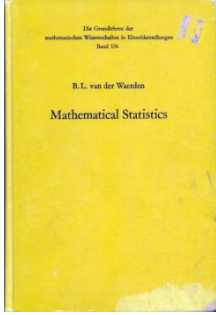
Statistics 101

Paul G. Plöger
SEE

Overview

1) **Various distributions of random Variables and their display**
2) Characterizing distributions; central tendency and dispersion
3) Some theorems on distributions (with / without models)
4) Standard error of empirical mean and empirical variance
5) Error propagation in regression for measurements with precision

Ex: The Quetelet Curve



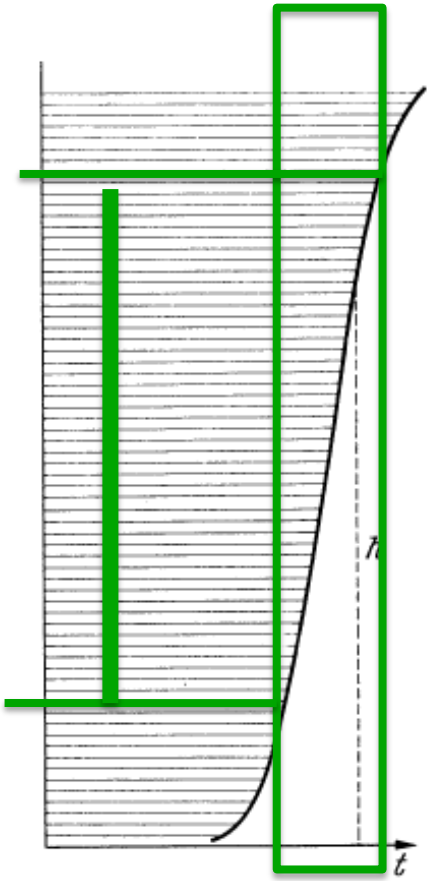


Fig. 11. Quetelet's curve

„I still remember vividly how my father took me one day as a boy to the outskirts of the city, where the willows stood on the bank and had me pick a hundred willow leaves at random. After throwing out those with damaged tips, 89 were left which we took home. We arranged them very carefully according to decreasing size like soldiers in rank and file.

Then my father drew a curved line through the tips and said, "This is the curve of Quetelet. From it you see how the mediocre always form the large majority and only a few stand out or are left behind."

B.L. van der Waerden, Mathematical Statistics, Springer, 1968

Two views on Statistics

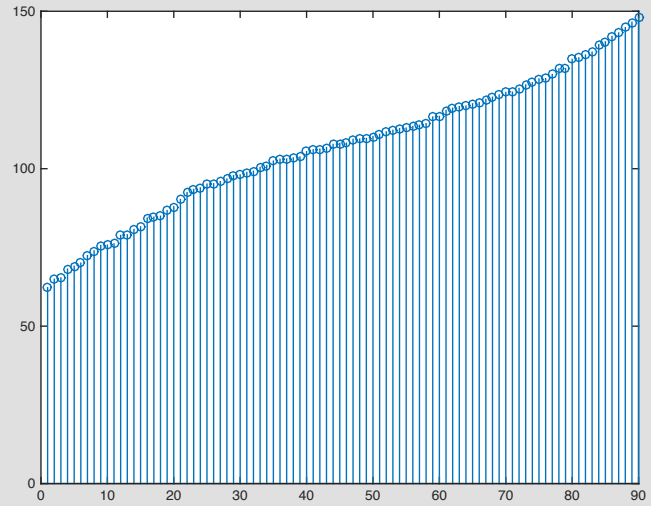
Statistical methods to describe data in form of diagrams, tables or individual parameters is called **descriptive statistics.**

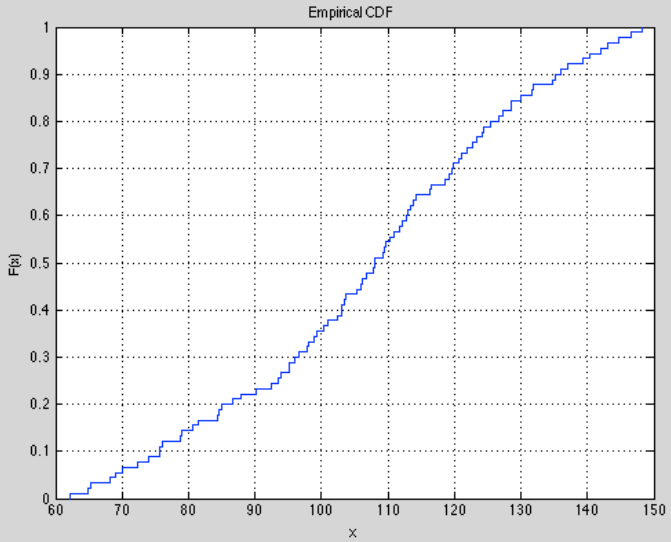
If we infer, based on these qualitative analysis techniques, from these given empirical data the validity of hypothesizes we talk about **deductive statistics**

Ex: Raw data table, Master list

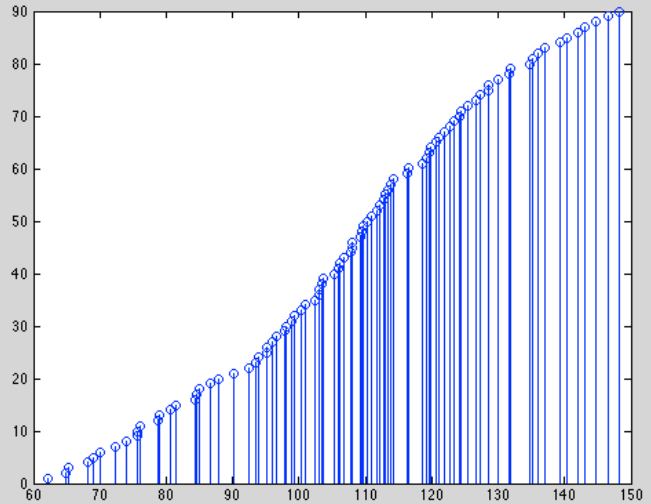
131.8	106.7	116.4	84.3	118.5	93.4	65.3	113.8	140.3
119.2	129.9	75.7	105.4	123.4	64.9	80.7	124.2	110.9
86.7	112.7	96.7	110.2	135.2	134.7	146.5	144.8	113.4
128.6	142.0	106.0	98.0	148.2	106.2	122.7	70.0	73.9
78.8	103.4	112.9	126.6	119.9	62.2	116.6	84.6	101.0
68.1	95.9	119.7	122.0	127.3	109.3	95.1	103.1	92.4
103.0	90.2	136.1	109.6	99.2	76.1	93.9	81.5	100.4
114.3	125.5	121.0	137.0	107.7	69.0	79.0	111.7	98.8
124.3	84.9	108.1	128.5	87.9	102.4	103.7	131.7	139.4
108.0	109.4	97.8	112.2	75.6	143.1	72.4	120.6	95.2

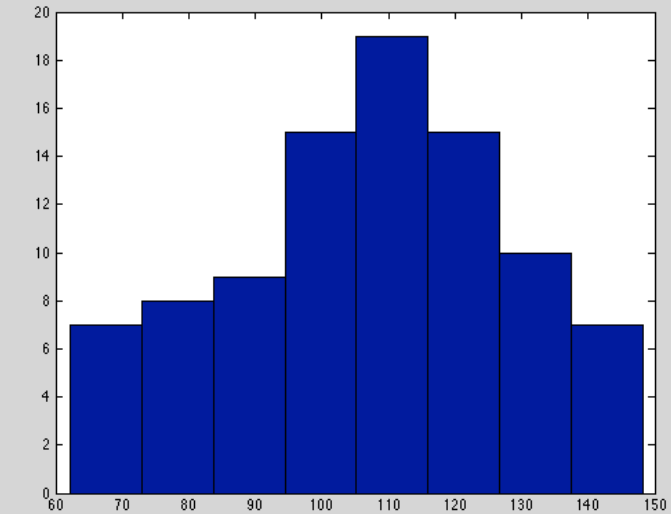
`Urdata(:)`





Some different views / plot types in MATLAB





stem plot

(empirical) cumulative distribution function

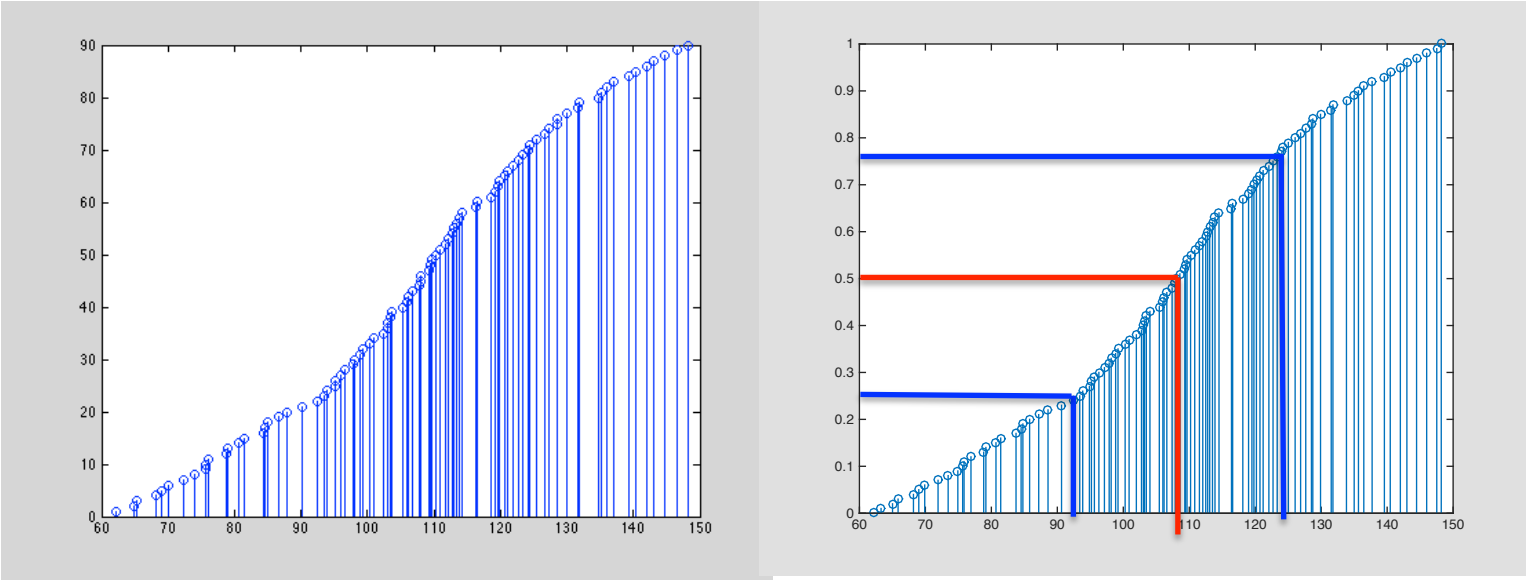
(quantile fct)

