Machine learning foundations II

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Learning goals

At the end of this lecture you will:

- Have a good understanding of the basic principles of machine learning (ML) and be able to apply them in the analysis of ML methods.
- Be able to design good experimental setups for developing ML models.
- Have a good understanding of the different evaluation measures for ML models.

Overview

Topics covered in this lecture:

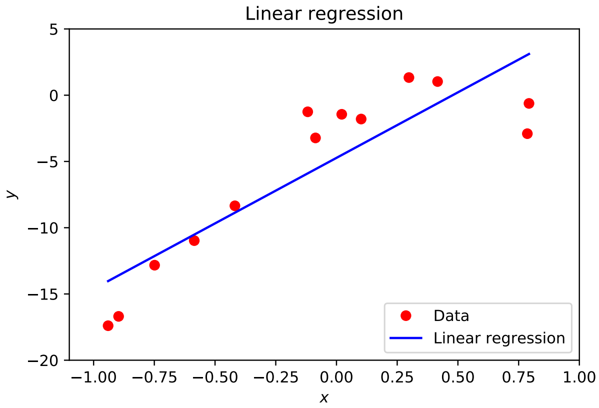
1. Model capacity, underfitting and overfitting
2. Model selection
3. Bias and variance trade-off
4. Maximum likelihood estimation
5. Supervised and unsupervised learning algorithms
6. Model evaluation
7. Ensambling

Model capacity, underfitting and overfitting

Materials:

- Chapter I.5.2 from Goodfellow et al., *Deep Learning*

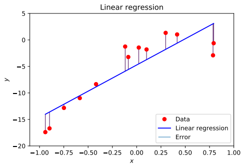
Linear regression

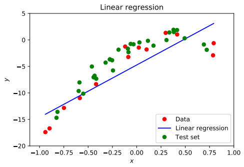


$$\hat{y} = \hat{w}_0 + \sum_{i=1}^{n} x_i \hat{w}_i$$
$$\hat{y} = \boldsymbol{x}^T \hat{\boldsymbol{w}}$$

Generalization

- The central challenge in machine learning is to design an algorithm which will perform well on new data (different from the training set data).
- This ability is called **generalization**.
- **Training error** is the error computed on the training set.
- During the training (learning) we aim at reducing the training error.
- If that is the end goal, we only have an optimization problem, not a machine learning one.



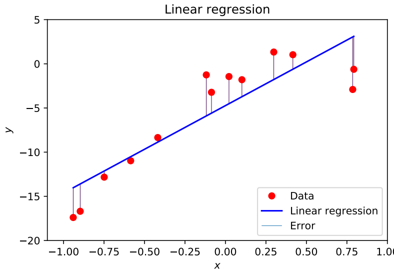


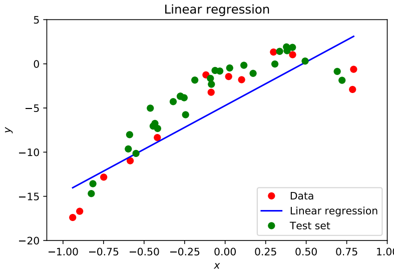
Generalization error

- **Generalization error**, also called **test error** is defined as the expected error on new, previously unseen data.
- Unlike in simple optimization, in machine learning our main goal is to minimize the **generalization error**.
- Usually the generalization error is estimated by measuring the performance on a **test data set** which must be independent from the training set.

Example: Linear regression

- Previously, we trained the model by minimizing the training error
$$\frac{1}{m^{(\text{train})}} \left\| \boldsymbol{X}^{(\text{train})} \hat{\boldsymbol{w}} - \boldsymbol{y}^{(\text{train})} \right\|_2^2$$
- We would like actually to minimize the test error
$$\frac{1}{m^{(\text{test})}} \left\| \boldsymbol{X}^{(\text{test})} \hat{\boldsymbol{w}} - \boldsymbol{y}^{(\text{test})} \right\|_2^2$$





Statistical learning theory

- **Statistical learning theory** provides methods to mathematically reason about the performance on the test set although we can observe only the training set.
- This is possible under some assumptions about the data sets
  - The training and test data are generated by drawing from a probability distribution over data sets. We refer to that as **data-generating process**.
  - **i.i.d. assumptions**
    - Examples in each data sets are **independent** from each other.
    - The training data set and the test data set are **identically distributed**, i.e., drawn from the same probability distribution.

Underfitting and overfitting

- The factor that determines how well a machine algorithm will perform is its ability to
  1. Make the training error small.
  2. Make the difference between the training and test error small.
- These two factors correspond to the two central challenges in machine learning: **underfitting** and **overfitting**.
- Underfitting occurs when the model is not able to produce a sufficiently small training error.
- Overfitting occurs when the gap between the training and test errors is too large.

