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INTRODUCTION TO DATA SCIENCE

Lecture 4

Prediction – Supervised Learning

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Instances and labels

- **Instances** are represented by their **attributes**

$$\mathbf{x} = (x_1, \dots, x_k) \in \mathcal{X}, \quad \mathcal{X} = \mathcal{X}_1 \times \cdots \times \mathcal{X}_k$$

- An instance belongs to a **class** or have a **value**. An instance a class or a value of which is known is called **labeled**

$$(\mathbf{x}, y) \in \mathcal{X} \times \mathcal{L}$$

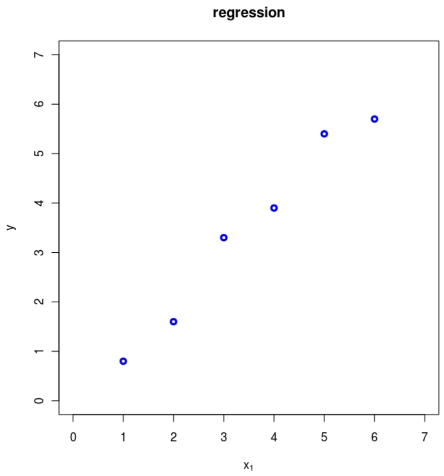
- Assume that labels are assigned according to some **unknown pattern** called labeling function

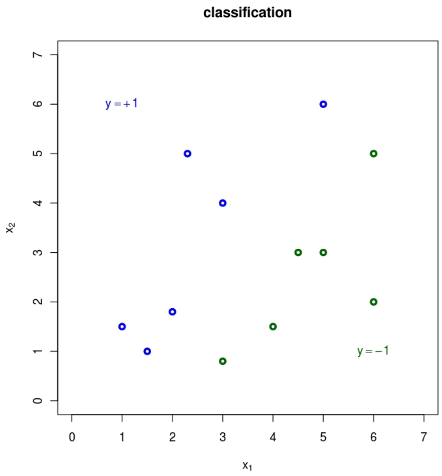
$$l : \mathcal{X} \to \mathcal{L}, \quad l(\mathbf{x}) = y$$

  - if $\mathcal{L} \subset \mathbb{Z}$[1] then l is a **classification** function (classifier)
  - if $\mathcal{L} \subset \mathbb{R}$ then l is a **regression** function (regressor)

[1] Important is, that we deal with discrete labels in case of classification.

Example





Train set and Modeling

The problem: The labeling function l is unknown.

- Good news: Even if l is not known, we have observed a sample of instances with their labels. Such a set of instances is called the **training sample**

$$\mathcal{S}^{tr} = \{(\mathbf{x}, y) | \mathbf{x} \in \mathcal{X}, y \in \mathcal{L}\}$$

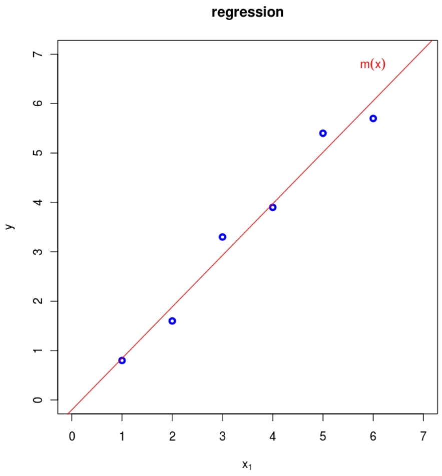
  which can be considered as an explicit definition of l.

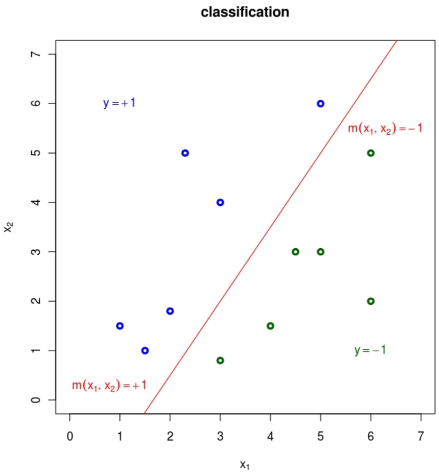
The solution: Try somehow, using $\mathcal{S}^{tr}$, to **model** l by a mapping

$$m : \mathcal{X} \to \mathcal{L}, \quad m(\mathbf{x}) = \hat{y}$$

such that m is as close to l as possible.

Example





The quality and the parameters of m

How do we express m?

- m is given by its **type** and **parameters** $\boldsymbol{\Theta}$
  - let's focus on linear models
    - $m^{\Theta}(\mathbf{x} = (x_1, \ldots, x_k)) = \theta_0 + \theta_1 x_1 + \cdots + \theta_k x_k$
    - $\Theta = (\theta_0, \theta_1, \ldots, \theta_k)$

How to measure if m approximates l well?

- **empirical error**[2]

$$err(m^{\Theta}, \mathcal{S}^{tr}) = \sum_{(\mathbf{x},y)\in\mathcal{S}^{tr}} l_r(y, m^{\Theta}(\mathbf{x})) = \sum_{(\mathbf{x},y)\in\mathcal{S}^{tr}} (y - m^{\Theta}(\mathbf{x}))^2$$

Modeling means[3] to choose a type of m and to find its parameters $\boldsymbol{\Theta}$ such that $err(m^{\Theta}, \mathcal{S}^{tr})$ is minimal.