histogram

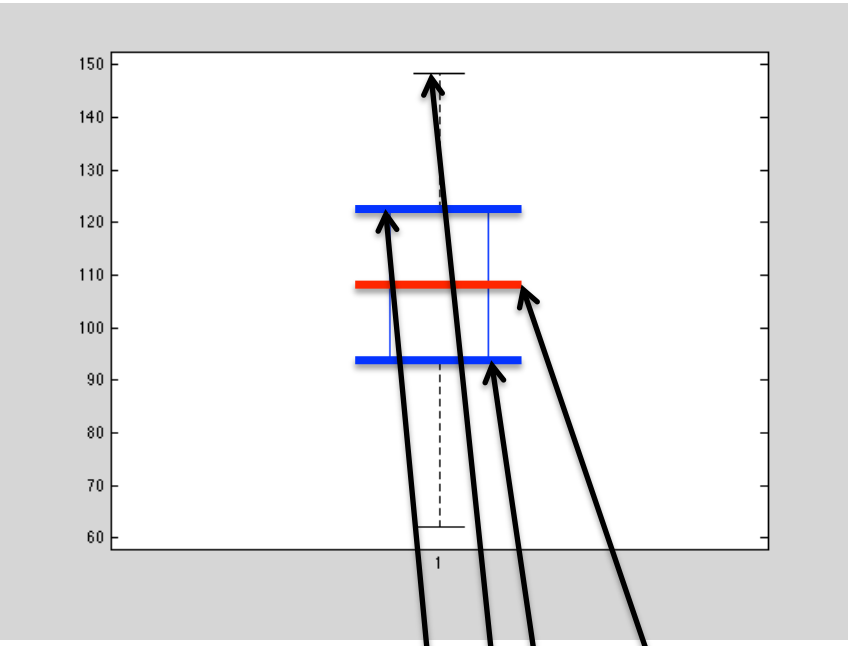
```
hist(Urdata(:),8);
stem(1:length(Urdata(:)),sort(Urdata(:)));
stem(sort(Urdata(:)),1:length(Urdata(:)));
cdfplot(Urdata(:))
```

```
import numpy as np
import statsmodels.api as sm
import matplotlib.pyplot as plt

sample = np.random.uniform(0, 1, 50)
ecdf = sm.distributions.ECDF(sample)

x = np.linspace(min(sample), max(sample))
y = ecdf(x)
plt.step(x, y)
plt.show()
```

Quantile is a scaled version of CDF
Quantile is inverse of CDF




```
stem(sort(Urdata(:)),1:length(Urdata(:)));
stem(quantile(Urdata(:),0:0.01:1),0:0.01:1)
```

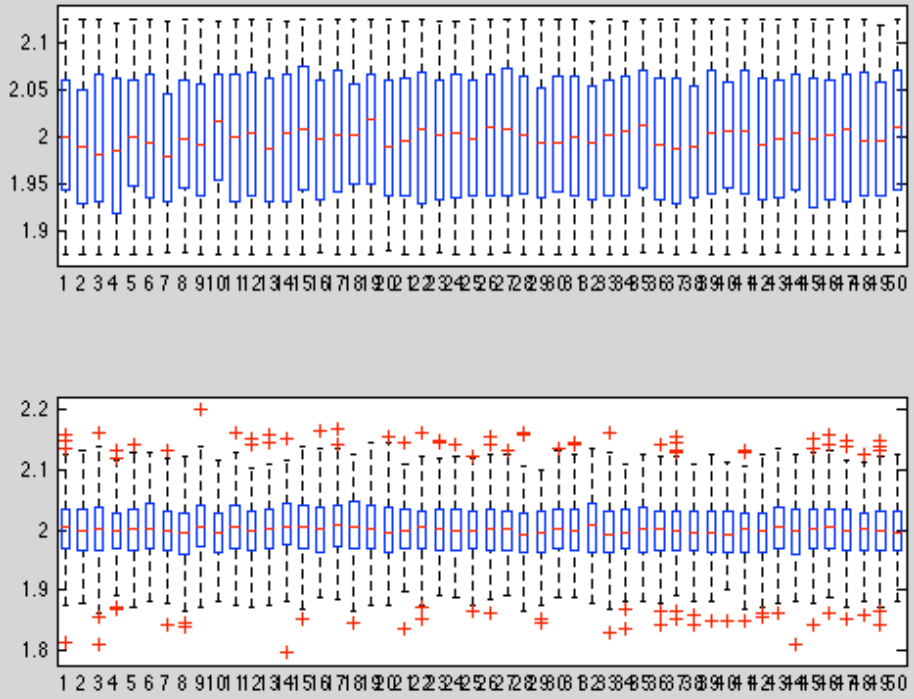


One of the easiest: boxplot

```
boxplot(Urdata(:))
```

It shows:

the median (red) (50% quantile)
the lower 25% quantile (lower box line: lbl)
upper 75% quantile (upper box line:ubl)
whiskers == median +/-1.5*(ubl-lbl)
outliers (data beyond wiskers ==
99.3 % coverage for normal distribution)



Good for overview spagetti data

```
spagetti_50 =(rand(250,50)-0.5)*0.25+2;
spagetti_50n = random('normal',2,0.05,250,50);
subplot(2,1,1);boxplot(spagetti_50);
subplot(2,1,2);boxplot(spagetti_50n)
%another example
PX=[ones(1,30)*0.2 ones(1,40)*1.2 ones(1,40)*2.4];
```

Basic Definitions and Facts from Statistics

A ***random variable X,Y,Z,...*** can be viewed as the name of a (real valued) experiment with a probabilistic outcome. Its value is the outcome of the experiment.

A ***probability distribution*** for a random variable ***Y*** specifies the probability $P(Y = y_i)$ that ***Y*** will take on the value y_i, for each possible value y_i.

The ***expected value***, or ***mean***, of a random variable ***Y*** is $E[Y] = \sum_i Pr(Y = y_i) \cdot y_i$. The symbol μ is commonly used to represent $E[Y]$.

The ***variance*** of a random variable is $Var(Y) = E[(Y - \mu_Y)^2]$. The variance characterizes the width or dispersion of the distribution about its mean.

The ***standard deviation*** of ***Y*** is $\sqrt{Var(Y)}$. The symbol σ_Y is often used used to represent the standard deviation of ***Y***.

The ***Binomial distribution*** gives the probability of observing ***r heads*** in a series of ***n independent coin tosses***, if the probability of heads in a single toss is ***p***.

The ***Normal distribution*** is a bell-shaped probability distribution that covers many natural phenomena.

The ***Central Limit Theorem*** is a theorem stating that the mean value of a large number of independent, identically distributed random variables ***approximately follows a Normal distribution***.

An ***estimator*** is a random variable ***Y*** used to estimate some parameter ***p*** of an underlying population.

The ***estimation bias of Y*** as an estimator for ***p*** is the quantity ***(E[Y] - p)***. An unbiased estimator is one for which the bias is zero.

A ***N% confidence interval*** estimate for parameter ***p*** is an interval that ***includes p*** with ***probability N%***.

A random variable X is a real – valued function:

$X : \Omega \to IR,$

$\omega \mapsto X(\omega)$

where ω is the result of an random experiment like e.g. measured runtime of an algorithm on a CPU with a cache. X needs to be measurable.

if F_X is a CDF then the function

$Q_X :]0,1[\to IR,$

$p \mapsto Q_X(p) = \min\{x \mid F_X(x) \geq p\}$

is called quantil function of F_X.

Q_X inverse of F_X in following sense:

$F_X(Q_X(p)) \geq p$ for $p \in]0,1[$ and

$Q_X(F_X(x)) \leq x$ for $x \in IR$

A probability measure P is a map from an algebra of sets $\mathcal{A}$

$P : \mathcal{A} \to IR,$

$A \mapsto P(A)$ which obeys: (Kolmogorov Axioms):

(1) $P(A) \geq 0$

(2) $P(\Omega) = 1$

(3) $P(A \cup B) = P(A) + P(B)$ if $A \cap B = \emptyset$

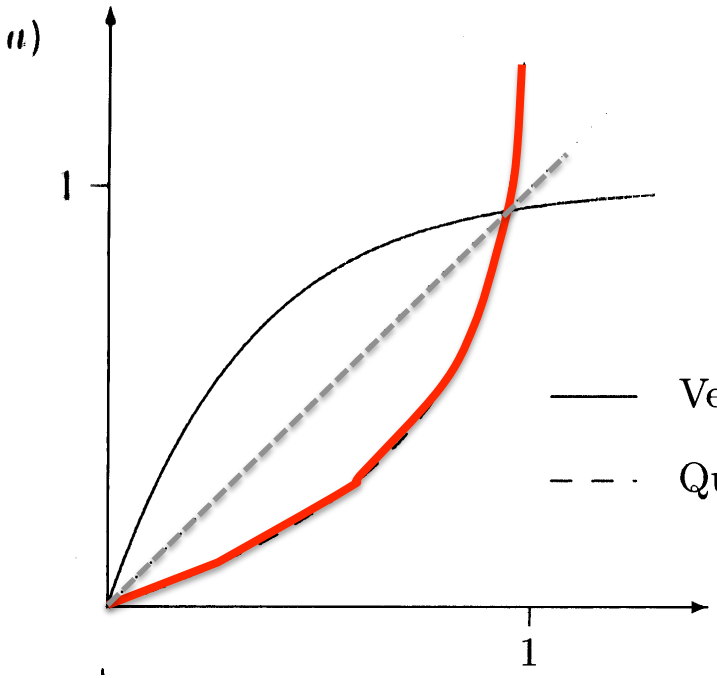
The cummulative distribution function (CDF) is defined as:

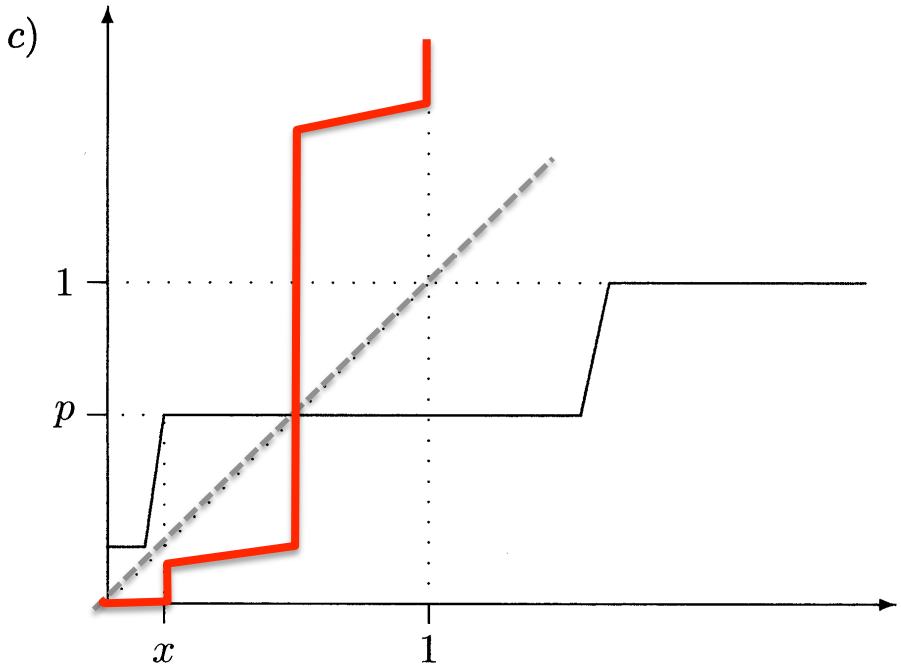
$F_X : IR \to [0,1],$

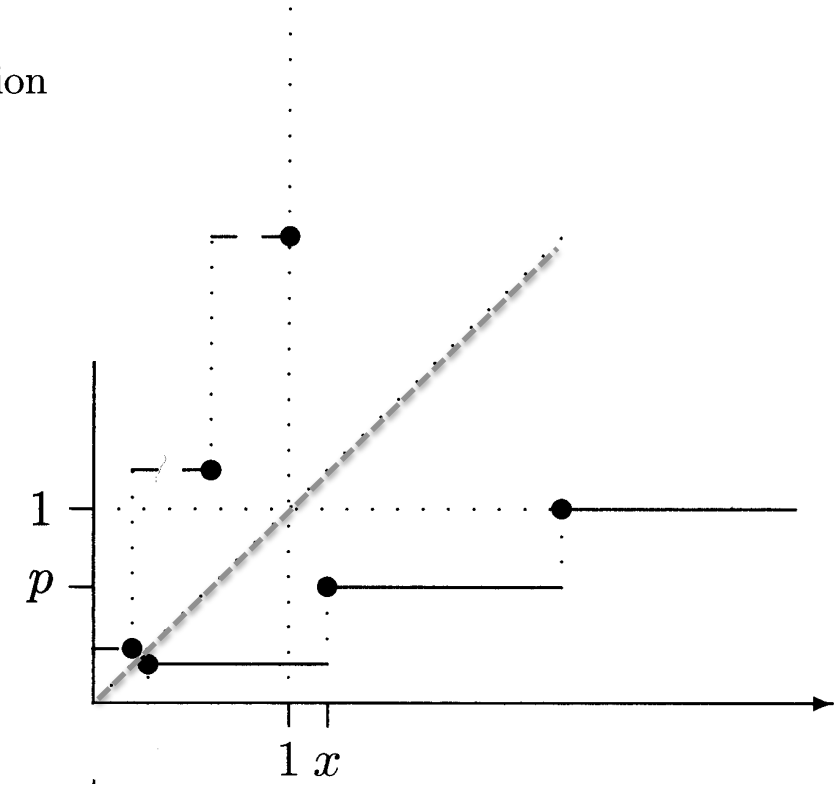
$x \mapsto F_X(x) := P(\{\omega \mid X(\omega) \leq x\})$

Random Variable, Cumulative distribution function, Quantile fct

Quantil == inverse CDF







Histogram, How to ?

With increasing size of the examined collective smaller category widths can be selected.

The larger the variation of the measured values (the difference between the largest and the smallest value), the wider the categories may be.

According to a a rule of thumb of Sturges (1926) the number of categories m (n = sample size) should be determined according to the relation $m \approx 1 + 3.32 \lg(n)$ where n is the sample size.

The maximum number of categories should not exceed 20 for reasons of clarity.

All categories should have the same width in general.

Overview

1) Various distributions of random Variables and their display
2) **Characterizing distributions; central tendency and dispersion**
3) Some theorems on distributions (with / without models)
4) Standard error of empirical mean and empirical variance
5) Error propagation in regression for measurements with precision

Graph versus Parameters

While the graph of a distribution stresses the WHOLE distribution (the whole collection of data is represented), statistical parameters should stress special, global, summarizing features of the underlying distribution.

It should represent „typical“ attributes, like the general tendency or variability i.e. the dispersion of the distribution.

I		II		III		IV	
X	Y	X	Y	X	Y	X	Y
10.0	8.04	10.0	9.14	10.0	7.46	8.0	6.58
8.0	6.95	8.0	8.14	8.0	6.77	8.0	5.76
13.0	7.58	13.0	8.74	13.0	12.74	8.0	7.71
9.0	8.81	9.0	8.77	9.0	7.11	8.0	8.84
11.0	8.33	11.0	9.26	11.0	7.81	8.0	8.47
14.0	9.96	14.0	8.10	14.0	8.84	8.0	7.04
6.0	7.24	6.0	6.13	6.0	6.08	8.0	5.25
4.0	4.26	4.0	3.10	4.0	5.39	19.0	12.50
12.0	10.84	12.0	9.13	12.0	8.15	8.0	5.56
7.0	4.82	7.0	7.26	7.0	6.42	8.0	7.91
5.0	5.68	5.0	4.74	5.0	5.73	8.0	6.89

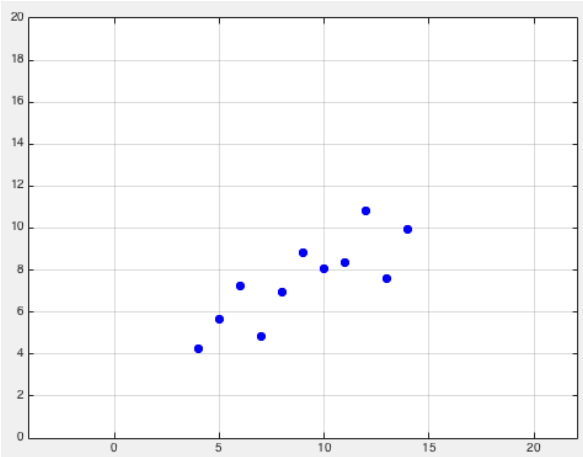
Interplay: graph versus parameters

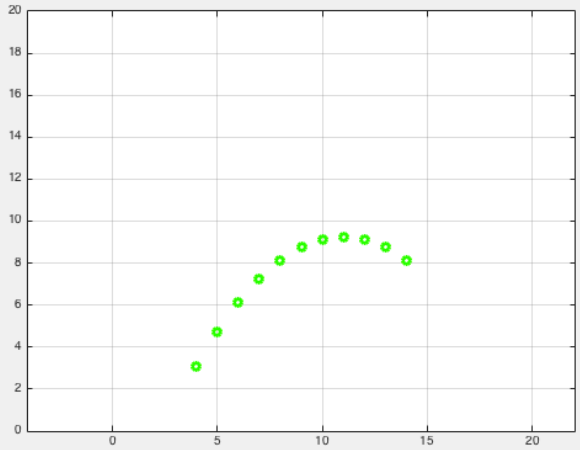
```
A=[
10.0000   8.0400   10.0000   9.1400   10.0000   7.4600   8.0000   6.5800
 8.0000   6.9500    8.0000   8.1400    8.0000   6.7700   8.0000   5.7600
13.0000   7.5800   13.0000   8.7400   13.0000  12.7400   8.0000   7.7100
 9.0000   8.8100    9.0000   8.7700    9.0000   7.1100   8.0000   8.8400
11.0000   8.3300   11.0000   9.2600   11.0000   7.8100   8.0000   8.4700
14.0000   9.9600   14.0000   8.1000   14.0000   8.8400   8.0000   7.0400
 6.0000   7.2400    6.0000   6.1300    6.0000   6.0800   8.0000   5.2500
 4.0000   4.2600    4.0000   3.1000    4.0000   5.3900  19.0000  12.5000
12.0000  10.8400   12.0000   9.1300   12.0000   8.1500   8.0000   5.5600
 7.0000   4.8200    7.0000   7.2600    7.0000   6.4200   8.0000   7.9100
 5.0000   5.6800    5.0000   4.7400    5.0000   5.7300   8.0000   6.8900]
```

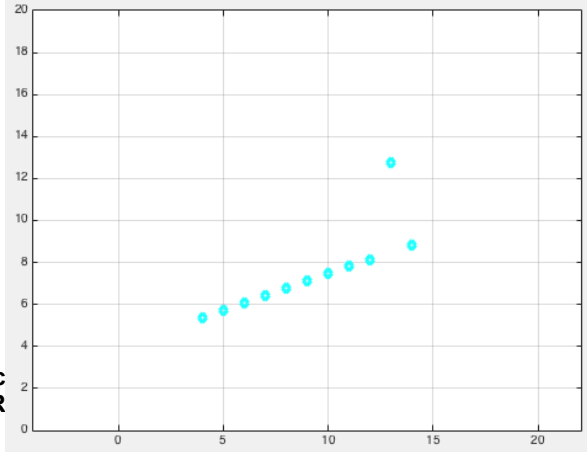
N=11
mean of X's = 9.0
mean of Y's = 7.5
equation of regression line: Y = 3 +0.5X
standard error of estimate of slope = 0.118
t = 4.24
sum of squares $X - X^{--}$ = 110.0
Regression sum of squares = 27.50
residual sum of squares of Y = 13.75
correlation coefficient = .82
r2 = .67

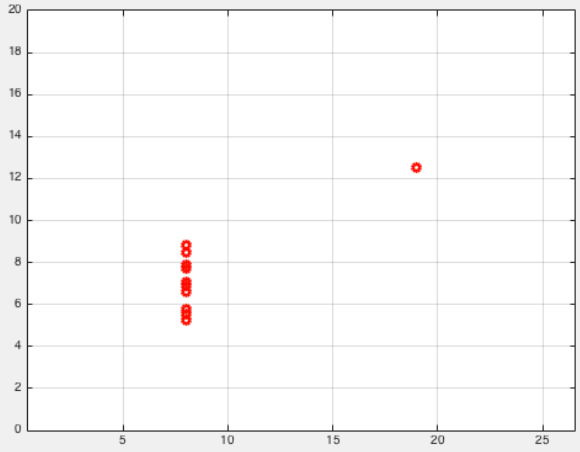
Interplay: graph versus parameters

```
clear
close
A=[
10.0000    8.0400   10.0000    9.1400   10.0000    7.4600    8.0000    6.5800
    8.0000    6.9500    8.0000    8.1400    8.0000    6.7700    8.0000    5.7600
   13.0000    7.5800   13.0000    8.7400   13.0000   12.7400    8.0000    7.7100
    9.0000    8.8100    9.0000    8.7700    9.0000    7.1100    8.0000    8.8400
   11.0000    8.3300   11.0000    9.2600   11.0000    7.8100    8.0000    8.4700
   14.0000    9.9600   14.0000    8.1000   14.0000    8.8400    8.0000    7.0400
    6.0000    7.2400    6.0000    6.1300    6.0000    6.0800    8.0000    5.2500
    4.0000    4.2600    4.0000    3.1000    4.0000    5.3900   19.0000   12.5000
   12.0000   10.8400   12.0000    9.1300   12.0000    8.1500    8.0000    5.5600
    7.0000    4.8200    7.0000    7.2600    7.0000    6.4200    8.0000    7.9100
    5.0000    5.6800    5.0000    4.7400    5.0000    5.7300    8.0000    6.8900];
figure
subplot(2,2,1);
plot(A(:,1),A(:,2),'*b','LineWidth',3)
grid on, axis([0,20,0,20]),  axis equal
subplot(2,2,2);
plot(A(:,3),A(:,4),'og','LineWidth',3)
grid on, axis([0,20,0,20]), axis equal
subplot(2,2,3);
plot(A(:,5),A(:,6),'dc','LineWidth',3)
grid on, axis([0,20,0,20]), axis equal
subplot(2,2,4);
plot(A(:,7),A(:,8),'or','LineWidth',3)
grid on, axis([0,20,0,20]), axis equal
```