Model capacity

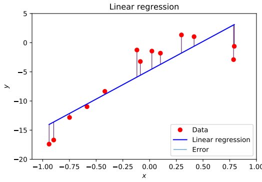
- A **capacity of the model** is its ability to fit a wide variety of functions.
- Low capacity models struggle to fit the training set (underfitting).
- Models with high capacity have danger to overfit the training data (e.g., by “memorizing” training samples).
- The capacity can be controlled by choosing its **hypothesis space**, i.e. the set of functions from which the learning algorithm is allowed to select the solution.
- Example: The linear regression algorithm has the set of all linear functions as its hypothesis space.

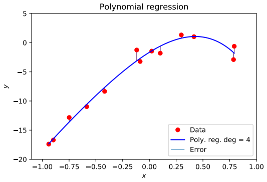
Polynomial regression

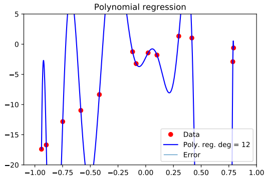
- The linear regression algorithm can be generalized to include all polynomial functions instead of just the linear ones.
- The linear regression model is then just a special case restricted to a polynomial of degree one: $\hat{y} = b + wx$.
- Moving to degree two to we obtain: $\hat{y} = b + w_1 x + w_2 x^2$.
  - This can be seen as adding a new feature x^2.
  - In fact, we can generalize this approach to create all sorts of hypothesis spaces, e.g.: $\hat{y} = b + w_1 x + w_2 \sin(x) + w_3 \sqrt{x}$.
- The **outuput** is still a **linear** function of the parameters, so in principle it can be trained in the same way as the linear regression.

Polynomial regression

A comparison of a linear, degree-4, and degree-12 polynomials as predictors

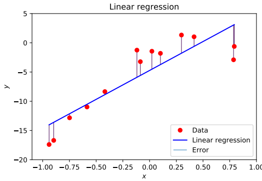


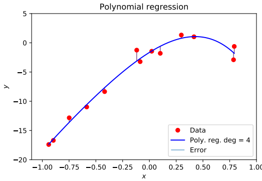


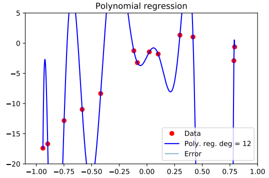


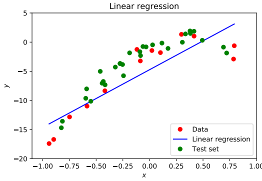
Polynomial regression

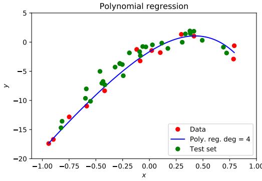
A comparison of a linear, degree-4, and degree-12 polynomials as predictors

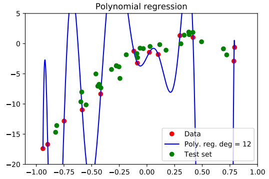












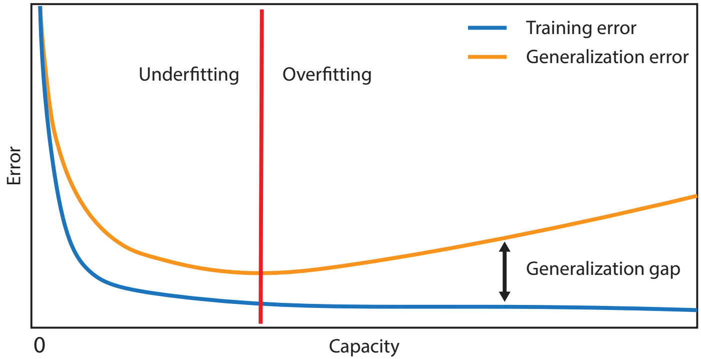
Overfitting and underfitting in polynomial estimation

- Models with low capacity are not up to the task.
- Models with high-capacity can solve a complex task, but when the capacity is too high for the concrete (training) task there is the danger of overfitting.
- In our example: the linear function is unable to capture the curvature so it undefits.
- The degree-12 predictor is capable of fitting the training data, but it also able to find infinitely many functions that pass through the same points, so it has high probability of overfitting.
- The degree-4 function is the right solution and it generalizes well on the new data.

Generalization and capacity

- Simpler functions generalize more easily, but we still need to choose a sufficiently complex hypothesis (function) to obtain small training error.
- Typically training error decreases with the increase of the model capacity until an (asymptotic) value is reached.
- The generalization error is U-shaped with the capacity range split in an underfitting and an overfitting zone(see next slide).

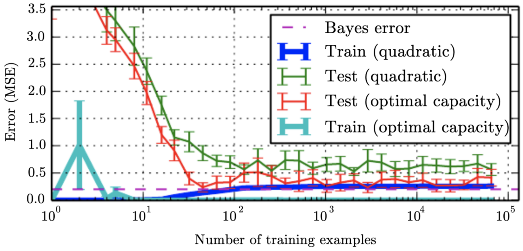
Generalization and capacity



Training set size

- Training and generalization error vary as the size of the training data set varies.
- Expected generalization error never increases as the size of the training set increases.
- Any fixed parametric model will asymptotically approach an error value that exceeds the so called Bayes error.
- It is possible for the model to have optimal capacity and still have a large gap between training and generalization errors.
- In that case the gap usually can be reduced with increasing the number of training examples.