- **least squares estimates** (LSE)

[2] $l_r(y, m^{\Theta}(\mathbf{x}))$ is a **regression loss** function.

[3] There are also some other issues important while we are modeling, we'll explain them later.

A generative model (1/2)

Let's $m^\Theta(\mathbf{x} = (x_1)) = \theta_0 + \theta_1 x_1$

- m^Θ approximates l with an error ϵ, i.e. $y = l(\mathbf{x}) = m^\Theta(\mathbf{x}) + \epsilon$
    - assume $\epsilon \sim N(0, \sigma^2)$, thus, $p(y|\mathbf{x}) \sim N(\theta_0 + \theta_1 x_1, \sigma^2)$

How is the data generated?

- assume the instances $(\mathbf{x}, y)$ are "sampled" independently
- the likelihood[4] of this sampling given parameters $\Theta = (\theta_0, \theta_1)$ is

$$L_{\mathcal{S}^{tr}}(\Theta) = \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(\mathbf{x}, y|\Theta) = \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(y|\mathbf{x}, \Theta)p(\mathbf{x}, \Theta)$$

Modeling means to choose a type of m and to find its parameters Θ such that $L_{\mathcal{S}^{tr}}(\Theta)$ is maximal.

- **maximum likelihood estimates** (MLE)

[4] i.e. the probability of the data ($\mathcal{S}^{tr}$)

A generative model (2/2)

$$\prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(\mathbf{x},y) = \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(y|\mathbf{x})p(\mathbf{x}) = \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(y|\mathbf{x}) \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(\mathbf{x})$$

since $p(\mathbf{x})$ doesn't depends on Θ, it's enough to maximize the **conditional likelihood**

$$L^{cond}_{\mathcal{S}^{tr}}(\Theta) = \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} p(y|\mathbf{x}) = \prod_{(\mathbf{x},y)\in\mathcal{S}^{tr}} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-m^{\Theta}(\mathbf{x}))^2}{2\sigma^2}}$$

this is equivalent to maximize the **conditional log-likelihood**

$$lnL^{cond}_{\mathcal{S}^{tr}}(\Theta) = \sum_{(\mathbf{x},y)\in\mathcal{S}^{tr}} ln\left(\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-m^{\Theta}(\mathbf{x}))^2}{2\sigma^2}}\right) \propto \min \sum_{(\mathbf{x},y)\in\mathcal{S}^{tr}} (y-m^{\Theta}(\mathbf{x}))^2$$

under the assumption of normality, MLE are the LSE

Gradient descent optimization

for more variables closed form solutions are bothersome

- *How to find a minimum of an "objective" function $f(\Theta)$?*
    - assume f is differentiable and convex

<u>Gradient descent</u>

```
input: $f, \alpha$, stopping criteria
initialize $\Theta$ (not with zeros)
repeat
    $\Theta \leftarrow \Theta - \alpha \frac{\partial f}{\partial \Theta}(\Theta)$
until approximate minimum is reached
return $\Theta$
```

stopping criteria

- $|\Theta^{old} - \Theta| < \epsilon$
- maximum number of iterations reached
- a combination of both

Stochastic gradient descent optimization

if f can be written as

$$f(\Theta) = \sum_{i=1}^{n} f_i(\Theta)$$

Stochastic gradient descent (SGD)

```
input: $f_i, \alpha,$ stopping criteria
initialize $\Theta$
repeat
    for all $i$ in random order do
        $\Theta \leftarrow \Theta - \alpha \frac{\partial f_i}{\partial \Theta}(\Theta)$
until approximate minimum is reached
return $\Theta$
```

α is a **hyper-parameter** of the “learning” algorithm

Prediction

The aim is not to *describe* the data but rather to **predict** labels on yet unseen instances.

- **generalization error** for regression[1]

$$err(m^\Theta) = E_{(\mathbf{x},y)}\{l_r(y, m^\Theta(\mathbf{x}))\} = \int_{\mathcal{X}} \int_{\mathcal{L}} l_r(y, m^\Theta(\mathbf{x})) p(\mathbf{x}, y) \, \mathrm{d}y \mathrm{d}\mathbf{x}$$

- generalization error for classification[2]

$$err(m^\Theta) = E_{(\mathbf{x},y)}\{l_c(y, m^\Theta(\mathbf{x}))\} = \int_{\mathcal{X}} \sum_{c \in \mathcal{L}} l_c(c, m^\Theta(\mathbf{x})) p(\mathbf{x}, y = c) \, \mathrm{d}y \mathrm{d}\mathbf{x}$$

Bayes predictor minimizes the generalization error

$$m_B = \arg\min_{m^\Theta} \; err(m^\Theta)$$

[1] $E_{(\mathbf{x},y)}\{l_r(y, m^\Theta(\mathbf{x}))\}$ is an expectation of the regression loss over $\mathcal{X} \times \mathcal{L}$.

[2] $l_c(y, m^\Theta(\mathbf{x}))$ is called **classification loss** and can be defined e.g. as $l_c(y, m^\Theta(\mathbf{x})) = 1 - \delta(y = m^\Theta(\mathbf{x}))$, with δ being a usual truth-indicator function.