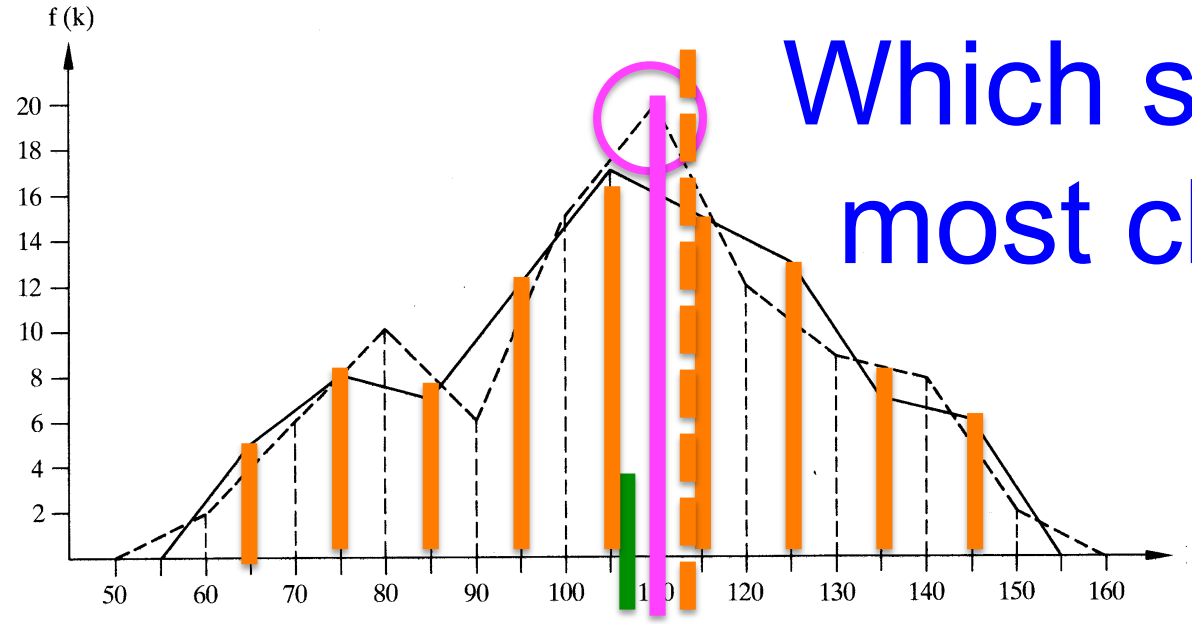


Abb. 1.1. Polygon der Häufigkeiten in Tab. 1.4 für 2 Reduktionslagen

Which single value is most charateristic?

Unimodal := one peak

Modal value: most frequent value of distribution:

```
[count,values]=hist(Urdata(:),11);
values(find(count == max(count)))
```

Median value: e.g. 50% are below this value:

```
quantile(Urdata(:),1/2) %or [1/4 ½ 3/4])
```

(emp.) Mean value: on average closest to the data:

```
1/length(Urdata(:))*sum(Urdata(:))
```

Example

Modal value of frequency distribution

Tabelle 1.6. Modalwert einer Häufigkeitsverteilung

	Meßwert (x)	Häufigkeit (f(x))
	11	2
	12	8
	13	18
	14	17
	15	22
Modalwert	16	28
	17	21
	18	11
	19	3

Median for grouped data

Tabelle 1.7. Medianwertbestimmung bei gruppierten Daten

Fehleranzahl (k)	Häufigkeit (f)	$f_{kum}(k)$
1– 20	3	3
21– 40	16	19
41– 60	12	31
61– 80	7	38
81–100	5	43
101–120	4	47
121–140	3	50

u=lower limit of category containing hit

Kb=interval width

F=count of cases in hit category, but below median

f_{MD}=case count in hit category

$$Md = u + \frac{\frac{n}{2} - F}{f_{MD}} Kb$$

EM = empirical mean = $\overline{x}$

It lies optimally „in middle“ i.e minimizing summed distance.

The mean equilibrates the difference to all elements

BUT also

mean is minimal for the sum of squared differences i.e.

$$\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

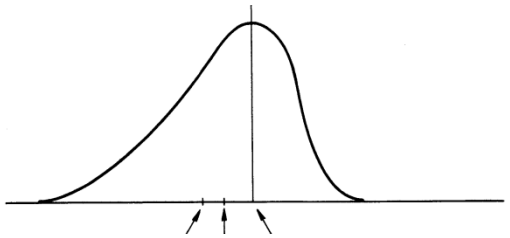
$$s_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \overline{x})^2$$

$$\sum(x_i - \overline{x}) = \sum x_i - \sum \overline{x} =$$

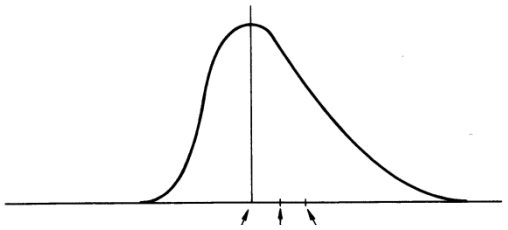
$$\sum x_i - n\overline{x} = \sum x_i - n\frac{1}{n}\sum x_i = 0$$

$$\min_c \sum (x_i - c)^2 = \overline{x}$$

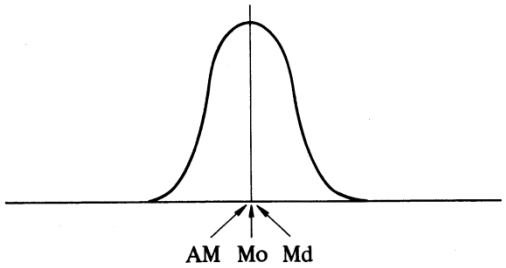
Compare Modal val., Median, EM



a rechtssteile



b linkssteile Verteilung



c symmetrische Verteilung

In case of symmetric distributions they are the same.

For biased ones (tilted in on direction) see left.

Dispersion I

AD = average deviation

$$AD = \frac{\sum_{i=1}^{n} (|x_i - \bar{x}|)}{n}.$$

Example

Tabelle 1.8. Berechnung einer AD-Streuung

Noten (x)	$(\lvert x_i - \bar{x} \rvert)$
3,3	0,8
1,7	0,8
2,0	0,5
4,0	1,5
1,3	1,2
2,0	0,5
3,0	0,5
2,7	0,2
3,7	1,2
2,3	0,2
1,7	0,8
2,3	0,2

$\sum_{i=1}^{n} x_i = 30$ $\qquad$ $\sum_{i=1}^{n} (|x_i - \bar{x}|) = 8,4$

$\bar{x} = 2,5$ $\qquad$ $AD = \frac{8,4}{12} = 0,70$

Dispersion II

Empirical variance

$$s^2 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n}.$$

Empirical standard deviation

$$s = \sqrt{s^2} = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n}}.$$

Remark:
For small n it‘s better to divide by (n-1)!
(Unbiased estimator!)

Example

Tabelle 1.9. Berechnung einer Varianz

Noten (x)	$x_i - \bar{x}$	$(x_i - \bar{x})^2$
3,3	0,8	0,64
1,7	−0,8	0,64
2,0	−0,5	0,25
4,0	1,5	2,25
1,3	−1,2	1,44
2,0	−0,5	0,25
3,0	0,5	0,25
2,7	0,2	0,04
3,7	1,2	1,44
2,3	−0,2	0,04
1,7	−0,8	0,64
2,3	−0,2	0,04
$\sum_{i=1}^{n} x_i = 30$	$\sum_{i=1}^{n} (x_i - \bar{x}) = 0$	$\sum_{i=1}^{n} (x_i - \bar{x})^2 = 7,92$
$\bar{x} = 2,5$		$s^2 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n} = \frac{7,92}{12} = 0,66$
		$s = \sqrt{0,66} = 0,81$

Overview

1) Various distributions of random Variables and their display
2) Characterizing distributions; central tendency and dispersion
3) **Some theorems on distributions (with / without models)**
4) Standard error of empirical mean and empirical variance
5) Error propagation in regression for measurements with precision

Tschebyscheff inequality

If X is a random variable with ***E(X)=μ*** and standard deviation σ, *k > 0* then it holds that:

$$P(|X-\mu| \leq k\sigma) \geq (1-\frac{1}{k^2})$$

This determines a lower bound of that part of data that falls within k number of std.-deviations from the mean. But taking complements (focus on data away from the mean, i.e. outliers):

$$P(|X-\mu| \geq k\sigma) \leq \frac{1}{k^2}$$

Patient in Hospital

Let X be the days of patients in hospital, expected value $\bar{x} = 10$, std variance $\sigma = 4$.

How likely is it, that a patient stays more then five and less then 10 days?

$$P(5 < X < 15) = P(|X - 10| < 5) \geq 1 - \frac{4*4}{5*5} = \frac{9}{25}$$

Estimate X inside 2 or 3 σ bounds

Just Tschebyscheff on P :

$$P\left(\mu - 2\sigma < X < \mu + 2\sigma\right) \geq \tfrac{3}{4} = 0.75$$

$$P\left(\mu - 3\sigma < X < \mu + 3\sigma\right) \geq \tfrac{8}{9} = 0.88$$

e.g. additional knowledge: P is normal =>

$$P\left(\mu - 2\sigma < X < \mu + 2\sigma\right) = 2\Phi(2) - 1 = 0.9544$$

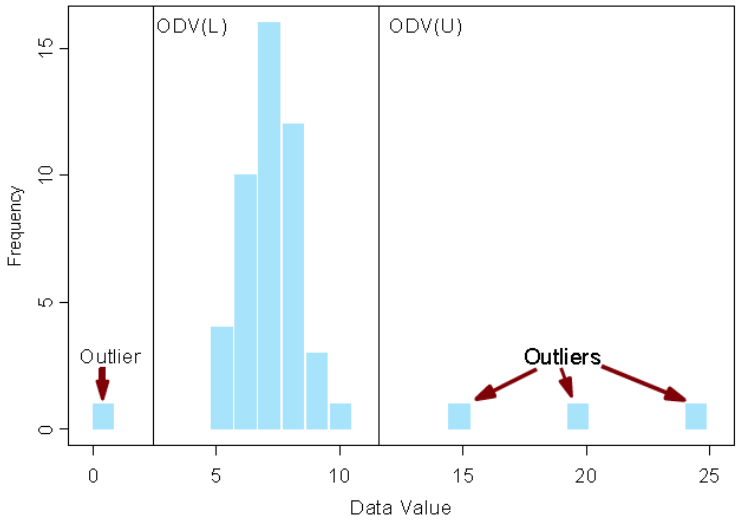
$$P\left(\mu - 3\sigma < X < \mu + 3\sigma\right) = 2\Phi(3) - 1 = 0.9974$$

