Lecture 10 – Summary and reflections

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Contents – Lecture 10

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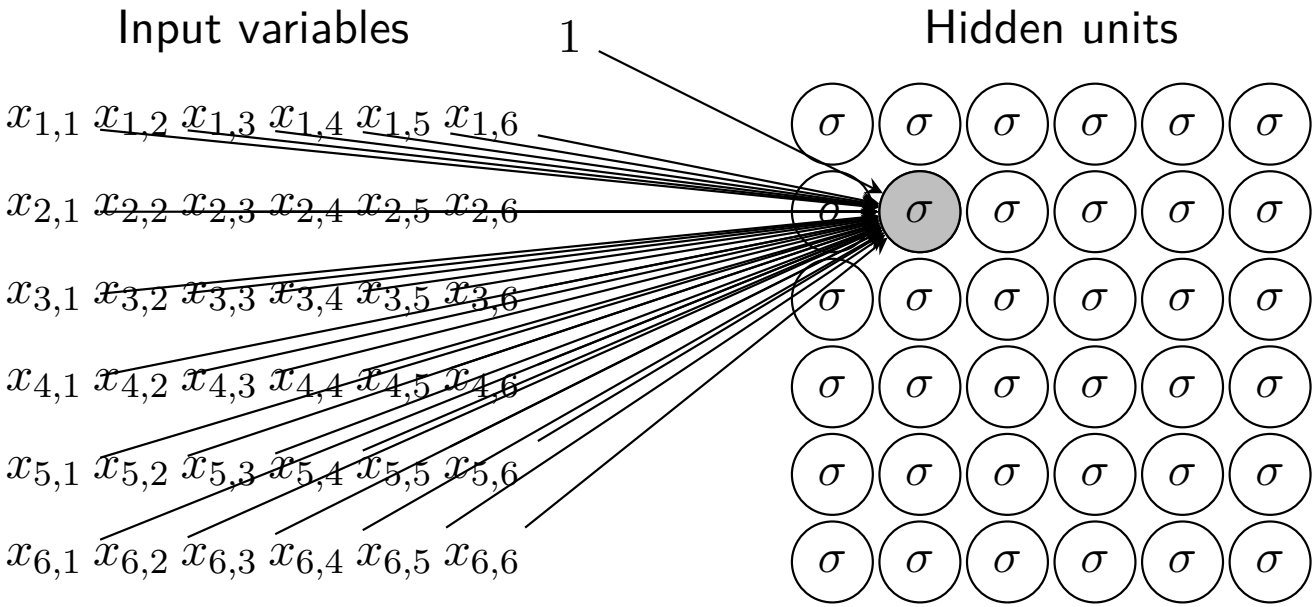
2. Summary of the course
3. Outlook: *a few words about things that we have not covered*
4. More machine learning!

Summary of Lecture 9 (I/IV)
Convolutional layer

Consider a hidden layer with 6×6 hidden units.