Regularization

The aim is to achieve low generalization error of the model

- it means, describe the available data[3] as well as possible
- but also, *don't fit the model to the noise* in the data
- i.e. try to get a smooth model

regularized linear regression

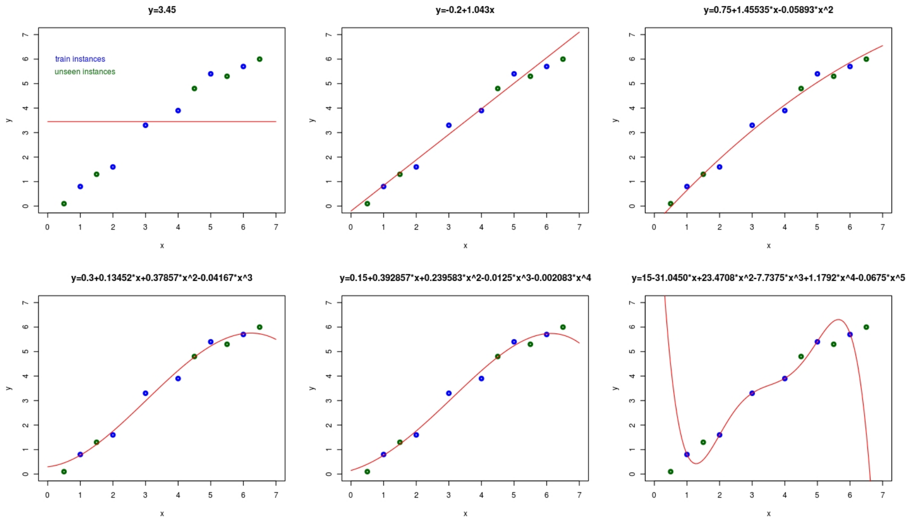
- the objective function[4] to optimize (minimize) is

$$f(\Theta) = \underbrace{\sum_{(\mathbf{x},y)\in\mathcal{S}^{tr}} (y - m^{\Theta}(\mathbf{x}))^2}_{\text{empirical error}} + \underbrace{\lambda\|\Theta\|^2}_{\text{regularization term}}$$

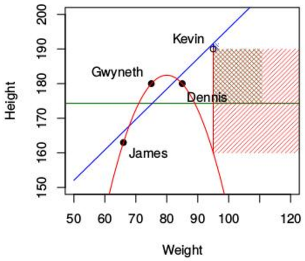
[3] Keep in mind that the available data is only the train set.

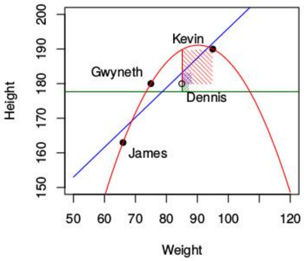
[4] λ is a hyper-parameter, while Θ is a parameter!

Example


y=3.45
train instances
unseen instances
y=-0.2+1.043x
y=0.75+1.45535*x-0.05893*x^2
y=0.3+0.13452*x+0.37857*x^2-0.04167*x^3
y=0.15+0.392857*x+0.239583*x^2-0.0125*x^3-0.002083*x^4
y=15-31.0450*x+23.4708*x^2-7.7375*x^3+1.1792*x^4-0.0675*x^5
x
y

Example


Kevin
Gwyneth
Dennis
James
Height
Weight
150 160 170 180 190 200
50 60 70 80 90 100 120


Kevin
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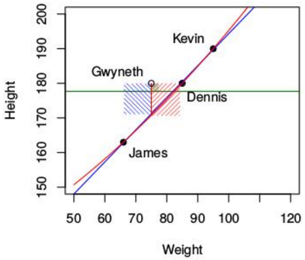
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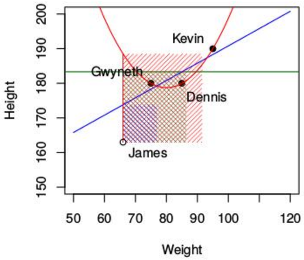

Kevin
Gwyneth
Dennis
James
Height
Weight
150 160 170 180 190 200
50 60 70 80 90 100 120

The quality of a model

According to Θ, we can have many **different models** m^{Θ}.

- Which model is the best one?
- Which properties a good model should have?
    - We need some quality indicators for a model…

One model could be trained using many **different training samples**.

- What would the results be in case of using $\mathcal{S}^{tr_2}$ or any other training sample instead of $\mathcal{S}^{tr_1}$?

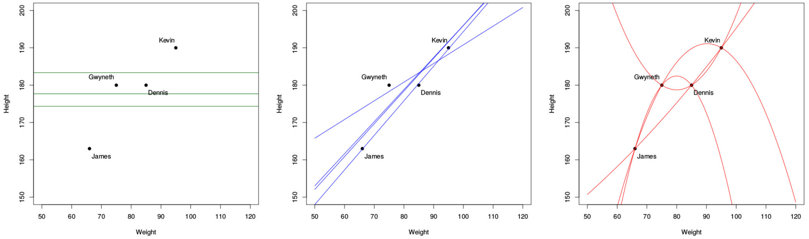
Bias and Variance

Bias

- measures, how $m^{\Theta,\mathcal{S}^{tr1}}, m^{\Theta,\mathcal{S}^{tr2}}, \ldots, m^{\Theta,\mathcal{S}^{trm}}$ differs from l
- determines, how generic the model m^{Θ} is

Variance

- measures, how $m^{\Theta,\mathcal{S}^{tr1}}, m^{\Theta,\mathcal{S}^{tr2}}, \ldots, m^{\Theta,\mathcal{S}^{trm}}$ differs frome each other
- determines, how stable the model m^{Θ} is



Underfitting vs. Overfitting

Bias

$$bias^2_{m^\Theta}(\mathbf{x}) = (\ l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x})\}\ )^2$$

Variance

$$variance_{m^\Theta}(\mathbf{x}) = \mathrm{E}_{\mathcal{S}^{tr}}\{\ (\ m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x})\}\ )^2\}$$

$\mathrm{E}_{\mathcal{S}^{tr}}\{\ X\ \}$ is an **expected value** of X over all training samples.