In practice we have to use empirical values

$$\mu \approx \bar{x} = \frac{1}{n}\sum x_i$$

$$\sigma^2 \approx s_x^2 = \frac{1}{n-1}\sum (x_i - \bar{x})^2$$

Example for outliers

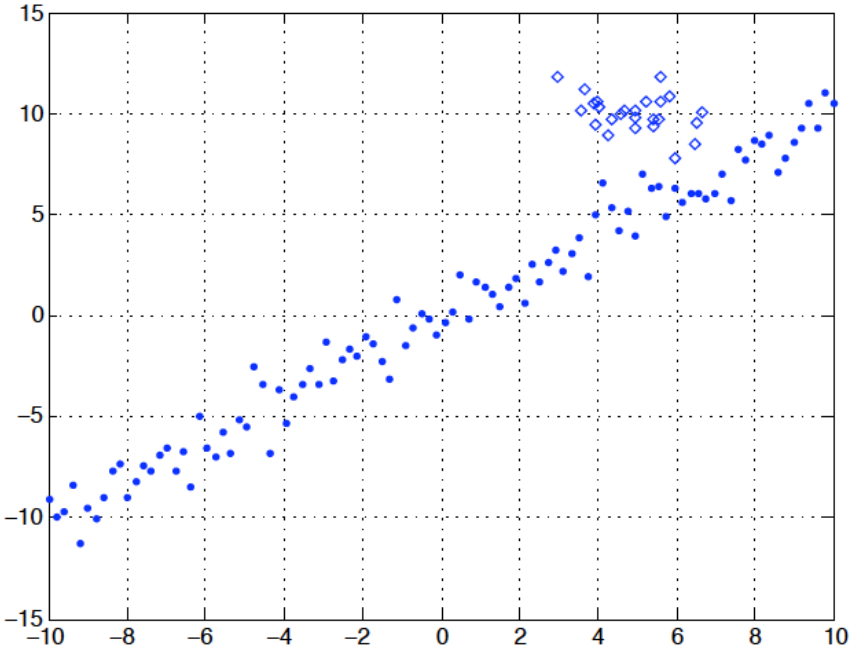


Ex: Tscheb. Outlier Algorithm

```
function [Rdata] = PGPremoveOutlier(PData,Pp1,Pp2)
%function [Rdata] = PGPremoveOutlier(Pdata,Pp1,Pp2)
%Pdata discrete, continuous
%Pp1 likelihood for expected outliers e.g. like 0.10, 0.05 , 0.01
%this will sort out bad data to get better mu and sigma
%Pp2 final likelihood for real outliers e.g. like 0.01, 0.001 , 0.0001
%all according to publ: Data Outlier Detection using the Chebyshev Theorem
%Brett G. Amidan, Thomas A. Ferryman, and Scott K. Cooley

%TODO check if its unimodal bcz then sharper bounds result

%%% phase 1
mu1= mean(PData);
sigma1 = std(PData);
k = inv(sqrt(Pp1));
ODV1U = mu1 + k*sigma1;
ODV1L = mu1 - k*sigma1;
NewData=PData(find(PData<=ODV1U));
NewData=NewData(find(NewData>=ODV1L));
```

```
%%% phase 2: calculate new u
%%% unbiased mu and sigma
mu2 = mean(NewData);
sigma2 = std(NewData);
k = inv(sqrt(Pp2));
ODV2U = mu2 + k*sigma2;
ODV2L = mu2 - k*sigma2;
NewNewData=NewData(find(NewData<=ODV2U));
Rdata=NewNewData(find(NewNewData>=ODV2L))
;
return
```

Outlier removal



Entropy **2009**, *11*, 560-585; doi:10.3390/e11040560

OPEN ACCESS

entropy

ISSN 1099-4300

www.mdpi.com/journal/entropy

Article

An Entropy-Like Estimator for Robust Parameter Identification

Giovanni Indiveri

Dipartimento Ingegneria Innovazione, University of Salento, Via Monteroni s.n., 73100 Lecce, Italy; E-Mail: giovanni.indiveri@unisalento.it; Tel.: +39 0832 29 7220; Fax +39 0832 29 7733

Received: 7 September 2009 / Accepted: 23 September 2009 / Published: 12 October 2009

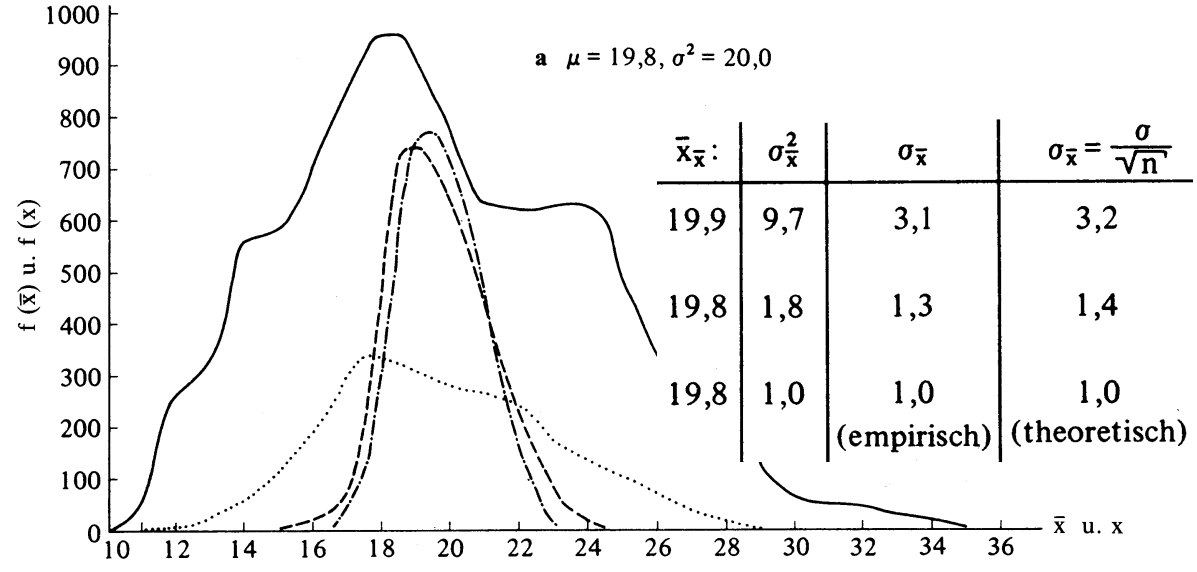
Abstract: This paper describes the basic ideas behind a novel prediction error parameter identification algorithm exhibiting high robustness with respect to outlying data. Given the low sensitivity to outliers, these can be more easily identified by analysing the residuals of the fit. The devised cost function is inspired by the definition of entropy, although the method in itself does not exploit the stochastic meaning of entropy in its usual sense. After describing the most common alternative approaches for robust identification, the novel method is presented together with numerical examples for validation.

Keywords: system identification; model fitting; data processing

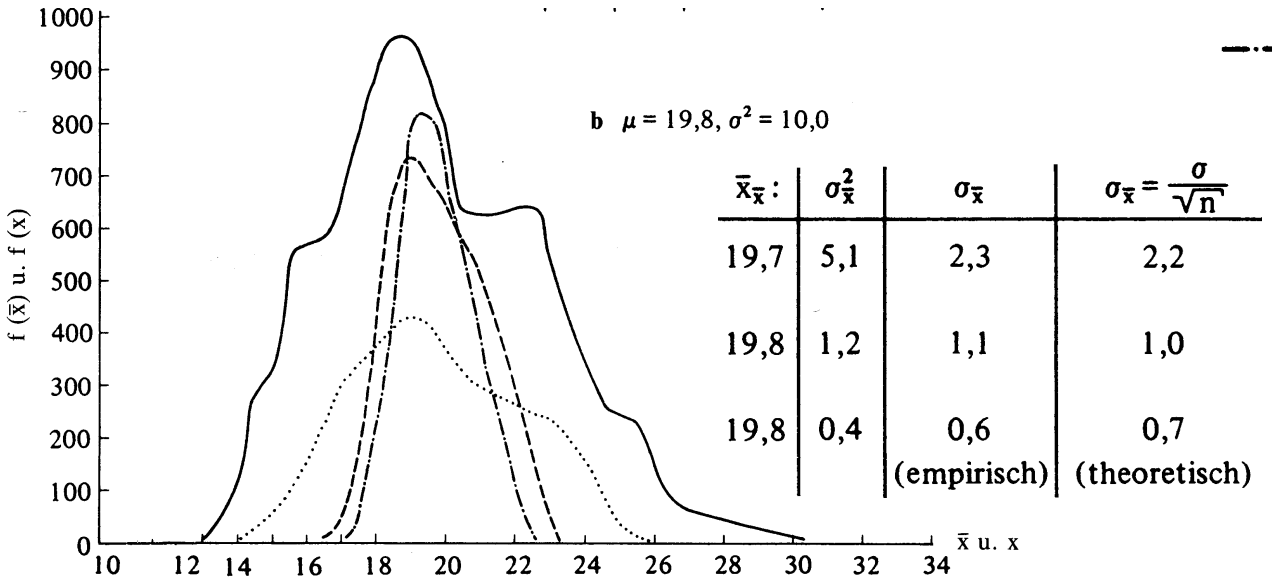
Overview

1) Various distributions of random Variables and their display
2) Characterizing distributions; central tendency and dispersion
3) Some theorems on distributions (with / without models)
4) **Standard error of empirical mean and empirical variance**
5) Error propagation in regression for measurements with precision

Example Std. error



$\bar{x}_{\bar{x}}$:	$\sigma^2_{\bar{x}}$	$\sigma_{\bar{x}}$	$\sigma_{\bar{x}} = \frac{\sigma}{\sqrt{n}}$
19,9	9,7	3,1	3,2
19,8	1,8	1,3	1,4
19,8	1,0	1,0 (empirisch)	1,0 (theoretisch)



$\bar{x}_{\bar{x}}$:	$\sigma^2_{\bar{x}}$	$\sigma_{\bar{x}}$	$\sigma_{\bar{x}} = \frac{\sigma}{\sqrt{n}}$
19,7	5,1	2,3	2,2
19,8	1,2	1,1	1,0
19,8	0,4	0,6 (empirisch)	0,7 (theoretisch)

- Population
- Mittelwerteverteilung von 200 Stichproben (n = 2)
- Mittelwerteverteilung von 200 Stichproben (n = 10)
- Mittelwerteverteilung von 200 Stichproben (n = 20)

Is dependent on σ of population
Is dependent on sample size

Standard Errors of mean / deviation

$\sigma_{\bar{x}}$ *is defined as "standard error of the mean".*

It is the standard deviation of equally sized samples

taken from one common population.

