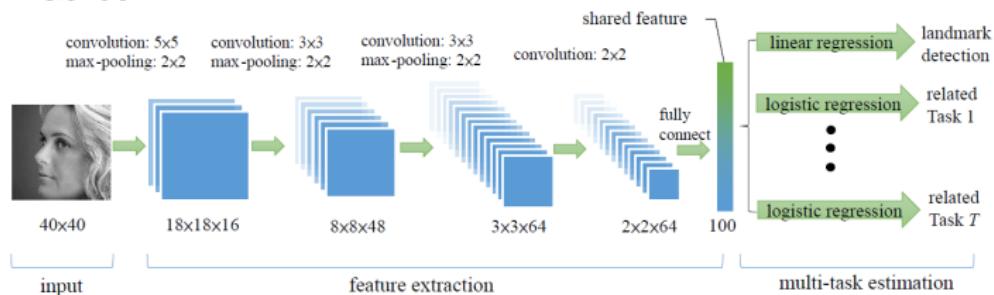
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Auxiliary tasks

- Additional tasks have own purpose or are just **auxiliary** to the original task
- Example: **Facial Landmark Detection** by Zhang et al. 2014 [20]
- Facial landmark detection impeded by occlusion and pose variances
- Simultaneously learn to estimate landmarks **and** “subly” related task:
 - Face pose
 - Smiling/not smiling
 - Glasses/no glasses (occlusion)
 - Gender



Network architecture

Auxiliary tasks (cont.)

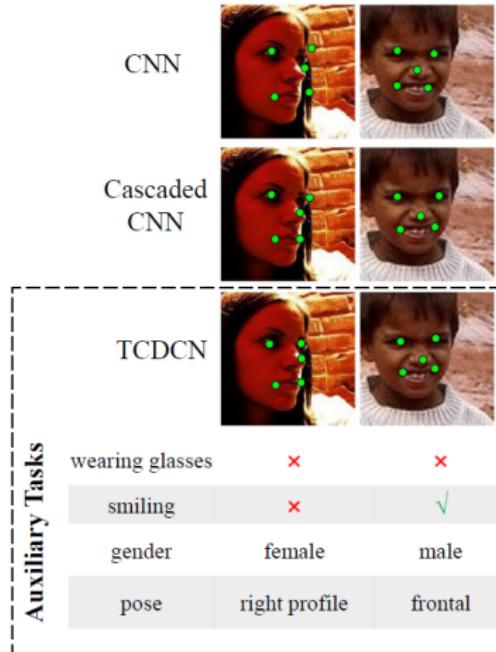
	CNN	CNN	CNN	CNN	CNN	CNN	CNN
	Cascaded CNN	Cascaded CNN	Cascaded CNN	Cascaded CNN	Cascaded CNN	Cascaded CNN	Cascaded CNN
	TCDCN	TCDCN	TCDCN	TCDCN	TCDCN	TCDCN	TCDCN
Auxiliary Tasks	wearing glasses	x	x	v	x	v	x
	smiling	x	v	x	x	x	x
	gender	female	male	female	female	male	male
	pose	right profile	frontal	frontal	left	frontal	frontal
							female

Landmark detection

Source: [20]

Auxiliary tasks (cont.)

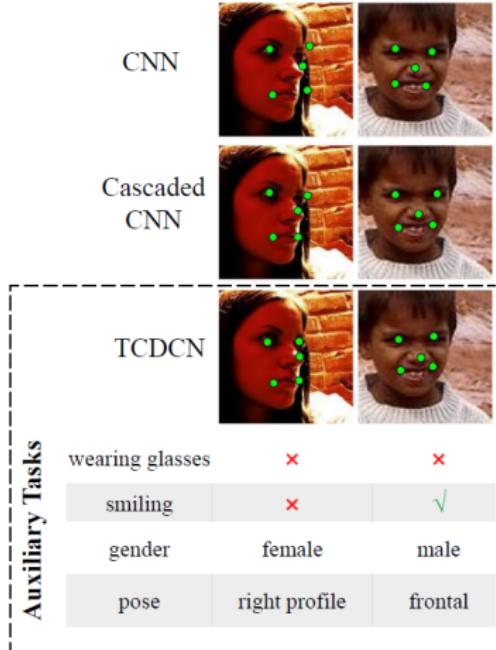
- Certain features difficult to learn for one task but easy for a related one [7]



Source: [20]

Auxiliary tasks (cont.)

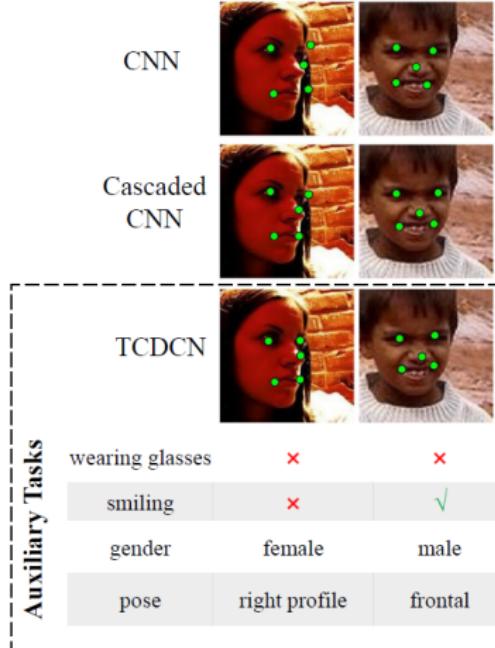
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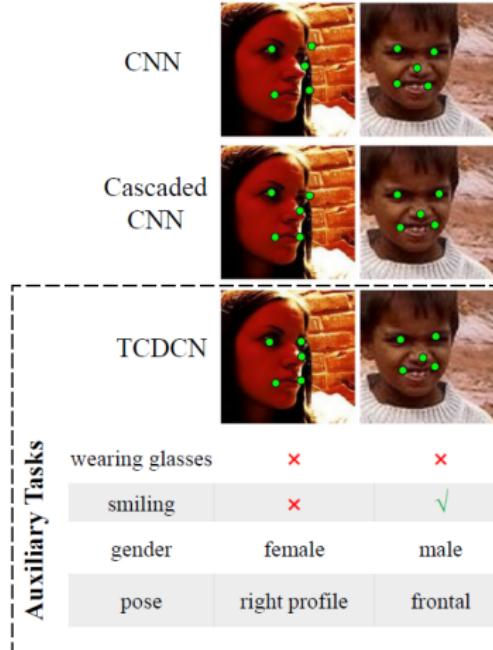
- Certain features difficult to learn for one task but easy for a related one [7]
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→ Task-based early-stopping



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Auxiliary tasks (cont.)

- Certain features difficult to learn for one task but easy for a related one [7]
- 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: [20]

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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