Underfitting

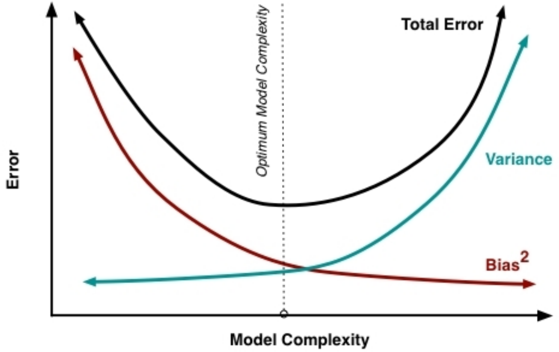
- when the model has high bias and low variance, i.e. is too general

Overfitting

- when the model has low bias and high variance, i.e. is too specific

The bias-variance tradeoff

Usually, the bias decreases with the **complexity** of the model, while variance increases with the complexity of the model. Thus, we need to find a tradeoff model, which is not too general nor too specific.



[1]

[1] image source: http://scott.fortmann-roe.com/

Error

What happens if we sum up the bias and the variance?[2]

$$
\begin{aligned}
& bias^2_{m^\Theta}(\mathbf{x}) + variance_{m^\Theta}(\mathbf{x}) = \\
&= (l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2 + \mathrm{E}_{\mathcal{S}^{tr}}\{(\hat{y} - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2\} \\
&= (l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2 + \mathrm{E}_{\mathcal{S}^{tr}}\{(\hat{y} - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2\} \\
&\quad + 2 \cdot (l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})(\mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\} - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\}) \\
&= (l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2 + \mathrm{E}_{\mathcal{S}^{tr}}\{(\hat{y} - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2\} \\
&\quad + 2 \cdot (l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})\mathrm{E}_{\mathcal{S}^{tr}}\{(\mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\} - \hat{y})\} \\
&= \mathrm{E}_{\mathcal{S}^{tr}}\{(l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})^2\} + \mathrm{E}_{\mathcal{S}^{tr}}\{(\mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\} - \hat{y})^2\}\} \\
&\quad + \mathrm{E}_{\mathcal{S}^{tr}}\{2 \cdot (l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\})(\mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\} - \hat{y})\} \\
&= \mathrm{E}_{\mathcal{S}^{tr}}\{(l(\mathbf{x}) - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\} + \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\} - \hat{y})^2\}\} \\
&= \mathrm{E}_{\mathcal{S}^{tr}}\{(l(\mathbf{x}) - \hat{y})^2\}
\end{aligned}
$$

We get the expected squared error of the model over all training samples w.r.t. the labeling.

[2] We will denote $m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x})$ as $\hat{y}$ for better readability on the next slides.

Noise in sampling

The error introduced on the previous slide deals with the labeling l.

- However, the precise values of l are unknown.
    - We should consider to use the observed labels from the training sample.

As we have seen, observations are usually noisy, i.e. $y = l(\mathbf{x}) + \epsilon$ for all $(\mathbf{x}, y) \in \mathcal{S}^{tr}$, where $\mathcal{S}^{tr}$ is an arbitrary sample of instances.

- there can be more instances with same attribute values but different labels
- note, that we don't care about where the noise came from
    - non-perfect measuring devices, human factor, etc.

$$noise(\mathbf{x}) = \mathrm{E}_{(\mathbf{x},y)}\{\, (y - l(\mathbf{x}))^2 \,\}$$

Noise in sampling

Usually, we assume a normally distributed sampling error $\epsilon \sim \mathcal{N}(0,1)$

- thus, $\mathrm{E}_{(\mathbf{x},y)}\{y\} = l(\mathbf{x})$

Let's rewrite the equations introduced before as

$$bias^2_{m^\Theta}(\mathbf{x}) = (\ \mathrm{E}_{(\mathbf{x},y)}\{y\} - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\}\ )^2$$

$$variance_{m^\Theta}(\mathbf{x}) = \mathrm{E}_{\mathcal{S}^{tr}}\{\ (\ \hat{y} - \mathrm{E}_{\mathcal{S}^{tr}}\{\hat{y}\}\ )^2\}$$

$$noise(\mathbf{x}) = \mathrm{E}_{(\mathbf{x},y)}\{\ (y - \mathrm{E}_{(\mathbf{x},y)}\{y\})^2\ \}$$

and sum them up

$$\underbrace{bias^2_{m^\Theta}(\mathbf{x}) + variance_{m^\Theta}(\mathbf{x})}_{\mathrm{E}_{\mathcal{S}^{tr}}\{(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})^2\}} + noise(\mathbf{x})$$