Training set size



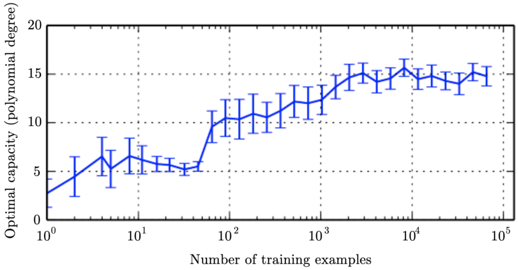


Figure from Goodfellow et al., *Deep Learning*

The No Free Lunch theorem

- **No Free Lunch Theorem** for machine learning (Wolpert, 1996):
  Averaged over all possible data-generating distributions every classification algorithm has the same error rate when tested on new unobserved data.
- In some sense, no machine algorithm is universally better than any other algorithm.
- An interesting, but mainly theoretical result.
- In practice we often have an information about the probability distributions we deal with and can tailor our algorithms to perform well with particular distributions.

Regularization

- In addition to increasing and decreasing of the hypothesis space, i.e., the capacity, we can influence the learning algorithm by **giving preference to one solution over another in the hypothesis space**.
- In case both functions are eligible we can define a condition to express preference about one of the functions.
- The unpreferred solution is chosen only if it gives significantly better performance with the training data.
- *More on regularization in the next lecture.*

Model selection

Materials:

- Chapter I.5.3 from Goodfellow et al., *Deep Learning*

Hyperparameters and validation sets

- **Hyperparameters** are settings that can be used to control the behaviour of the algorithm.
- In general, the hyperparameters are not modified by the learning algorithm itself.
- **Example**: In **polynomial regression** the degree of the polynomial is a **capacity** hyperparameter.
- A setting can be chosen to be hyperparameter when it is **difficult to optimize** or - more often - when its derivation from the training set **can lead to overfitting**.
  - Example: in polynomial regression we can always fit the data better with a higher degree polynomial.

Choice of training, validation, and test sets

- The **validation set** is used during training to predict the behaviour (generalization error) of the algorithm on new data, i.e., on the test set and to chose the hyperparameters.
- Ideally these two sets are disjoint.
- The validation set is chosen from the training data.
- The training data is split in two disjoint subsets.
- One subset is used to learn the parameters of the algorithm and the other is the validation set.
- The subset used to learn the parameters is still typically called a **training set**.

Choice of training, validation, and test sets

- **Question**: How large should the validation set be?
- Since the validation set is used to determine the hyperparameters it will typically underestimate the generalization error.
- However, it will usually better predict the generalization error than the training set.
- After the completion of the hyperparameters optimization we can estimate the generalization error using the test data.
- In practice the testing should be done also on different test data to avoid the test data becoming "stale".

Choice of training, validation, and test sets

Training	Validation	Test
Used to find the optimal **parameters** of the model.	Used to find the optimal **model** (hyper-parameters).	Used to estimate the **performance** of the optimal model.
w	$f(\cdot)$	$\|\|\hat{y} - y\|\|$

Cross-validation

- Dividing the data set into disjoint training and test sets can result in a result in a too small validation and/or test set.
- In such cases all data is used to estimate the generalization error.
- We use procedures that repeat the training and testing on different randomly chosen subsets or splits of the original data set.
- The most common such procedure is the **k-fold cross-validation**.

Cross-validation

- The original data is partitioned into k (disjoint) subsets.
- The average error can be estimated by taking the average over k trials.
- In trial i, the i-th subset is used as test set and the rest as training set.
- Problem: no unbiased estimators of the variance of such average error exist, but there are approximations that are used in practice.

Bias and variance trade-off

Materials:

- Chapter I.5.4 from Goodfellow et al., *Deep Learning*

Point estimation

- For efficient design of learning algorithms it is useful to have formal characterizations of notions like generalization, overfitting and underfitting.
- To this end we introduce some definitions.
- **Point estimation** is the attempt to provide the single "best" prediction of some quantity of interest.
- The quantity of interest can be a single parameter, parameter vector of some model, e.g., the weights $\boldsymbol{w}$ in the linear regression model.
- It can also be a whole function, e.g., the linear function or polynomial of some degree, like in the polynomial regression.

Point estimation

- Given a parameter $\boldsymbol{\theta}$ we denote its point estimate with $\hat{\boldsymbol{\theta}}$.
- As usual, let $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ be m independent and identically distributed (i.i.d.) data points.
- A **point estimator** or **statistic** is any function of the data

$$\hat{\boldsymbol{\theta}}_m = g(\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)})$$

- This definition is very general. For instance, that the value returned by g need not be close to the true value $\boldsymbol{\theta}$. Also g might return a value which is outside the values that $\boldsymbol{\theta}$ is allowed to have.