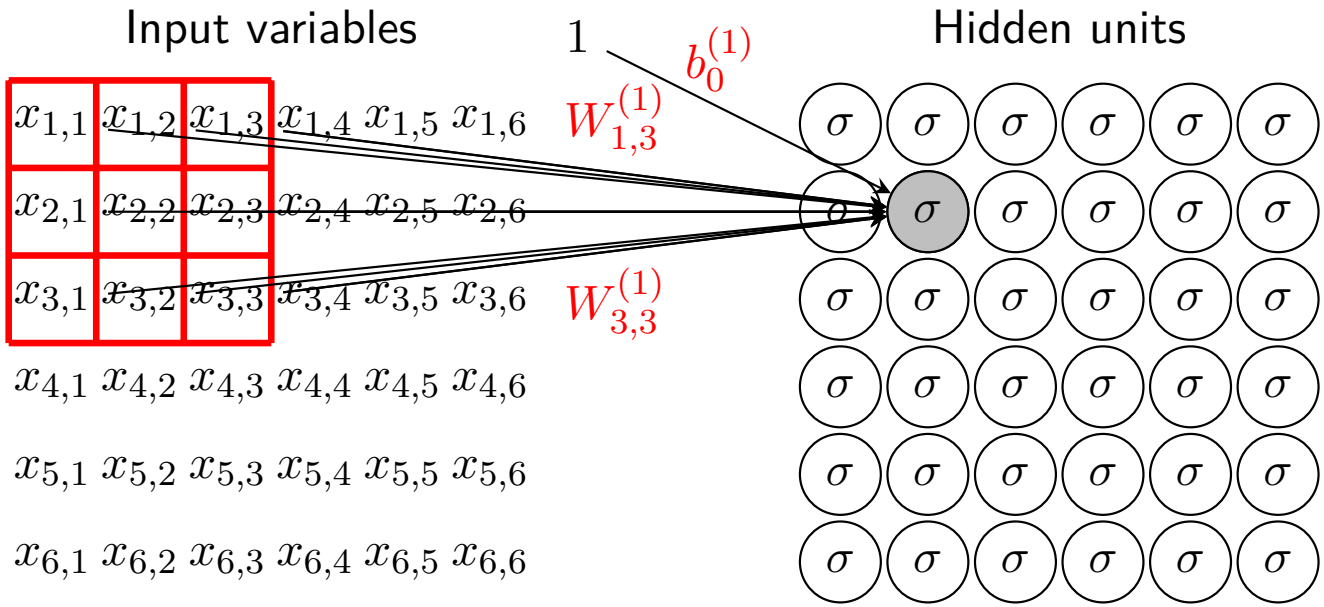
- **Dense layer**: Each hidden unit is connected with **all pixels**. Each pixel-hidden-unit-pair has its own **unique parameter**.



Summary of Lecture 9 (I/IV)
Convolutional layer

Consider a hidden layer with 6×6 hidden units.

- **Dense layer**: Each hidden unit is connected with **all pixels**. Each pixel-hidden-unit-pair has its own **unique parameter**.
- **Convolutional layer**: Each hidden unit is connected with a **region of pixels** via a set of parameters, so-called **kernel**. Different hidden units have the **same set of parameters**.



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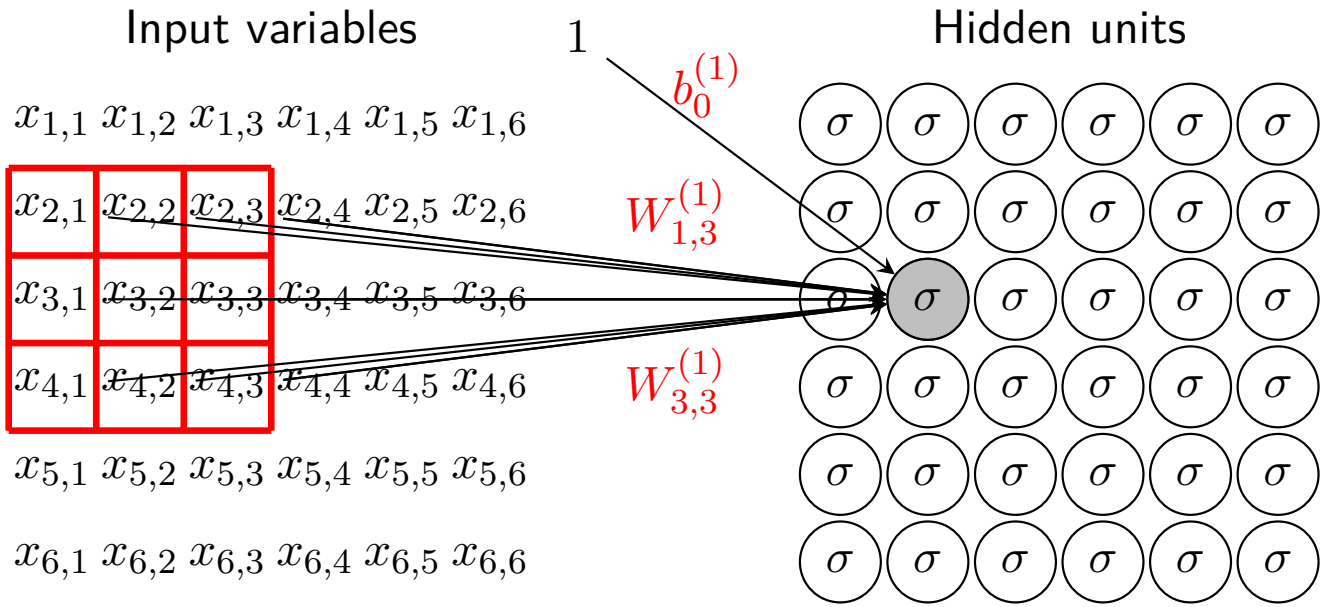