if σ *of population is known :*

$$\sigma_{\bar{x}} = \sqrt{\frac{\sigma^2}{n}} = \frac{\sigma}{\sqrt{n}}$$

but in general σ *itself must be estimated :*

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1} \quad s.t.$$

$$\hat{\sigma}_{\bar{x}} = \sqrt{\frac{\hat{\sigma}^2}{n}} = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n(n-1)}}$$

the smaller $\hat{\sigma}_{\bar{x}}$ *is the better has* μ *been estimated*

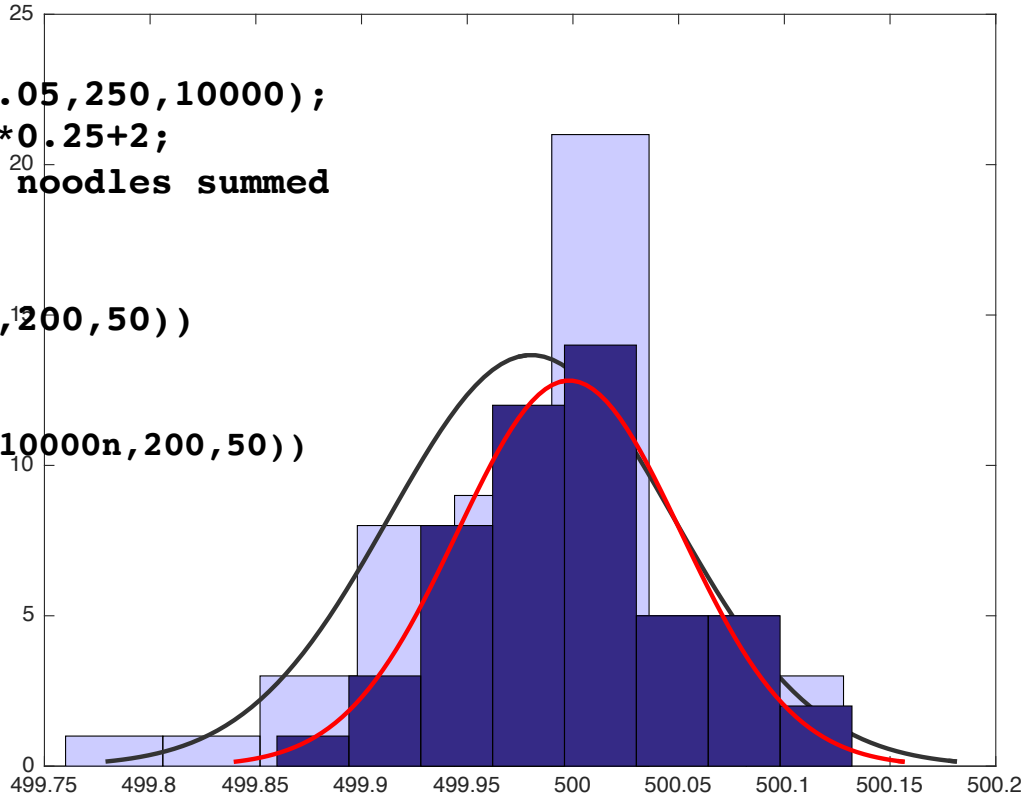
standard error of the standard deviation :

$$\hat{\sigma}_s = \sqrt{\frac{\hat{\sigma}^2}{2n}}$$

```
function[RDist]=PGPStdErrorOfMeanv2(Pdist,PStichSampleSize,PStichRepeatCnt)
%PDist : 1 dim == Grundgesamtheit
%PStichSamplesize: each sample drawn from Pdist has this size, e.g. M=200
%PStichRepeatCnt : how many samples used to calc. the mean zB n=50
boxNum=length(Pdist);
RDist = zeros(1,PStichRepeatCnt);
for k=1:PStichRepeatCnt % for clarity programmed as for lop
%grab a random sample from distribution via randperm and sum it
    cur_sum = sum(Pdist(...
randperm(boxNum,PStichSampleSize)));
    RDist(k)= cur_sum/ PStichSampleSize;
end
return
```

Which spagetti factory makes better 500g packages?

```
spagetti_10000n = random('normal',2,0.05,250,10000);
spagetti_10000 =(rand(250,10000)-0.5)*0.25+2;
%weight distrb. of 10k boxes with 250 noodles summed
box_10000n = sum(spagetti_10000n);
box_10000 = sum(spagetti_10000);
histfit(PGPStdErrorOfMeanv2(box_10000,200,50))
h(1).FaceColor = [.8 .8 1];
h(2).Color = [.2 .2 .2];
hold on histfit(PGPStdErrorOfMeanv2(box_10000n,200,50))
```

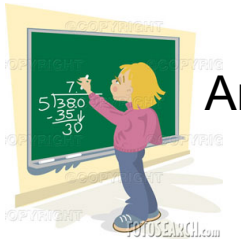


Overview

1) Various distributions of random Variables and their display
2) Characterizing distributions; central tendency and dispersion
3) Some theorems on distributions (with / without models)
4) Standard error of empirical mean and empirical variance
5) **Error propagation in regression for measurements with precision**

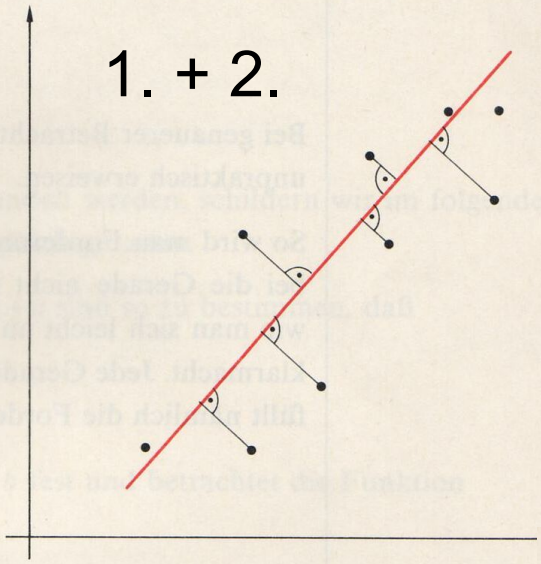
Observation

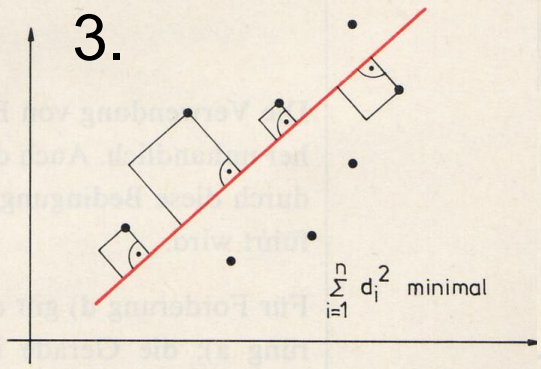
Many metrics

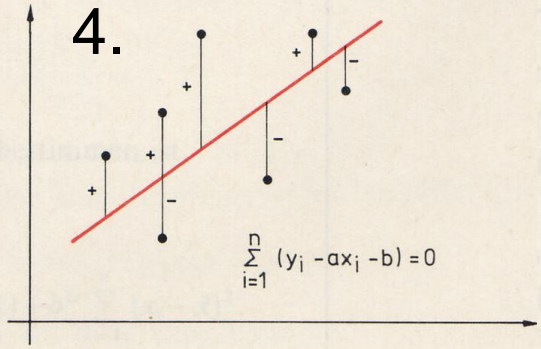


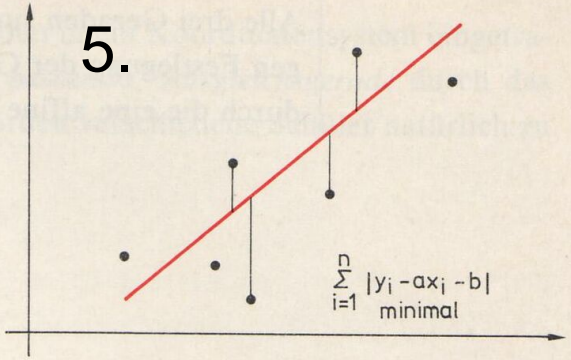
Argue

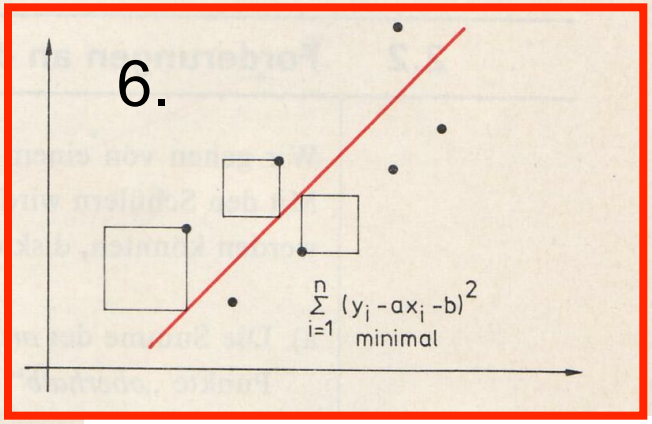
1. Sum of distances above == sum of distances below
2. Sum of orthogonal distances is minimal
3. Sum of squares is minimal
4. sum of straight line displacements is zero
5. sum of absolut values of line displacements is minimal
6. Sum of squares of straight line displacements is minimal











Derivation

$$F(a,b) = \sum_i (y_i - (ax_i + b))^2 \overset{!}{=} minimum$$

$$\frac{\partial}{\partial b} F(a,b) = -2\sum_i (y_i - ax_i - b) = 0$$

$$\Rightarrow nb = \sum_i y_i - a\sum_i x_i$$

$$\Rightarrow b = \frac{1}{n}\sum_i y_i - a\frac{1}{n}\sum_i x_i = E[Y] - aE[X]$$

$$\frac{\partial}{\partial a} F(a,b) = \frac{\partial}{\partial a}\sum_i (y_i - (ax_i + E[Y] - aE[X]))^2 =$$

$$\frac{\partial}{\partial a}\sum_i \left[(y_i - E[Y]) - a(x_i - E[X])\right]^2 =$$

$$\frac{\partial}{\partial a}\sum_i (y_i - E[Y])^2 - 2a(y_i - E[Y])(x_i - E[X]) + a^2(x_i - E[X])^2 =$$

$$-2\sum_i (y_i - E[Y])(x_i - E[X]) + 2a\sum_i (x_i - E[X])^2 = 0$$

$$\Rightarrow a = \frac{\sum_i (y_i - E[Y])(x_i - E[X])}{\sum_i (x_i - E[X])^2}$$

data model:

y = f(x)= ax +b

Covariance

What happens if y_i are measured with uncertainties

Use the following abbrev.:

$$S = \sum_i \frac{1}{\sigma_i^2}$$

$$S_y = \sum_i \frac{y_i}{\sigma_i^2}$$

$$S_x = \sum_i \frac{x_i}{\sigma_i^2}$$

$$S_{xy} = \sum_i \frac{y_i x_i}{\sigma_i^2}$$

$$S_{xx} = \sum_i \frac{x_i x_i}{\sigma_i^2}$$

$$\Delta = SS_{xx} - S_x^2$$

y_i with variances σ_i

Assume the measurements of y_i have different σ_i.

weight them according to their variance.

using the new statistics :

$$a = \frac{S_y S_{xx} - S_{xy} S_x}{\Delta} \qquad b = \frac{SS_{xy} - S_x S_y}{\Delta}$$

How do Errors in a and b depend on errors in y_i?