Expected squared error

$$
\begin{aligned}
&\mathrm{E}_{\mathcal{S}^{tr}}\{(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})^2\}+\mathrm{E}_{(\mathbf{x},y)}\{(y-\mathrm{E}_{(\mathbf{x},y)}\{y\})^2\}\\
&=\mathrm{E}_{(\mathbf{x},y)}\{(y-\mathrm{E}_{(\mathbf{x},y)}\{y\})^2\}+\mathrm{E}_{\mathcal{S}^{tr}}\{(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})^2\}\\
&\quad+\mathrm{E}_{\mathcal{S}^{tr}}\{2\cdot(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\mathrm{E}_{(\mathbf{x},y)}\{y\})(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})\}\\
&=\mathrm{E}_{\mathcal{S}^{tr}}\{\mathrm{E}_{(\mathbf{x},y)}\{(y-\mathrm{E}_{(\mathbf{x},y)}\{y\})^2\}\}+\mathrm{E}_{\mathcal{S}^{tr}}\{\mathrm{E}_{(\mathbf{x},y)}\{(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})^2\}\\
&\quad+\mathrm{E}_{\mathcal{S}^{tr}}\{\mathrm{E}_{(\mathbf{x},y)}\{2\cdot(y-\mathrm{E}_{(\mathbf{x},y)}\{y\})(\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})\}\}\\
&=\mathrm{E}_{\mathcal{S}^{tr}}\{\mathrm{E}_{(\mathbf{x},y)}\{(y-\mathrm{E}_{(\mathbf{x},y)}\{y\}+\mathrm{E}_{(\mathbf{x},y)}\{y\}-\hat{y})^2\}\}\\
&=\mathrm{E}_{\mathcal{S}^{tr}}\{\mathrm{E}_{(\mathbf{x},y)}\{(y-\hat{y})^2\}\}
\end{aligned}
$$

We get the expected squared error of the model over all training samples and all instances w.r.t. the observed labeling.

- known labels for observed instances

Test set, RMSE and MAE

In practice, we train a model m^{Θ} on a train set $\mathcal{S}^{tr}$ and test its error on a so-called **test sample** $\mathcal{S}^{te}$ defined as

$$\mathcal{S}^{te} \subset \mathcal{X} \times \mathcal{L} \setminus \mathcal{S}^{tr}$$

Root mean squared error (regression)

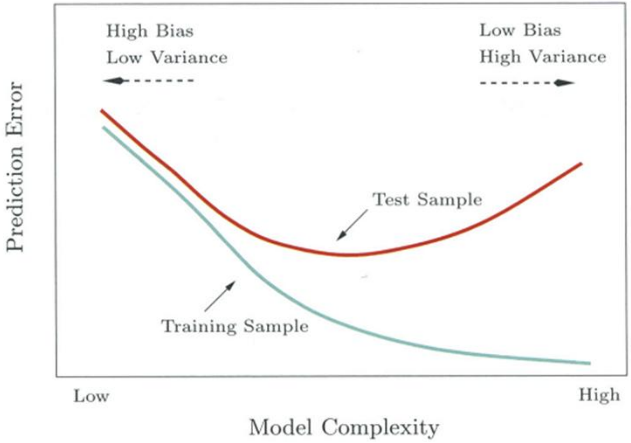
$$rmse(m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x}), \mathcal{S}^{te}) = \sqrt{\frac{\sum_{(\mathbf{x},y)\in\mathcal{S}^{te}} (m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x}) - y)^2}{|\mathcal{S}^{te}|}}$$

Mean absolute error (classification)

$$mae(m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x}), \mathcal{S}^{te}) = \frac{\sum_{(\mathbf{x},y)\in\mathcal{S}^{te}} I(m^{\Theta,\mathcal{S}^{tr}}(\mathbf{x}) \neq y)}{|\mathcal{S}^{te}|}$$

where $I(\cdot) = 1$ if the condition $(\cdot)$ holds, otherwise $I(\cdot) = 0$.

Bias-variance, test set, train set, . . .



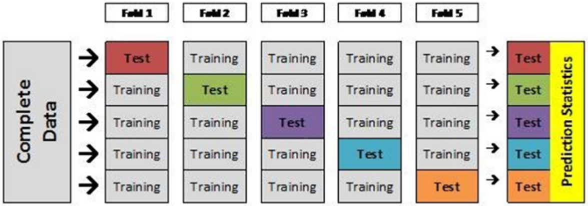
[3]

[3] image from Google images.

Cross-validation

A small complication: As usual, we have only one training and one test set on the input! Moreover, the labels of instances in the test set are "hidden"[1] to the model.

- Question: How can we get the model with the least expected error?
  - i.e. evaluating over all training samples and all instances...
- Answer: Try to simulate learning over "more" training sets and "more" instances.
  - i.e. creating more (smaller) training sets from the original one...



[1] The test set should be usually used for the final evaluation of the model but not for tuning it (selection of a best technique or good parameters, etc.)

k-fold Cross-validation

One possible alternative[2]:

1. Split (systematically or randomly) the training sample $\mathcal{S}^{tr}$ to k parts of similar size
$$\mathcal{S}^{tr} = \bigcup_k \mathcal{S}_k^{tr}$$
2. choose those hyper-parameters Ξ such that[3]
$$\Xi = \underset{m^{\Xi}}{arg\,min} \left\{ \frac{1}{k} \sum_{i=1}^{k} err(m^{\Theta,\Xi,\bigcup_{1\leq j\leq k, j\neq i} \mathcal{S}_j^{tr}}, \mathcal{S}_i^{tr}) \right\}$$
   - $\mathcal{S}_i^{tr}$ is called **validation fold**.
3. "re-learn" the final m^{Θ} using Ξ on the whole training set $\mathcal{S}^{tr}$

[2] Ξ denotes the hyper-parameters of the model.