Point estimation

- Of course, a good estimator is still a function that returns values close to $\boldsymbol{\theta}$.
- Since the data is drawn from a random process, point estimate $\hat{\boldsymbol{\theta}}$ is considered to be a random variable and $\boldsymbol{\theta}$ is fixed, but unknown parameter.

Function estimation

- In **function estimation**, we assume that there is a (true) function that describes the (approximate) relationship between $\boldsymbol{x}$ and $\boldsymbol{y}$

$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

  where ϵ is the part of $\boldsymbol{y}$ which is not predictable from $\boldsymbol{x}$
- The goal is to find the **function estimate** (**model**) $\hat{f}$ which is a good approximation of f.
- The linear regression and polynomial regression can be seen both illustrate scenarios that can be interpreted as either estimating a parameter $\boldsymbol{w}$ or estimating a function $\hat{f}$.

Bias

- A bias of an estimator $\hat{\boldsymbol{\theta}}_m$ is defined as

$$\text{bias}(\hat{\boldsymbol{\theta}}_m) = \mathbb{E}(\hat{\boldsymbol{\theta}}_m) - \boldsymbol{\theta}$$

  where the expectation is over the data and $\boldsymbol{\theta}$ is the true underlying value.
- An estimator $\hat{\boldsymbol{\theta}}_m$ is **unbiased** if $\text{bias}(\hat{\boldsymbol{\theta}}_m) = 0$. Note that this implies $\mathbb{E}(\hat{\boldsymbol{\theta}}_m) = \boldsymbol{\theta}$.
- $\hat{\boldsymbol{\theta}}_m$ is **asymptotically unbiased** if $\lim_{m\to\infty} \text{bias}(\hat{\boldsymbol{\theta}}_m) = 0$ (implying $\lim_{m\to\infty} \mathbb{E}(\hat{\boldsymbol{\theta}}_m) = \boldsymbol{\theta}$).

Bias: example

- **Example**: Consider samples $\{x^{(1)}, \dots, x^{(m)}\}$ i.i.d distributed according to the Gaussian distribution

$$p(x^{(i)}; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{x^{(i)} - \mu}{\sigma^2}\right)$$

- The **sample mean** is a common estimator of the Gaussian mean parameter

$$\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} x(i)$$

Bias: example

We compute the bias as expectation by substituting the Gaussian distribution in the formula

$$\begin{aligned}
\mathrm{bias}(\mu_m) &= \mathbb{E}[\mu_m] - \mu \\
&= \mathbb{E}\left[\tfrac{1}{m}\textstyle\sum_{i=1}^{m} x^{(i)}\right] - \mu \\
&= \left(\tfrac{1}{m}\textstyle\sum_{i=1}^{m} \mathbb{E}[x^{(i)}]\right) - \mu \\
&= \left(\tfrac{1}{m}\textstyle\sum_{i=1}^{m} \mu\right) - \mu \\
&= \mu - \mu = 0
\end{aligned}$$

The sample mean is an unbiased estimator of Gaussian mean parameter.

Bias: example

- **Example**: Estimators of the variance of a Gaussian distribution
- We compare two different estimators of the variance σ^2 parameter
- **Sample variance**

$$\hat{\sigma}^2 = \frac{1}{m} \sum_{1}^{m} \left(x^{(i)} - \hat{\mu}_m \right)^2$$

  where $\hat{\mu}$ is the sample mean.
- We are interested in computing

$$\text{bias}(\hat{\sigma}_m^2) = \mathbb{E}[\hat{\sigma}_m^2] - \sigma^2$$

Bias: example

- First we evaluate $\mathbb{E}[\hat{\sigma}_m^2]$:

$$\mathbb{E}[\hat{\sigma}_m^2] = \mathbb{E}\left[\frac{1}{m}\sum_{1}^{m}\left(x^{(i)} - \hat{\mu}_m\right)^2\right] = \frac{m-1}{m}\sigma^2$$

- Back to the bias

$$\text{bias}(\hat{\sigma}_m^2) = \mathbb{E}[\hat{\sigma}_m^2] - \sigma^2 = \frac{m-1}{m}\sigma^2 - \sigma^2 = -\frac{\sigma^2}{m}$$

- Therefore the sample variance is a **biased** estimator.

Bias: example

- The **unbiased variance estimator** is defined as

$$\tilde{\sigma}^2 = \frac{1}{m-1} \sum_{1}^{m} \left(x^{(i)} - \hat{\mu}_m \right)^2$$

- Indeed

$$\mathbb{E}[\tilde{\sigma}_m^2] = \mathbb{E}\left[\frac{1}{m-1} \sum_{1}^{m} \left(x^{(i)} - \hat{\mu}_m \right)^2 \right] = \frac{m-1}{m-1}\sigma^2 = \sigma^2$$

and the bias is 0.

Variance and standard error

- Another important feature of an estimator is its variance.
- The **variance** of an estimator is simple its statistical variance $\text{Var}(\hat{\theta})$ over the training set as a random variable.
- Alternatively we can compute the **standard error** (the square root of the variance) $\text{SE}(\hat{\theta})$.
- The variance or the standard error provide a measure how much the estimate would vary as we resample the data independently from the underlying data generating process.
- We would prefer a relatively low variance of the estimator.