Observe the general law to propagate variances:

$$\sigma_F^2 = \sum_i \sigma_i^2 \left(\frac{\partial F}{\partial y_i} \right)^2$$

using the new abbreviations:

$$a = \frac{S_y S_{xx} - S_{xy} S_x}{\Delta} \qquad b = \frac{S S_{xy} - S_x S_y}{\Delta}$$

Now:

$$\sigma_a^2 = \sum_i \sigma_{y_i}^2 \left(\frac{\partial a}{\partial y_i} \right)^2 \qquad \frac{\partial a}{\partial y_i} = \frac{S_{xx} - S_x x_i}{\sigma_{y_i}^2 \Delta} \Rightarrow \ldots \Rightarrow \sigma_a^2 = \frac{S}{\Delta}$$

$$\sigma_b^2 = \sum_i \sigma_{y_i}^2 \left(\frac{\partial b}{\partial y_i} \right)^2 \qquad \frac{\partial b}{\partial y_i} = \frac{S_x x_i - S_x x_i}{\sigma_{y_i}^2 \Delta} \Rightarrow \ldots \Rightarrow \sigma_b^2 = \frac{S_{xx}}{\Delta}$$

How do a and b vary if yi ‘s vary?

Reverse Argument

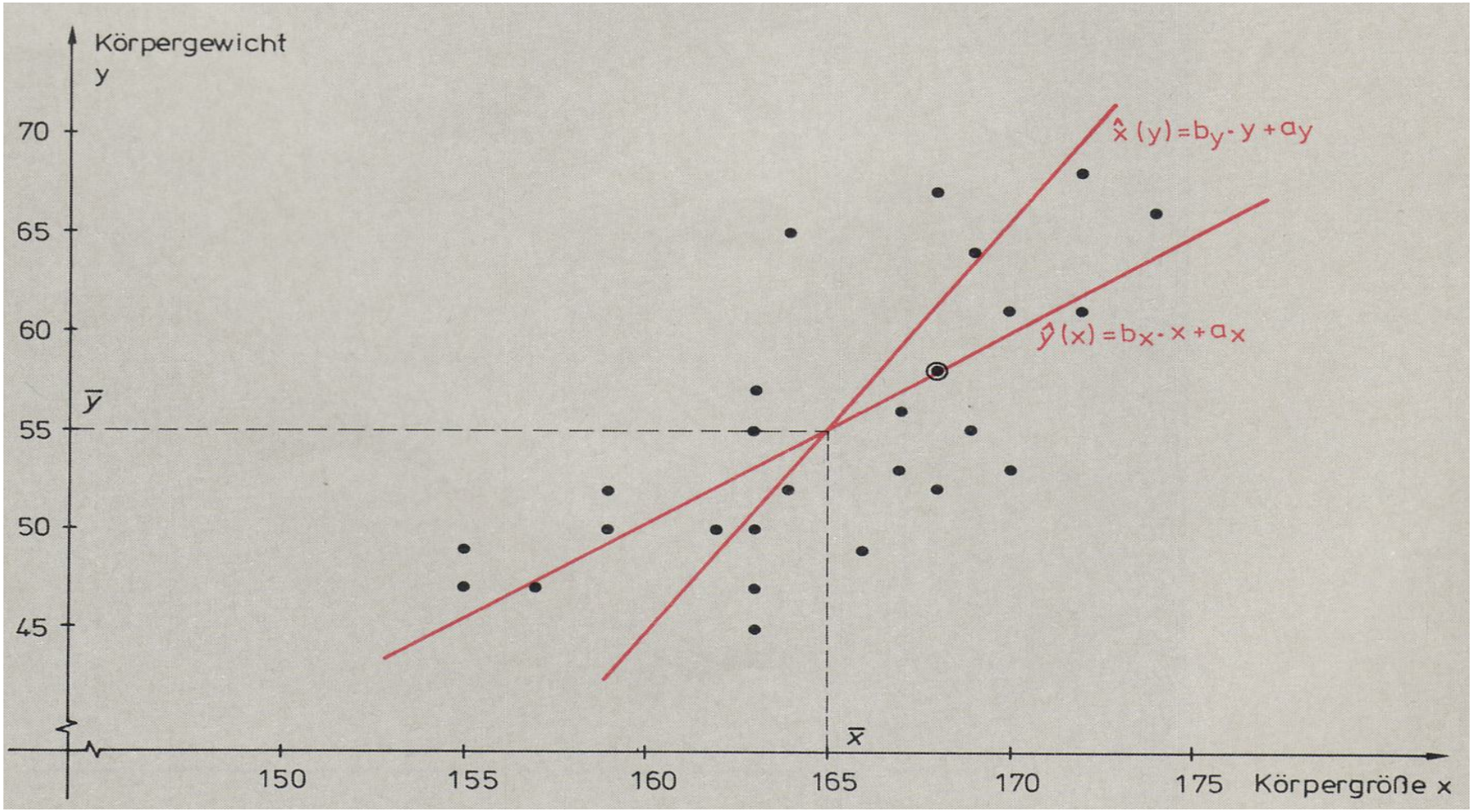
by the very same reasoning we can build: x(y)=by+a (dependency of feature X on feature Y)

solution

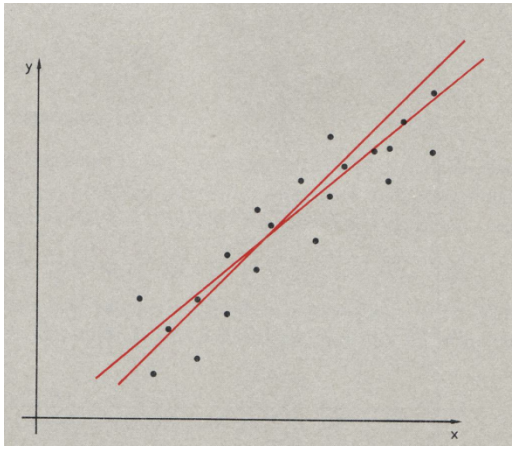
$$a = E[X] - bE[Y]$$

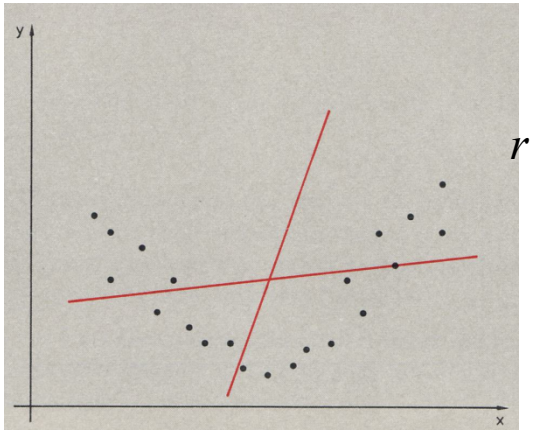
$$b = \frac{\sum_i (y_i - E[Y])(x_i - E[X])}{\sum_i (y_i - E[Y])^2}$$

Both Regression Lines



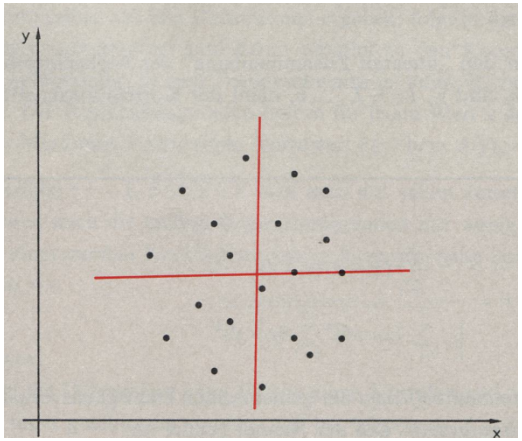
Possible Intersections

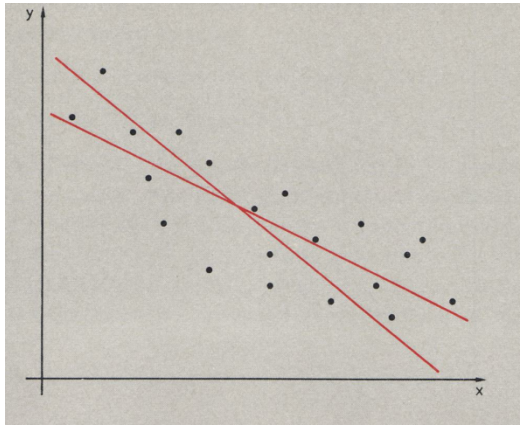




$$r = \frac{\sum_i (x_i - E[X])(y_i - E[Y])}{\sqrt{\sum_i (x_i - E[X])^2}\sqrt{\sum_i (y_i - E[Y])^2}}$$

correlation coefficient r





unit vectors
scalar product

cos of enclosed angle
-1<= r <=1

Summary

the regression line measures a linear trend in the given data

the covariance is an important part in the regression line

the correlation coefficient indicates, how much these trends agree in the given two data series.

Testing Hypothesis

1) How to construct tests?
2) How confident can we be?
3) How many samples needed? (sample size)

Let X be a random variable,
$X_1,...,X_N$ a sample from X,
θ a parmeter (unknown).
Then – given α – find (confidence) interval $[\hat{\theta}_L, \hat{\theta}_U]$ s.t.:

$$P(\hat{\theta}_L \le \theta \le \hat{\theta}_U) = 1 - \alpha$$

($1-\alpha$ confidence level)
observe:
if $x_1, x_2, ..., x_n$ are values of $X_1,...,X_N$
then $\hat{\theta}_L = g_l(x_1, x_2, ..., x_n)$ and
$\hat{\theta}_U = g_u(x_1, x_2, ..., x_n)$ are bounds of the confidence interval.

Intervall estimation

$$P(\overline{X} - \varepsilon \le \mu \le \overline{X} + \varepsilon) = 0.95$$

gilt. Mit den realisierten Werten der Stichprobe ist der Punktschätzwert $\overline{x}$ eine Zahl und das Schätzintervall $[\overline{x} - \varepsilon, \overline{x} + \varepsilon]$ ein gewöhnliches Intervall.

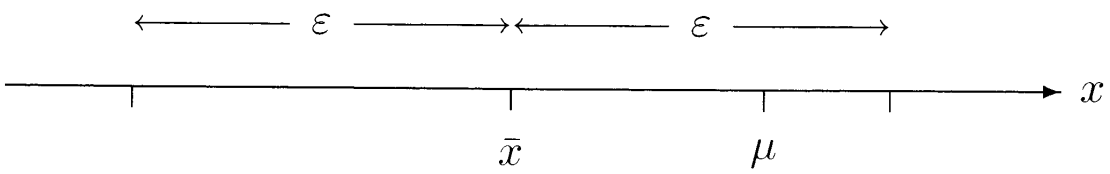


Abbildung 5.1: Schätzintervall für μ im Beispiel 5.7

Required sample size to find μ

Given:

a required width b of confidence interval at confidence level (1-a).

a distribution X first normal, then relaxed.

let X be a random variable.

$X_1,..,X_n$ *a sample thereof*, $\sigma^2 = V[X] = E[(X-\mu)^2]$

to find $\mu = E[X]$ *at confidence level* $(1-\alpha)$

and in confidence interval $\hat{\theta}_U - \hat{\theta}_L \le 2b$

distinguish two cases :

1) *assume* $X \sim N(\mu,\sigma^2)$, σ^2 *known. Then every* $n \ge n_{\min} = \frac{u^2_{1-\alpha/2}\sigma^2}{b^2}$ *gives a confidence interval of at most* $2b$ *width.* $u()$ *is quantile of* $N(0,1)$ *at* $(1-\alpha/2)$.