[3] $m^{\Theta,\Xi,\bigcup_{1\leq j\leq k, j\neq i} \mathcal{S}_j^{tr}}$ denotes a model whose parameters Θ were learned using hyper-parameters Ξ on the sample $\bigcup_{1\leq j\leq k, j\neq i} \mathcal{S}_j^{tr}$.

Bayes Classifier

Let's have $C_1, \ldots, C_K$ mutually exclusive and exhaustive classes

prior probability $P(C_i)$

- probability that an arbitrary instance is labeled with class C_i

likelihood $P(\mathbf{x}|C_i)$

- probability that an arbitrary instance belonging to class C_i is associated with the instance $\mathbf{x}$

evidence $P(\mathbf{x})$

- probability that the instance $\mathbf{x}$ is seen regardless of its class

posterior probability $P(C_i|\mathbf{x})$

- probability that the instance $\mathbf{x}$ is labeled with class C_i

$$P(C_i|\mathbf{x}) = \frac{P(\mathbf{x}|C_i)P(C_i)}{P(\mathbf{x})}$$

for $\mathbf{x}$ **predict** C_i for which $P(C_i|\mathbf{x})$ is maximal

Discriminant function

in case of K classes, classification can be seen as an implementation of K discriminant functions $g_1(\mathbf{x}), \ldots, g_K(\mathbf{x})$ such that

- for $\mathbf{x}$ **predict** C_i for which $g_i(\mathbf{x})$ is maximal

binary classification

- $K = 2$, i.e. labels of instances belong to $\mathcal{L} = \{0, 1\}$
- e.g. $g_1(\mathbf{x}) = P(\mathbf{x}|C_1)P(C_1)$ and $g_2(\mathbf{x}) = P(\mathbf{x}|C_2)P(C_2)$
- a single discriminant is enough

$$g(\mathbf{x}) = g_1(\mathbf{x}) - g_2(\mathbf{x})$$

- for $\mathbf{x}$ predict C_1 if $g(\mathbf{x}) > 0$, and predict C_2 if $g(\mathbf{x}) < 0$

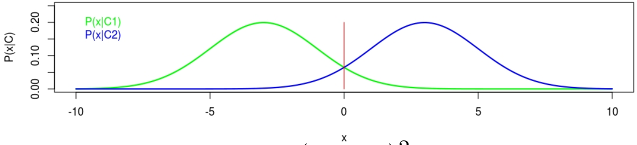
decision boundary

- separates the feature space into **decision regions**
- $g(\mathbf{x}) = 0$ for any $\mathbf{x}$ lying on the decision boundary

Example

one dimensional feature space, two classes

- assume equal priors, i.e. $P(C_1) = P(C_2)$
- assume normal likelihoods, i.e. $P(\mathbf{x}|C_i) = \mathcal{N}(\mu_i, \sigma_i^2)$
    - assume equal standard deviations, i.e. $\sigma_1^2 = \sigma_2^2$
- $g_i(\mathbf{x}) = logP(\mathbf{x}|C_i) + logP(C_i)$



$$g_i(\mathbf{x}) = \underbrace{-\frac{1}{2} log\ 2\pi}_{\text{constant}} \underbrace{-log\ \sigma_i}_{\text{equal variances}} - \frac{(x-\mu_i)^2}{\underbrace{2\sigma_i^2}_{\text{equal variances}}} \underbrace{+logP(C_i)}_{\text{equal priors}} = -(x-\mu_i)^2$$

- we use the estimates m_i for μ_i, i.e. $g_i(\mathbf{x}) = -(x-m_i)^2$
    - assign $\mathbf{x}$ to the class C_i with the nearest mean m_i
- decision boundary, where $g_1(\mathbf{x}) = g_2(\mathbf{x})$, i.e. $\mathbf{x} = \frac{m_1+m_2}{2}$

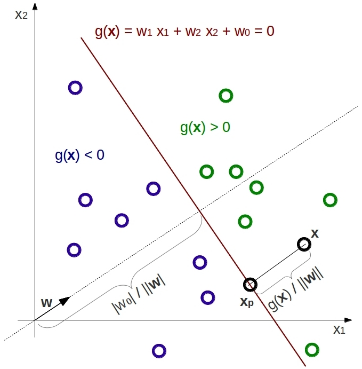
Linear classifier

linear discriminant function – a hyperplane

- $g(\mathbf{x}) = g_1(\mathbf{x}) - g_2(\mathbf{x}) = (\mathbf{w}_1^T\mathbf{x} + w_{10}) - (\mathbf{w}_2^T\mathbf{x} + w_{20})$

$$g(\mathbf{x}) = (\mathbf{w}_1 - \mathbf{w}_2)^T\mathbf{x} + (w_{10} - w_{20}) = \mathbf{w}^T\mathbf{x} + w_0$$

- assign $\mathbf{x}$ to the class C_1 if $g(\mathbf{x}) > 0$, and to C_2 if $g(\mathbf{x}) < 0$



Linear classifier – properties

Let $\mathbf{x}_1, \mathbf{x}_2$ be two points on the hyperplane

- $g(\mathbf{x}_1) = \mathbf{w}^T\mathbf{x}_1 + w_0 = 0 = \mathbf{w}^T\mathbf{x}_2 + w_0 = g(\mathbf{x}_2) \Longrightarrow \mathbf{w}^T(\mathbf{x}_1 - \mathbf{x}_2) = 0$
    - $\mathbf{w}$ is orthogonal to the hyperplane, i.e. **defines** its **direction**