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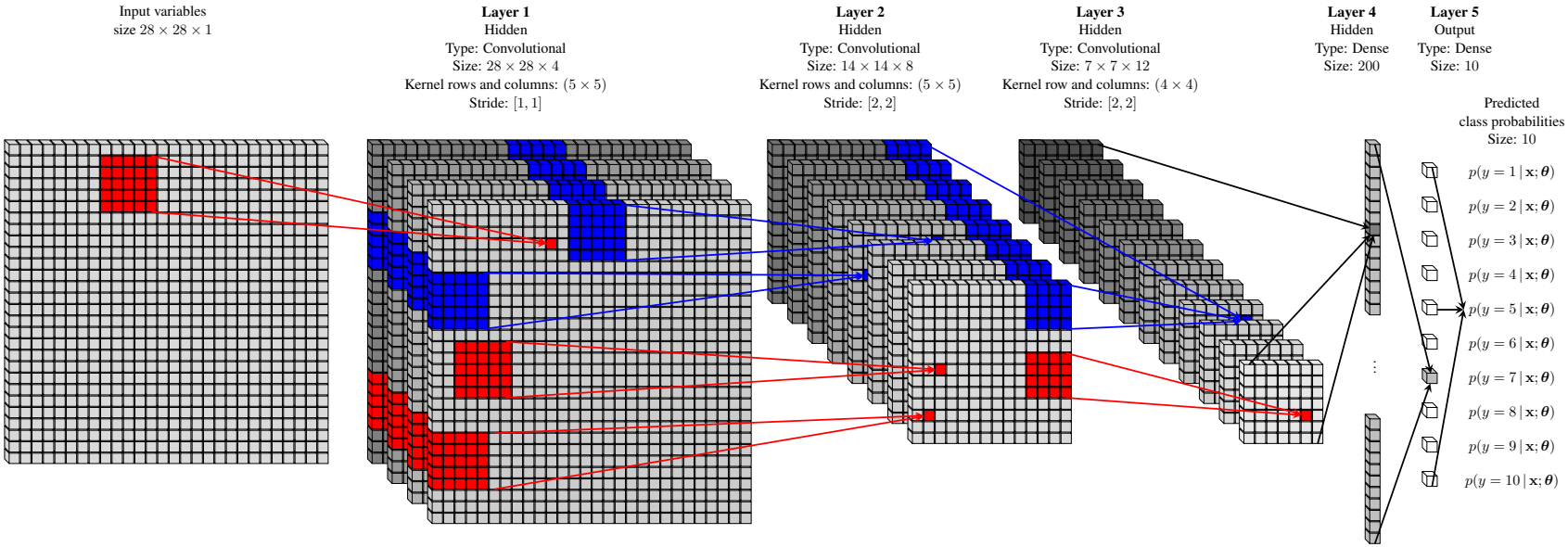
Summary of Lecture 9 (II/IV)
Convolutional neural network (CNN)

A full CNN usually consist of

- multiple convolutional layers (here three),...
- ...and a few final dense layers (here two).



Summary of Lecture 9 (III/IV)
Training a neural network

We train a network by considering the optimization problem

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}), \qquad J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L(\mathbf{x}_i, \mathbf{y}_i, \boldsymbol{\theta})$$

- $\boldsymbol{\theta}$ – all parameters of the network
- $\widehat{\boldsymbol{\theta}}$ – the estimated parameters
- $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{n}$ – the training data
- $L(\mathbf{x}_i, \mathbf{y}_i, \boldsymbol{\theta})$ – the loss function (for example cross-entropy)
- $J(\boldsymbol{\theta})$ – the cost function

Summary of Lecture 9 (IV/IV)
Stochastic gradient descent

At each optimization step we need to compute the gradient

$$\mathbf{g}_t = \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_t) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\theta}} L(\mathbf{x}_i, \mathbf{y}_i, \boldsymbol{\theta}_t).$$

Challenge - n is big - expensive to compute gradient.
Solution: For each iteration, we only use a small random batch of the data set – a **mini-batch** – to compute the gradient $\mathbf{g}_t$. This procedure is called the **stochastic gradient descent**.