Variance and standard error

- The standard error of the mean estimator is given as

$$\mathrm{SE}(\hat{\mu}) = \sqrt{\mathrm{Var}\left[\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right]} = \frac{\sigma}{\sqrt{m}}$$

  where σ is the true variance of the distribution, i.e., the samples $x^{(i)}$.
- Neither the square root of the sample variance nor the square root of the unbiased estimator of the variance give an unbiased estimate of the standard deviation.
- Both approaches underestimate the true standard deviation.
- However, for large m the approximation works quite well.

Variance and standard error

- Often the generalization error is estimated based on the sample mean of the error on the test set.
- The accuracy of the estimate depends on the number of the examples.
- From the statistical theory (central limit theorem) we know that the mean is distributed with normal distribution for which we can establish confidence intervals.
- For instance, the 95% confidence interval is given by

$$[\hat{\mu_m} - 1.96\mathrm{SE}(\hat{\mu}_m), \hat{\mu_m} + 1.96\mathrm{SE}(\hat{\mu}_m]$$

- Then we can say that algorithm A is better than algorithm B of the confidence upper bound for the error of A is less than the corresponding lower bound of B.

Trading off bias and variance to minimize mean squared error

- Bias and variance measure two different sources of error in an estimator.
- Bias measures the expected deviation with the true value of the estimator.
- Variance provides a measure of the deviation from the expected value of the estimator depending on the particular data sampling.

Trading off bias and variance to minimize mean squared error

- Often we need to make a trade-off between these two.
- The most common way to do this is via cross-validation.
- An alternative is to compare the **mean squared error** (MSE) of the estimates.

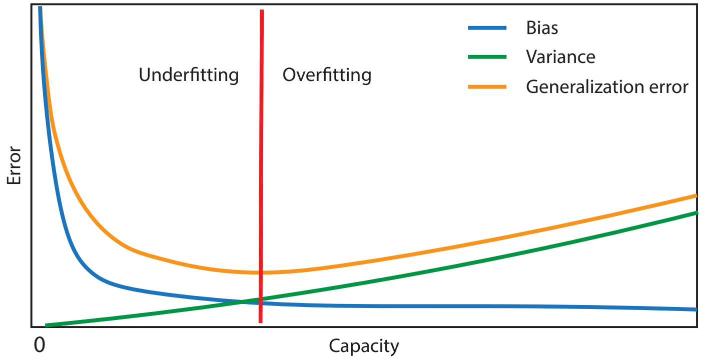
$$\text{MSE} = \mathbb{E}[(\hat{\theta}_m - \theta)^2] = \text{bias}(\hat{\theta}_m)^2 + \text{Var}(\hat{\theta}_m)$$

- The smaller MSE the better - so minimizing both the bias and variance is always preferable.

Bias and variance

- Our original goal was to provide a mathematical support for the notions of capacity, underfitting, and overfitting.
- Indeed there is a close relationship between these three concepts and bias and variance.
- When generalization error is measured by MSE (and hence indirectly via bias and variance) increasing capacity tends to increase variance and decrease bias.
- Again the generalization as a function of capacity is given by an U-shaped curve.

Bias and variance



Consistency

- So far we considered fixed size of the training data sets.
- We expect that as the number m of training examples grows the estimators will converge to the true value of the parameters.
- More formally this is captured in the notion of **consistency**

  $$\text{plim}_{m\to\infty}\hat{\theta}_m = \theta$$

  where plim denotes convergence in probability: for any $\epsilon > 0$, $P(\mid \hat{\theta}_m - \theta \mid > \epsilon) \to 0$ as $m \to \infty$.
- For consistent models the bias decreases as m increases, however a decreasing bias (when m increases) does not imply consistency.

Maximum likelihood estimation

Materials:

- Chapter I.5.5 from Goodfellow et al., *Deep Learning*

Maximum likelihood estimation

- We would like to have some principle from which we can derive good estimator functions for a large scale of models.
- The **maximum likelihood estimation** is the most common such principle.
- Given observation data and a corresponding (statistical) model our goal is to find the parameter vector which imply the highest probability to obtain the data.