Let $\mathbf{x}_p$ be the projection of $\mathbf{x}$ on the hyperplane, i.e. $g(\mathbf{x}_p) = 0$

- $\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{||\mathbf{w}||}$, where r is the distance of $\mathbf{x}$ from the hyperplane
    - $g(\mathbf{x}) = g(\mathbf{x}_p + r\frac{\mathbf{w}}{||\mathbf{w}||}) = \mathbf{w}^T(\mathbf{x}_p + r\frac{\mathbf{w}}{||\mathbf{w}||}) + w_0 = \underbrace{\mathbf{w}^T\mathbf{x}_p + w_0}_{g(\mathbf{x}_p)=0} + r\frac{\mathbf{w}^T\mathbf{w}}{||\mathbf{w}||}$
    - $g(\mathbf{x}) = r||\mathbf{w}|| \Longrightarrow r = \frac{g(\mathbf{x})}{||\mathbf{w}||}$

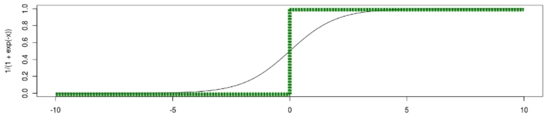
Let $\mathbf{x} = \mathbf{0}$

- $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 \Longrightarrow \underbrace{\frac{g(\mathbf{x})}{||\mathbf{w}||}}_{r_\mathbf{0}} = \underbrace{\frac{\mathbf{w}^T\mathbf{x}}{||\mathbf{w}||}}_{0} + \frac{w_0}{||\mathbf{w}||} \Longrightarrow r_\mathbf{0} = \frac{w_0}{||\mathbf{w}||}$
    - w_0 **defines** the **distance** of the hyperplane from the origin

Logistic regression (1/2)

Can be the probability $P(C = 1|\mathbf{x})$ approximated by a linear function?

- $P(C = 0|\mathbf{x}) = 1 - P(C = 1|\mathbf{x})$ in a binary case
- find parameters $\mathbf{w}, w_0$ such that $P(C = 1|\mathbf{x}) = (\mathbf{w}^T\mathbf{x} + w_0) + \epsilon$
  - problem: a simple regression model can predict values outside the interval[4] $[0, 1]$
    - solution: use a **sigmoid logistic function** $s(t) = \frac{1}{1+e^{-t}}$



- **logistic regression model**

$$P(C = 1|\mathbf{x}) = s(\mathbf{w}^T\mathbf{x} + w_0) + \epsilon = \frac{1}{1 + e^{-(\mathbf{w}^T\mathbf{x}+w_0)}} + \epsilon$$

[4] Probabilities should lie between 0 and 1.

Logistic regression (2/2)

Maximum lilelihood estimate

- instances $(\mathbf{x}_i, c_i) \in \mathcal{S}^{tr}$ in a training set, where $c_i \in \{0, 1\}$
- Bernoulli distribution for binary targets
- conditional likelihood with $\Theta = (\mathbf{w}, w_o)$

$$L^{cond}_{\mathcal{S}^{tr}}(\Theta) = \prod_{(\mathbf{x}_i, c_i) \in \mathcal{S}^{tr}} p(C = c_i | \mathbf{x}_i) =$$

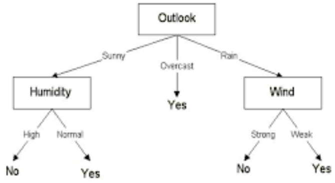
$$= \prod_{(\mathbf{x}_i, c_i) \in \mathcal{S}^{tr}} p(C = 1 | \mathbf{x}_i)^{c_i} \, (1 - p(C = 1 | \mathbf{x}_i))^{(1 - c_i)}$$

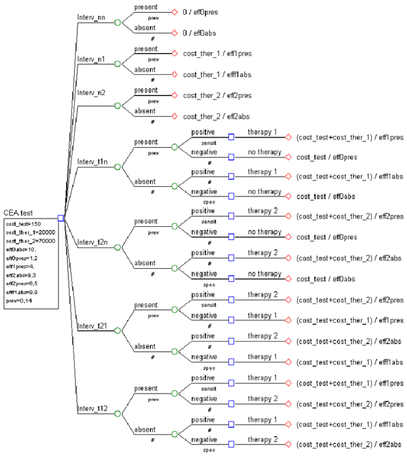
- conditional log-likelihood $ln \, L^{cond}_{\mathcal{S}^{tr}}(\Theta)$ to maximize is

$$\sum_{(\mathbf{x}_i, c_i) \in \mathcal{S}^{tr}} \Big(c_i \, ln(\frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + w_0)}}) + (1 - c_i) \, ln \big(1 - \frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + w_0)}} \big) \Big)$$