Training data (reshuffled)

$\mathbf{x}_{19}$	$\mathbf{x}_{16}$	$\mathbf{x}_{18}$	$\mathbf{x}_6$	$\mathbf{x}_9$	$\mathbf{x}_{13}$	$\mathbf{x}_1$	$\mathbf{x}_{14}$	$\mathbf{x}_{20}$	$\mathbf{x}_{11}$	$\mathbf{x}_3$	$\mathbf{x}_8$	$\mathbf{x}_7$	$\mathbf{x}_{12}$	$\mathbf{x}_4$	$\mathbf{x}_{17}$	$\mathbf{x}_5$	$\mathbf{x}_{10}$	$\mathbf{x}_2$	$\mathbf{x}_{15}$
$\mathbf{y}_{19}$	$\mathbf{y}_{16}$	$\mathbf{y}_{18}$	$\mathbf{y}_6$	$\mathbf{y}_9$	$\mathbf{y}_{13}$	$\mathbf{y}_1$	$\mathbf{y}_{14}$	$\mathbf{y}_{20}$	$\mathbf{y}_{11}$	$\mathbf{y}_3$	$\mathbf{y}_8$	$\mathbf{y}_7$	$\mathbf{y}_{12}$	$\mathbf{y}_4$	$\mathbf{y}_{17}$	$\mathbf{y}_5$	$\mathbf{y}_{10}$	$\mathbf{y}_2$	$\mathbf{y}_{15}$

Iteration: 6

Epoch: 2

This course

Machine learning gives computers the ability to
solve problems without being explicitly programmed
for the task at hand. This is done by **learning from examples**,

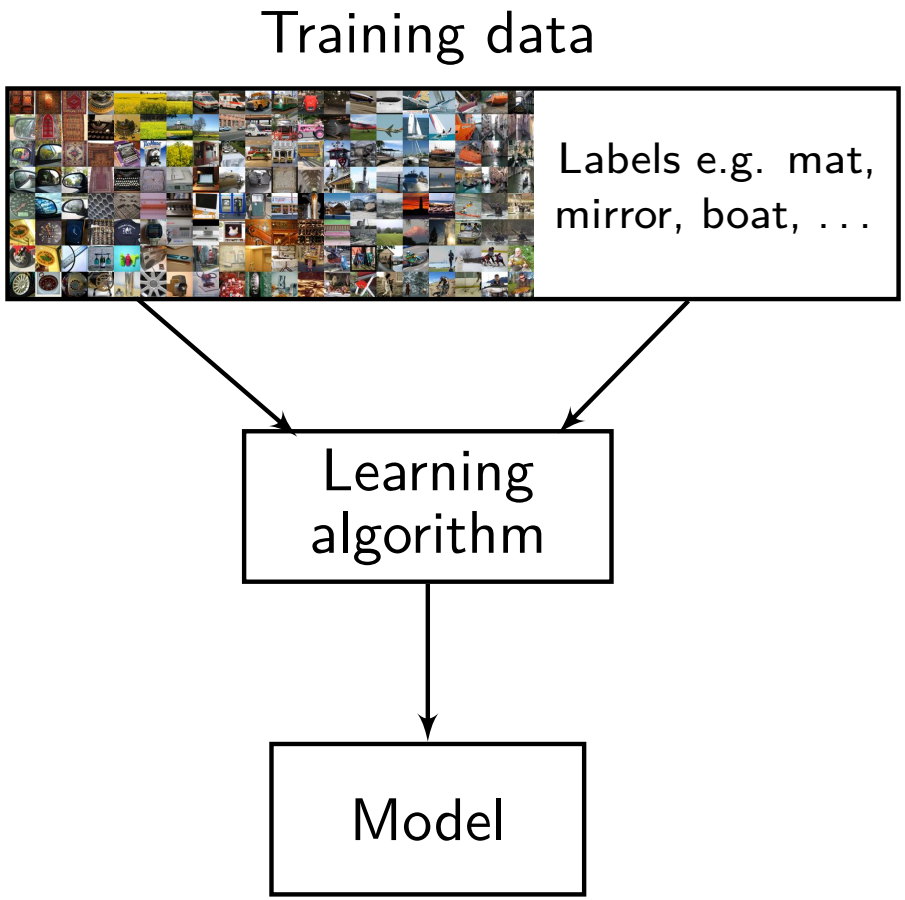
i.e. from training data.