Maximum likelihood estimation

- Consider a set of m examples $\mathbb{X} = \{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(m)}\}$ drawn independently from the true but unknown distribution $p_{\text{data}}(\mathbf{x})$.
- Let $p_{\text{model}}(\mathbf{x}; \boldsymbol{\theta})$ be a parametric family of probability distributions, i.e., for each $\boldsymbol{\theta}$ we get a different distribution p_{model}.
- $p_{\text{model}}(\boldsymbol{x}; \boldsymbol{\theta})$ maps any configuration $\boldsymbol{x}$ to a real number estimating the (true) probability $p_{\text{data}}(\boldsymbol{x})$

Maximum likelihood estimation

- The maximum likelihood estimator for $\boldsymbol{\theta}$ is then defined as

$$\boldsymbol{\theta}_{\mathrm{ML}} = \mathrm{argmax}_{\boldsymbol{\theta}} p_{\mathrm{model}}(\mathbb{X}; \boldsymbol{\theta}) = \mathrm{argmax}_{\boldsymbol{\theta}} \prod_{i=1}^{m} p_{\mathrm{model}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

  Note that also the empirical distribution $\hat{p}_{\mathrm{data}}$ is implicitly present in the formula through $\boldsymbol{x}^{(i)}$.
- A more convenient equivalent optimization problem is obtained by taking logarithm of the product

$$\boldsymbol{\theta}_{\mathrm{ML}} = \mathrm{argmax}_{\boldsymbol{\theta}} p_{\mathrm{model}}(\mathbb{X}; \boldsymbol{\theta}) = \sum_{i=1}^{m} \log p_{\mathrm{model}} \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Maximum likelihood estimation

- We can further rescale by dividing the expression by m

$$\boldsymbol{\theta}_{\text{ML}} = \text{argmax}_{\boldsymbol{\theta}} p_{\text{model}}(\mathbb{X}; \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x} \sim \hat{p}_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x}; \boldsymbol{\theta})$$

- In this way the problem is expressed as an equivalent expectation problem (now the empirical distribution $\hat{p}_{\text{data}}$ becomes explicit).

Maximum likelihood estimation

- Perhaps more straightforwardly, the maximum likelihood estimation can be seen as minimizing the dissimilarity between $\hat{p}_{\text{data}}$ and p_{model}.
- The degree of dissimilarity is given by the KL-divergence

$$D_{\text{KL}}(\hat{p}_{\text{data}} \| p_{\text{model}}) = \mathbb{E}_{\mathbf{x} \sim \hat{p}_{\text{data}}}[\log \hat{p}_{\text{data}}(\boldsymbol{x}) - \log p_{\text{model}}(\boldsymbol{x})]$$

- Only the term of the right is function of the model, so it is the only one which needs to be minimized

$$-\mathbb{E}_{\mathbf{x} \sim \hat{p}_{\text{data}}}[\log p_{\text{model}}(\boldsymbol{x})]$$

  which is equivalent with the maximization problem from the previous slide.
- It boils down to minimizing the **cross-entropy** between the two distributions.

Maximum likelihood estimation

- **The maximum likelihood estimation can be seen as an attempt to make the model distribution** p_{model} **to match the empirical distribution** $\hat{p}_{\text{data}}$.
- Ideally we would like to match the data generating distribution p_{data}, but we do not have access to it.

Conditional log likelihood and mean square error

- The maximal likelihood estimator can be generalized to estimate a conditional probability $P(\mathbf{y} \mid \mathbf{x}; \boldsymbol{\theta})$.
- Let all inputs be given by $\boldsymbol{X}$ and all observed outputs by $\boldsymbol{Y}$. Then the conditional maximum likelihood estimator is

$$\boldsymbol{\theta}_{\text{ML}} = \arg\max_{\theta} P(\boldsymbol{Y} \mid \boldsymbol{X}; \boldsymbol{\theta})$$

- If the examples are assumed to be i.i.d., then this can be decomposed into

$$\boldsymbol{\theta}_{\text{ML}} = \arg\max_{\theta} \sum_{i=1}^{m} \log P(\boldsymbol{y}^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Example: linear regression as maximum likelihood

- The linear regression seen as an algorithm that learns to take an input $\boldsymbol{x}$ and produce output $\hat{y}$.
- This function from $\boldsymbol{x}$ to $\hat{y}$ is chosen to minimize the mean squared error.
- This criterion was introduced more or less arbitrarily.
- We revisit linear regression from the point of view of maximal likelihood.
- We think of the model as producing a conditional distribution $p(y \mid \boldsymbol{x})$ instead of a single prediction $\hat{y}$.

Example: linear regression as maximum likelihood

- With an infinitely large training set we might see several examples whit the same input $\boldsymbol{x}$ but different y.
- The learning algorithm needs to fit the distribution to all these y corresponding to the same $\boldsymbol{x}$.
- To derive the linear regression algorithm we assume $p(y \mid \boldsymbol{x}) = \mathcal{N}(y; \hat{y}(\boldsymbol{x}; \boldsymbol{w}), \sigma^2)$, where $\hat{y}(\boldsymbol{x}; \boldsymbol{w})$ gives the (prediction of the) mean of the normal distribution and σ is fixed to some chose constant.
- The parameter vector θ corresponds in this case to $\boldsymbol{w}$.

Example: linear regression as maximum likelihood

- By substituting (the full Gaussian function version of) $p(y \mid \boldsymbol{x})$ in the conditional log-likelihood formula we obtain

$$\sum_{i=1}^{m} \log p(\boldsymbol{x}^{(i)} \mid y^{(i)}; \boldsymbol{\theta}) = -m \log \sigma - \frac{m}{2} \log(2\pi) - \sum_{i=1}^{m} \frac{\left\| \hat{y}^{(i)} - y^{(i)} \right\|^2}{2\sigma^2}$$

  where $\hat{y}^{(i)}$ is the linear regression on the i-th input $\boldsymbol{x}^{(i)}$.