Popular Prediction Models

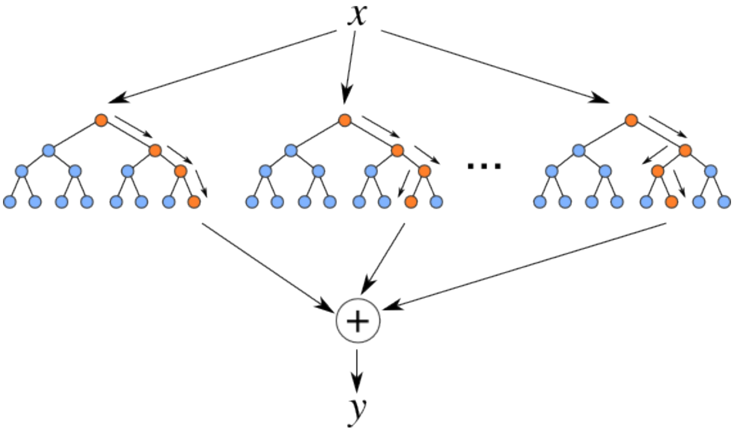
Decision Trees





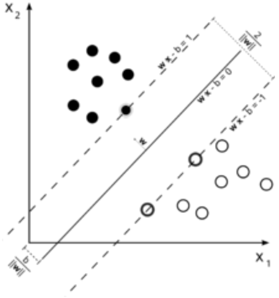
Popular Prediction Models

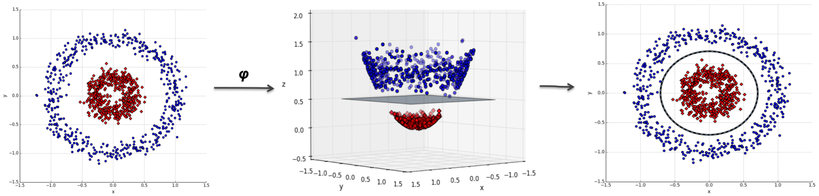
Random Forests



Popular Prediction Models

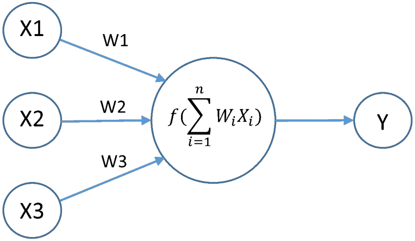
Support Vector Machines

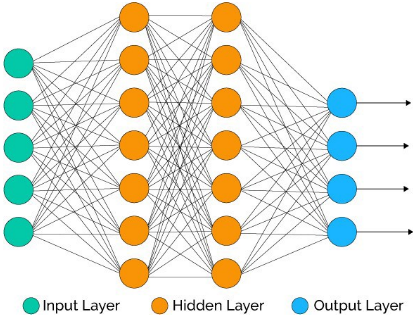




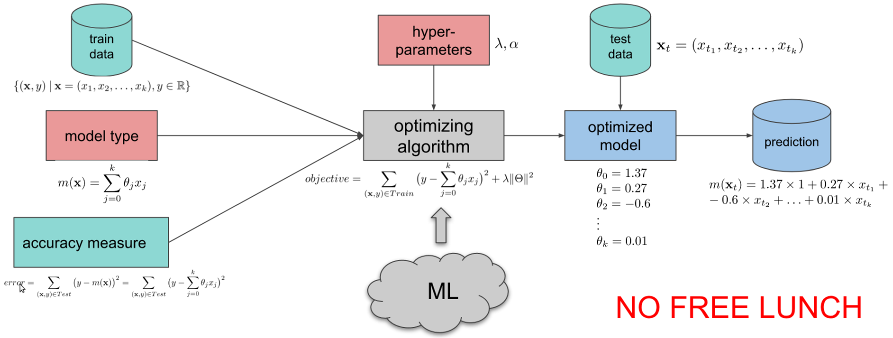
Popular Prediction Models

Neural Networks





Modeling – Recap



train data
$\{(\mathbf{x},y) \mid \mathbf{x}=(x_1,x_2,\ldots,x_k), y \in \mathbb{R}\}$
model type
$m(\mathbf{x}) = \sum_{j=0}^{k} \theta_j x_j$
accuracy measure
$error = \sum_{(\mathbf{x},y)\in Test} (y-m(\mathbf{x}))^2 = \sum_{(\mathbf{x},y)\in Test} (y-\sum_{j=0}^{k}\theta_j x_j)^2$
hyper-parameters
λ, α
optimizing algorithm
$objective = \sum_{(\mathbf{x},y)\in Train} (y-\sum_{j=0}^{k}\theta_j x_j)^2 + \lambda\|\Theta\|^2$
ML
test data
$\mathbf{x}_t = (x_{t_1}, x_{t_2}, \ldots, x_{t_k})$
optimized model
$\theta_0 = 1.37$
$\theta_1 = 0.27$
$\theta_2 = -0.6$
$\vdots$
$\theta_k = 0.01$
prediction
$m(\mathbf{x}_t) = 1.37 \times 1 + 0.27 \times x_{t_1} + - 0.6 \times x_{t_2} + \ldots + 0.01 \times x_{t_k}$

NO FREE LUNCH

Thanks for your attention

References

- Pang-Ning Tan, Michael Steinbach, and Vipin Kumar (2005). Introduction to Data Mining. Addison-Wesley Longman Publishing Co., Inc.
- Ethem Alpaydin (2009). Introduction to Machine Learning. The MIT Press.
- Jiawei Han, Micheline Kamber and Jian Pei (2011). Data Mining: Concepts and Techniques. Morgan Kaufmann.
- Tom Mitchell (1997). Machine Learning. McGraw Hill.

2 Homeworks

1. Home study of the basic principles for the following methods
   - Decision Trees
   - Support Vector Machines
   - Neural Networks
2. Use some regression techniques for the chosen regression dataset to predict the target attribute
3. Use some classification techniques for the chosen regression dataset to predict the target attribute

Questions?

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