Data on its own is typically useless, it is only when we can extract knowledge from the data that it becomes useful.

Specifically, we have studied **supervised learning** methods, in which we build a **model** of the relationship between an input variable x and an output variable y.

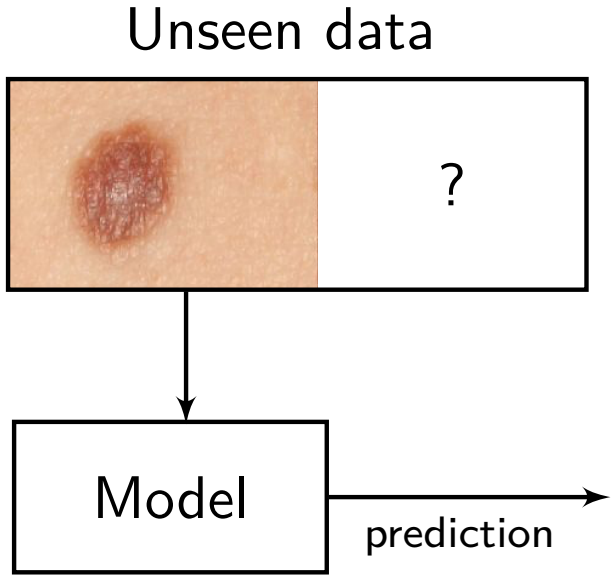
Supervised Machine Learning

Learning a model from labeled data.



Supervised Machine Learning

Using the learned model on new previously unseen data.



The model must **generalize** to new unseen data.

Inputs and outputs

The **input** $\mathbf{x}$ is composed of all the ***available*** variables which are believed to be relevant for predicting the value of the **output** y.

We have considered the case where we have p input variables, $\mathbf{x} = (x_j)_{j=1}^{p}$, and one output variable y.

Both the inputs x_j and the output y can be either

- **numerical/quantitative** (can be ordered), or
- **categorical/qualitative** (takes values in an unordered set).