- By comparing with the mean squared error

$$\text{MSE}_{\text{train}} = \frac{1}{m} \sum_{i=1}^{m} \left\| \hat{y}^{(i)} - y^{(i)} \right\|^2$$

  one can see that maximizing the log-likelihood with respect to $\boldsymbol{w}$ results with the same estimate of $\boldsymbol{x}$ as minimizing MSE. (The third term in the log-likelihood forumula, needs to be as small as possible.)

Properties of maximum likelihood

- It can be shown that the maximum likelihood estimator is the best asymptotically, i.e. as $m \to \infty$, in terms of its convergence rate.
- **Property of consistency**: as the number of training examples approaches infinity the maximum likelihood estimate of a parameter converges towards the true parameter value.
- The maximum likelihood estimator has the property of consistency provided:
  - The true distribution p_{data} is in the model family $p_{\text{model}}(\cdot; \boldsymbol{\theta})$
  - p_{data} corresponds to exactly one value of $\boldsymbol{\theta}$

Supervised and unsupervised learning algorithms

Materials:

- Chapters I.5.6 and I.5.7 from Goodfellow et al., *Deep Learning*

Supervised learning algorithms

- Learning algorithms that learn based on a given training examples $\boldsymbol{x}$ and their corresponding outputs $\boldsymbol{y}$.
  - Linear and logistic regressions
  - Support vector machines
  - k-nearest neighbours
  - Decision trees

Unsupervised learning algorithms

- Unsupervised algorithms experience only "features", but not supervision feedback.
- The distinction with the supervised algorithms is not always clear since there is no good test to distinguish if something is a feature or a target provided by the supervisor.
- Rule of thumb: in unsupervised algorithms no human annotation is needed for the training examples.
  - Principal component analysis
  - k-means clustering
  - t-Distributed Stochastic Neighbor Embedding
  - Generative adversarial networks

Model evaluation

Materials:

- Fawcett, “An introduction to ROC analysis”

Model evaluation

- To quantitatively evaluate a machine learning algorithm we need to define a **performance measure**.
- Usually the performance measure is specific to the task carried out by the algorithm.
- For classification tasks a natural measure is the model **accuracy**.
- The **accuracy** is defined as the proportion of examples for which the model produces the correct output.
- An equivalent (complementary) measure is the **error rate** defined as the proportion of incorrect outputs.

Model evaluation

- The best way to evaluate a machine learning algorithm is by applying it to a **test set** data which has not been seen before.
- Ideally there should be **no overlap** between the **test set** and the **training set** used to obtain the model.

Binary classification

- We consider **binary classification** problems, i.e., problems using only two classes/
- Formally each input example $x^{(i)}$ needs to be mapped into one element of the set $\{\boldsymbol{p}, \boldsymbol{n}\}$ of **true** classes.
- A **classification model** (**classifier**) is a function from the input examples to from the set $\{\boldsymbol{Y}, \boldsymbol{N}\}$ of **predicted classes** or **hypothesized classes**.
- $\boldsymbol{p}, \boldsymbol{n}$ correspond to $\boldsymbol{Y}, \boldsymbol{N}$, respectively.

Binary classification

- For a given classifier there are four possible outcomes.
- If the true class of $x^{(i)}$ is $\boldsymbol{p}$ and the predicted class is $\boldsymbol{Y}$ then we have a **true positive** (TP); if it was classified $\boldsymbol{N}$, then we have a **false negative** (FN).
- Symmetrically, a $x^{(i)}$ with true class $\boldsymbol{n}$ which is assigned a predicted class $\boldsymbol{N}$ is a **true negative** (TN); if the predicted class is $\boldsymbol{Y}$, then it is a false positive (FP).

Confusion matrix

These four combinations can be put together in a **confusion matrix**, also called **contingency table**.

		True class	
		p	***n***
Predicted class	***Y***	True positives (TP)	False positives (FP)
	N	False negatives (FN)	True negatives (TN)

Binary classifications metrics

- Using the four basic categories of prediction outcomes (TP, FP, TN, FN) we can derive various **measures** of performance of classification models.
- For instance the accuracy can be defined as

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}$$

- Also quite frequently used measures are

$$Sensitivity = \frac{TP}{TP + FN} \quad Specificity = \frac{TN}{TN + FP} \quad Precision = \frac{TP}{TP + FP}$$

Binary classification metrics

- Sensitivity is also called **recall**, **true positive rate** or **hit rate**
- In medical contexts the sensitivity can be interpreted as a measure of the extent to which diseased individuals are incorrectly diagnosed.
- In general: measures the proportion of the target group the method is able to detect, i.e. how sensitive is to this group.
- Specificity is also called **true negative rate** or **selectivity**.
- In medical contexts the specificity can be interpreted as a measure of the extent to which healthy individuals are correctly diagnosed.
- The precision tells us which proportion of the positive predictions is correct.