Regression and classification

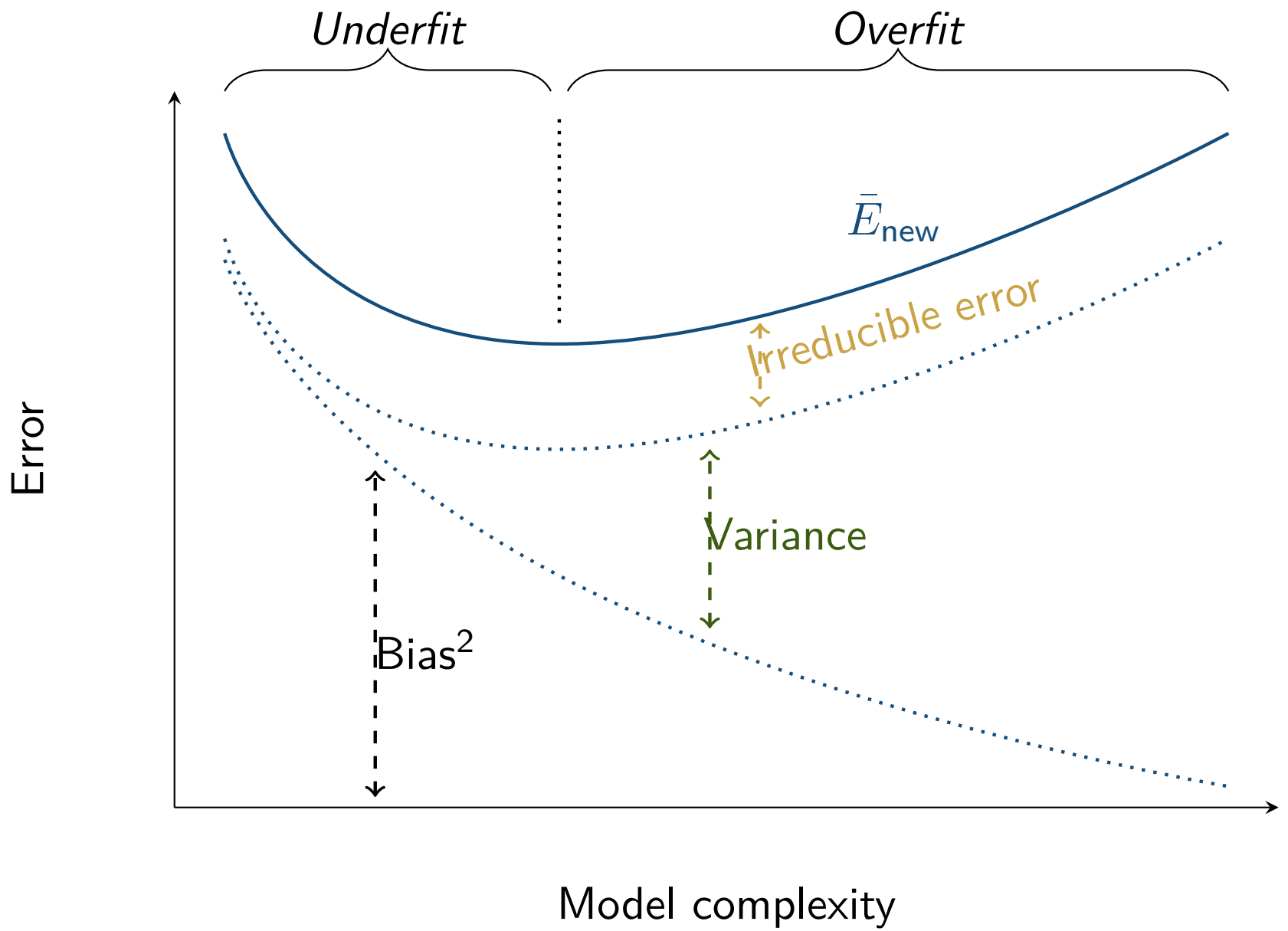
	Regression	**Classification**
Output, y	**numerical**	**categorical**
Inputs, x_j	numerical or categorical	numerical or categorical
Model("conceptual")	$y = f(\mathbf{x}) + \varepsilon$	$p(y = k \mid \mathbf{x})$, $k = 1, \ldots, K$

Bias-variance

- E_{new}: How well a method will perform for unseen data.
- Bias: The inability of a **model** to describe the training data.
- Variance: How sensitive a **model** is to noise in training data.

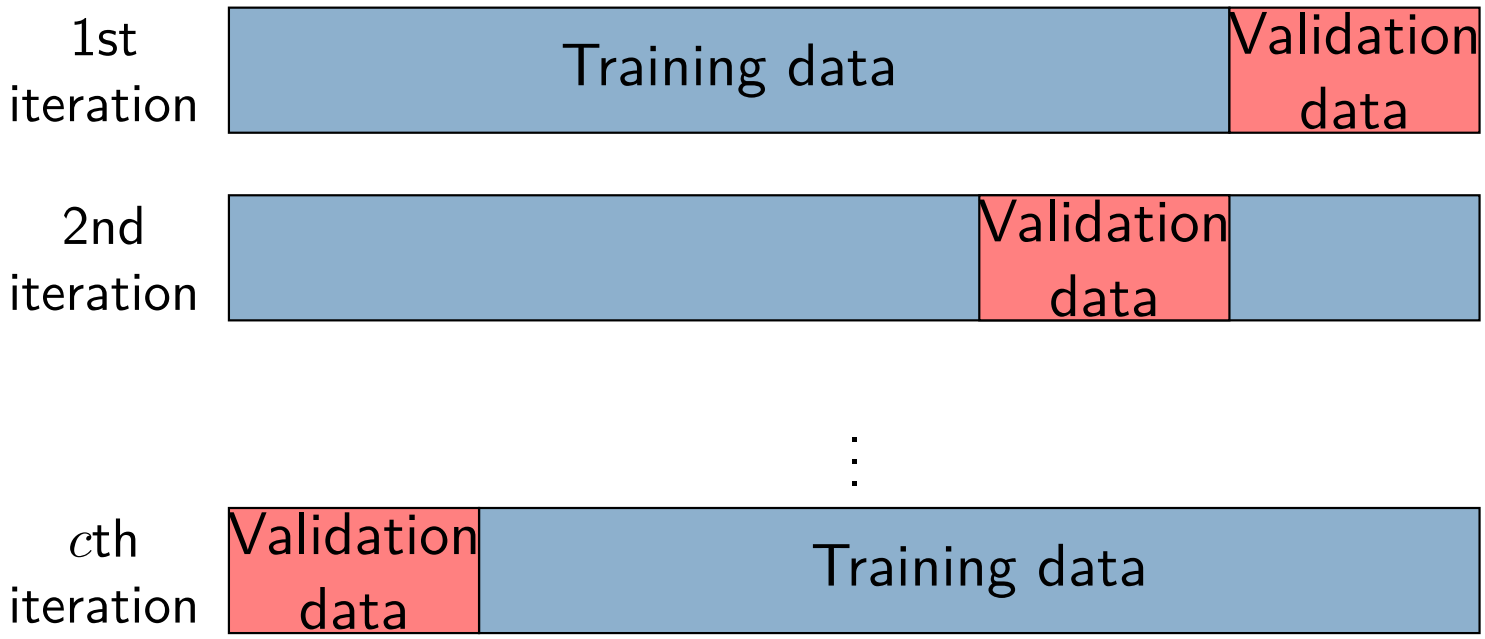
$$E_{\text{new}} = \text{bias}^2 + \text{variance} + \text{irreducible error}$$

Bias-variance



Cross validation

To estimate E_{new}, we can use cross-validation.



When using cross validation to select, e.g., inputs and hyperparameters, there is a risk of overfitting! (But it can still be the best available option . . .)

Regularization

Regularization offers a way to decrease the model complexity (and hence risk of overfitting)

- **Ridge Regression**: add a penalty term $\lambda \|\boldsymbol{\theta}\|_2^2$
- **LASSO:** add a penalty term $\lambda \|\boldsymbol{\theta}\|_1$ – can result in ***sparse*** solutions

Select λ, e.g. by cross validation!

There are also other ways to change the model complexity:

- Increase k in k-NN
- Boosting

Parametric vs. nonparametric models

Parametric models

- Parameterized by a **finite-dimensional parameter $\boldsymbol{\theta}$**
- Training/learning the model = estimating $\widehat{\boldsymbol{\theta}}$
- Once $\widehat{\boldsymbol{\theta}}$ is estimated, the predictions depend only on $\widehat{\boldsymbol{\theta}}$ (not the training data)
- ***ex)*** Linear regression, LDA, QDA, Neural Networks

Nonparametric models

- The model **flexibility** is allowed to **grow** with the amount of available data
- **Predictions depend directly on the training data**
- Can be viewed as having an infinite number of parameters
- ***ex)*** k-NN, CART

Ensemble methods

Ensemble methods are a type of "meta algorithms":

> Construct **one powerful model** from multiple **base models** (=ensemble members), each of which may perform poorly on its own!

We have encountered two such approaches:

1. **Bagging:** Reduce variance of low-bias/high-variance models by **bootstrap aggregation**
2. **Boosting:** Construct **weak base models** sequentially, so that each model tries to **correct the mistakes** of the previous one

A toolbox of methods

	Regression	Classification	Non-parametric	Parametric	Ensemble
Linear regression	✓			✓	
Logistic regression		✓		✓	
LDA		✓		✓	
QDA		✓		✓	
k-NN	✓	✓	✓		
CART	✓	✓	✓		
Random Forests	✓	✓	✓		✓
AdaBoost		✓		(✓)	✓
(Deep) Neural nets	✓	✓		✓	

Summary for the exam (in one slide)

- Classification and regression problem formulations
- Parametric and non-parametric models
- Inputs and outputs / numerical and categorical and variables
- Decision boundaries / linear vs. nonlinear classifiers
- Cross-validation (the purpose!) and model testing
- Bias-variance trade-off / model flexibility / over-fitting
- Regularization / ridge regression and LASSO
- The **different methods** discussed throughout the course

Summary for life

What should you remember from statistical machine learning?