Binary classification metrics

- Sometimes the above mentioned measures are not sufficient.
- For example, in a population in which the percentage of healthy individuals is much larger than the diseased individuals, it is easy to achieve high specificity by trivially classifying each patient as healthy.
- We can obtain more objective evaluation by combing metrics.
- The metrics F_1 is the harmonic mean (average) of the precision and recall (sensitivity)

$$\frac{2}{F_1} = \frac{1}{Precision} + \frac{1}{Recall} \text{ or } F_1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}$$

Areas under the curve measures

- (Binary) classifications often depend on some parameter (e.g., threshold).
- Hence on way to combine two metrics is by assigning them to the axes of a coordinate system and varying this parameter to construct a graphical plot.
- We obtain a curve (actually, most of the time series of points) such that each point corresponds to a particular parameter value.
- The area under the curve is a measure of how good is the classification.

Receiver Operating Characteristic (ROC) curve

- The ROC curve plots the true positive rate (sensitivity) versus the false positive rate (1 - specificity).

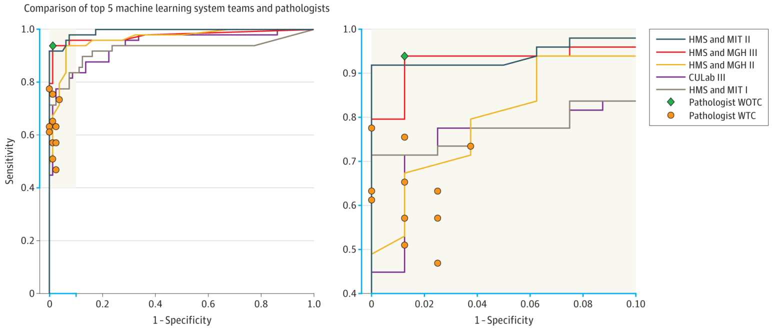


Figure from Bejnordi et al., “Diagnostic assessment of deep learning algorithms for detection of lymph node metastases in women with breast cancer”

Receiver Operating Characteristic (ROC) curve

- There are several characteristic points points in the ROC space:
    - (0,0) corresponds to the strategy of never making a positive classification.
    - (1,1) is the opposite: unconditionally issuing a positive classification.
    - (0,1) represents perfect classification.
    - Obviously we strive to achieve this ideal point as as a result have as much as possible area under the curve covered (ideally it should cover the whole square corresponding to the ROC space)
- A less common example of a measure combination into a graphical plot is the precision-recall plot (recall on the x-axis, precision on the y-axis).

Ensambling

Materials:

- Chapter II.7.11 from Goodfellow et al., *Deep Learning*

Bagging and other ensemble methods

- **Bagging** (short for **b**ootstrap **agg**regat**ing**) is a technique for reducing of the generalization error by combining several models.
- Train models separately and let them vote on the right output.
- An example of a general strategy in machine learning called **model averaging**.
- Methods using this strategy are called *ensemble methods*.
- The rationale behind the combining of models is that usually different models will not make the same error.

Bagging

- Different ensemble methods compose the ensemble of models in different ways.
- One way would be to choose the models, training algorithms and objective functions as different as possible.
- In contrast, begging allows the same kind of model, algorithm and objective function to be reused several times.

Bagging

- Bagging constructs k different data sets.
- Each data set
  - has the same size as the original set and
  - is constructed by sampling with repetition from the original data set
- For each data set a different model is produced.
- Each model reflects the differences between the (training) data sets.

Bagging example

Training an “8 detector” with two resampled datasets: a “cartoon” example.

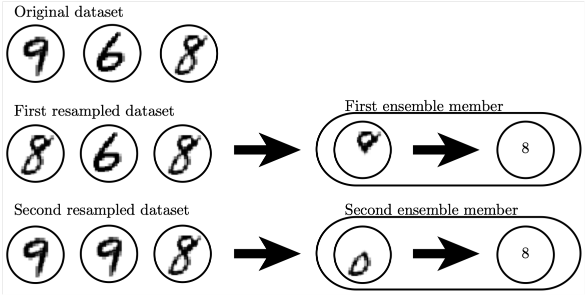


Figure from Goodfellow et al., *Deep Learning*

Model averaging for neural networks

- Neural networks profit from model averaging even when they are trained on the same data set.
- This is because with random initialization, minibatches (subsets of the training set), hyperparameters, non-determinism in the implementation a sufficient variety between the models can be achieved.

Model averaging in general

- In general, it is considered that model averaging always improves the generalization error.
- In theory, with sufficient computer memory and time one can always improve the results by combining several methods.
- Therefore, when testing/benchmarking (new) methods it is considered "fair" to use only a single model.
- Machine learning contests are usually won by using model averaging.
- **Boosting** is similar to ensembling, only the models (neural networks) are added **incrementally** to the ensemble.

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