- The problem formulations: **regression** and **classification**
- The **existence** of different types of methods
- The **bias-variance trade-off** and **cross validation**
- The **possibilities**: Machine learning can be used for an extremely wide range of applications and data types

The TSTF principle: **Try simple things first!**

Outlook: Unsupervised learning

Regression and classification are **supervised learning** problems – The models are trained using both inputs $\mathbf{x}$ and outputs y.

Unsupervised learning methods tries to find patterns in ***unlabeled*** data, i.e. we train the models from just the $\mathbf{x}$.

- Dimensionality reduction / manifold learning
- Cluster analysis
- Generative model learning[1]
- Blind source separation

[1] e.g. `https://www.thispersondoesnotexist.com/`

Outlook: Reinforcement learning

A **reinforcement learning** system is asked to take ***actions*** that influence its ***environment*** in order to maximize a ***reward***.

Contrary to supervised learning,

- the correct input/output pair is not revealed
- learning has to be carried out based on the reward feedback
- often a focus on online performance
  ($\Rightarrow$ exploration-exploitation trade-off)

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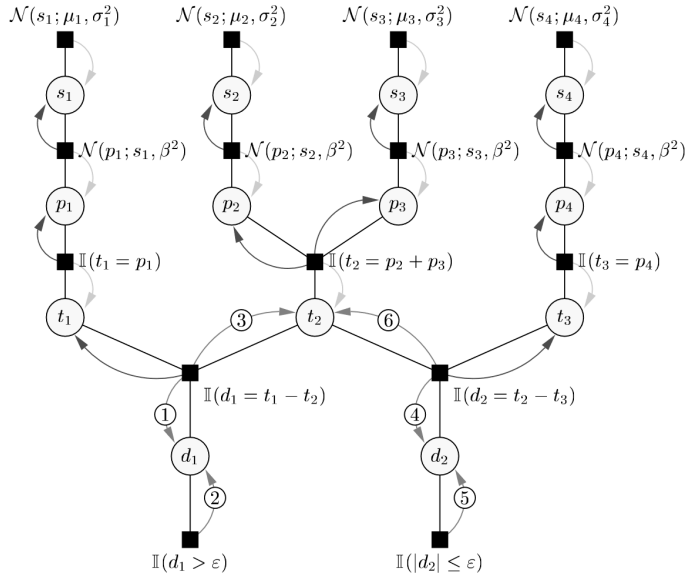
Advanced probabilistic machine learning

Contents (very brief):

- Probabilistic/Bayesian modeling
- Bayesian linear regression
- Graphical models
- Gaussian processes
- Variational inference
- Monte Carlo methods
- Unsupervised learning
- Variational autoencoders



Examination: Mini-project, lab, oral exam.

When: Period 1.

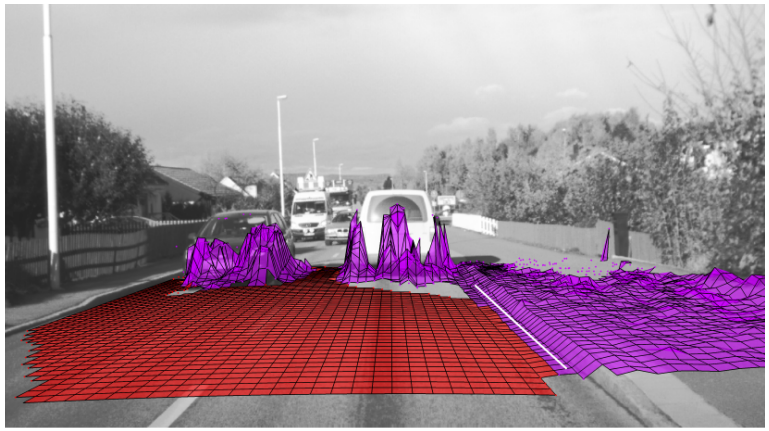
Info: `http://www.it.uu.se/edu/course/homepage/apml/`

Welcome!

Our Machine Learning research – ultrabrief

- Monte Carlo methods (especially sequential Monte Carlo)
- Deep learning
- Gaussian processes
- The use of probabilistic programming
- Applications: Autonomous driving (with Autoliv), digital pathology (with Sectra), etc.

We take a particular interest in nonlinear dynamical systems.



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Thank you!

Machine learning gives computers the ability to
solve problems without being explicitly programmed
for the task at hand.

Thank you for your attention and good luck in the future!!!