2) *now X arbitrary,* σ^2 *known, then choose* $n \ge n^*_{\min} = \max\{40, n_{\min}\}$. *If* σ^2 *unknown replace* σ^2 *by* s^2 *gotten from different estimator.*

Spice bags

Assume:

$X_i \sim N(\mu, 25), \sigma^2 = 25$ known

a) A sample of size n=20 finds $\bar{x}$ =99.35 gr Find confidence interval at level (1-0.01)=0.99

b) Find n_{min} using the maximum width of 1 for the confidence intervall

$$a)\ \hat{\theta}_{L,U} = \bar{X} \mp u_{1-\alpha/2}\frac{\sigma}{\sqrt{n}}$$

$$using\ n = 20, \sigma^2 = 25, u_{1-\alpha/2} = u_{0.995} = 2.58$$

$$\bar{x} = 99.35$$

$$\hat{\theta}_{L,U} = 99.35 \mp 2.58\frac{5}{\sqrt{20}} = 99.35 \mp 2.88$$

$$\Rightarrow interval\ is: [96.47, 102.23]$$

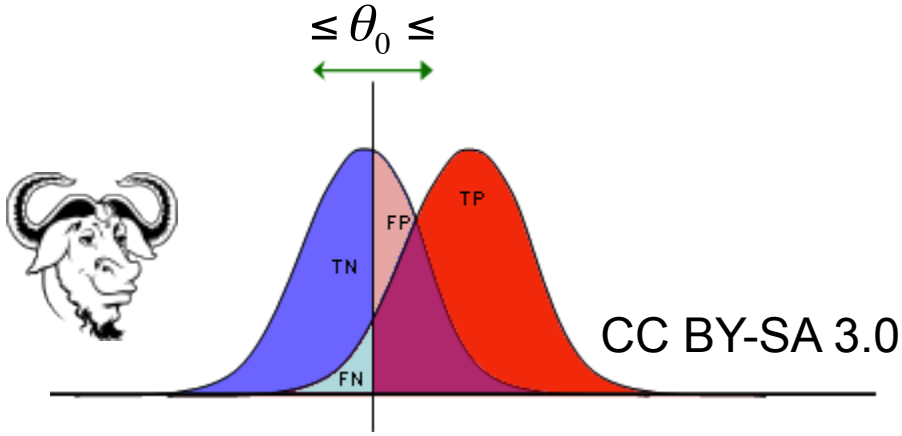
$$b)\ 2b = 1 \Rightarrow b = 0.5, u_{1-\alpha/2} = 2.58, \sigma^2 = 25,$$

$$n_{\min} = \frac{u_{1-\alpha/2}^2\sigma^2}{b^2} = \frac{2.58^2 \cdot 25}{0.25} = 665.64$$

$$n \geq 666$$

Example

ROC Continuous Example: Fever Bound => flue yes / no



Classifier prediction (Hypothesized class)	Evidence (True Class) pos	neg
Hit	TP	FP
Miss	FN	TN
Column totals	P	N

Classifier: Decide on disease by varying diagnosis temperature θ_0:

What is the "best" classifier value to indicate: you have the flue?

Red: true positive **(TP)**
high temperature and will have flue
[if a pos. instance is classified as Hit.]

Light blue: false negative **(FN)**
too low temp, but will get the flue
[if a pos. instance is classified as Miss.]

Strong blue: true negative **(TN)**
too low temp, and no flue
[if a neg. instance is classified as Miss.]

Light red: false positives **(FP)**
high temperature but never get it
[if a neg. instance is classified as Hit.]

From Confusion table to ROC graph

Hypothesized class	True class: p	True class: n
y	True Positives	False Positives
n	False Negatives	True Negatives
Column totals	P	N

$$\text{FP rate} = \frac{FP}{N}$$

$$\text{TP rate} = \frac{TP}{P} = \text{Recall}$$

ROC graph uses for x axis == FP rate

ROC graph uses for y axis == TP rate

$$\text{Precision} = \frac{TP}{TP+FP}$$

F-score= Precision * Recall

$$\text{Accuracy} = \frac{TP+TN}{P+N}$$

From Confusion table to ROC graph

		Condition (as determined by "Gold standard")		
		Condition Positive	Condition Negative	
Test Outcome	Test Outcome Positive	**True Positive**	**False Positive** (Type I error)	Precision = Σ True Positive / Σ Test Outcome Positive
	Test Outcome Negative	**False Negative** (Type II error)	**True Negative**	Negative predictive value = Σ True Negative / Σ Test Outcome Negative
		Sensitivity = Σ True Positive / Σ Condition Positive	**Specificity** = Σ True Negative / Σ Condition Negative	Accuracy

Co Wikipedia (en):
„ROC“, CC BY-SA 3.0

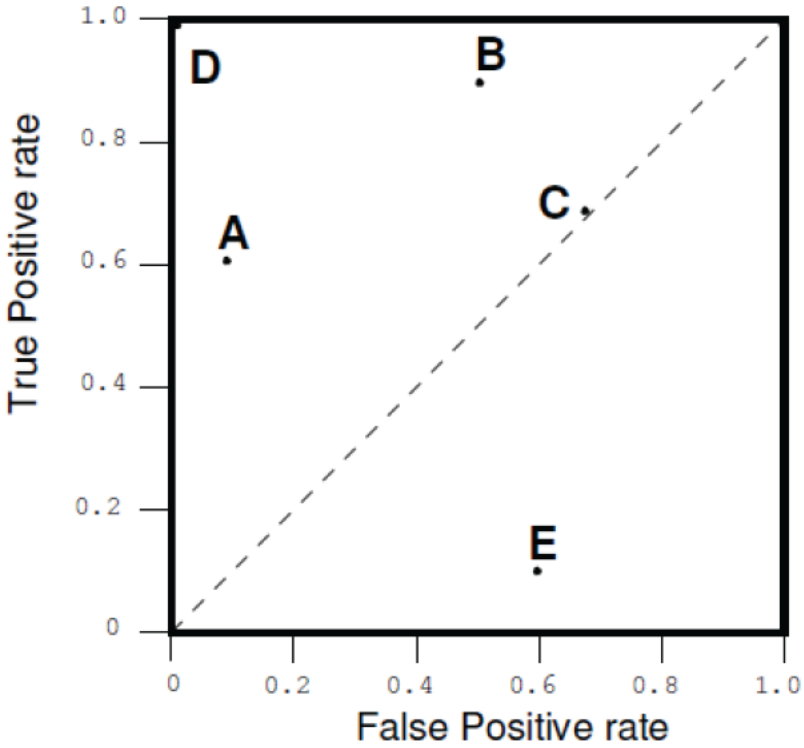
ROC graphs

ROC graphs are two-dimensional graphs in which TP rate is plotted on the Y axis and FP rate is plotted on the X axis.

A ROC graph depicts relative trade-offs between benefits (true positives) and costs (false positives).

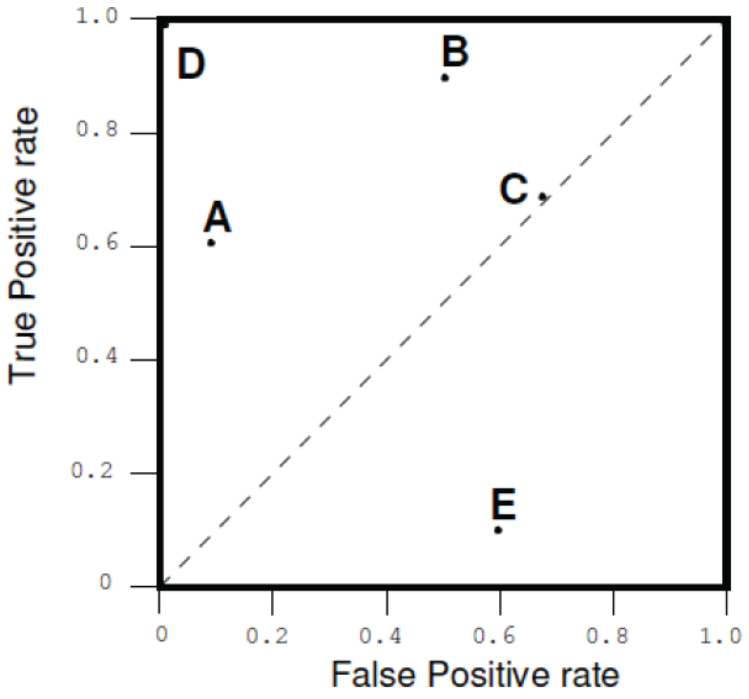
A discrete classier is one that outputs only a class label. Each discrete classier produces a pair (FP rate, TP rate), which corresponds to a single point in ROC space.

From:
ROC Graphs: Notes and Practical Considerations for Data Mining Researchers
Tom Fawcett,Intelligent Enterprise Technologies Laboratory, HP Laboratories Palo Alto,
slides from GIC 09



A basic ROC graph showing five discrete classifiers.

Important Points in ROC space



From:
ROC Graphs: Notes and Practical Considerations for Data Mining Researchers
Tom Fawcett,Intelligent Enterprise Technologies Laboratory, HP Laboratories Palo Alto,
slides from GIC-09

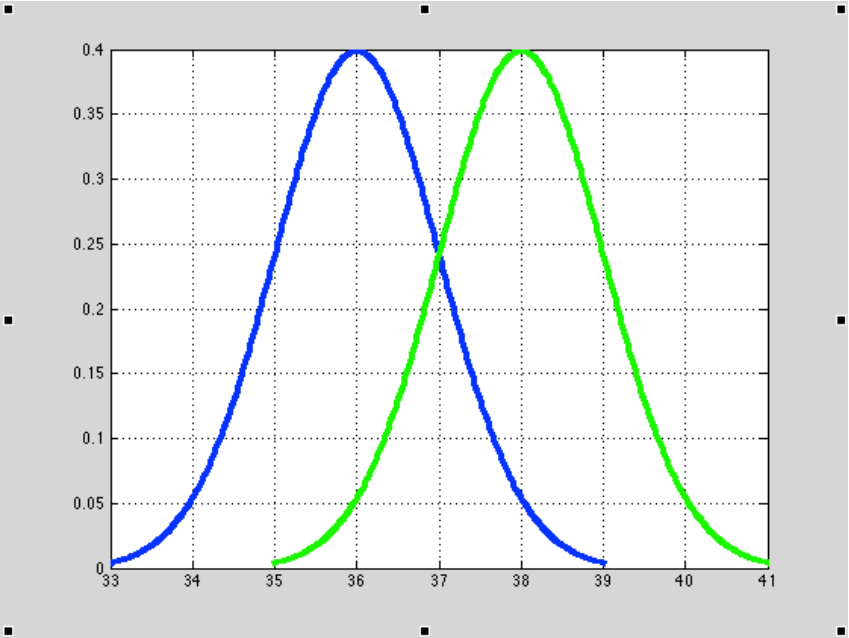
The lower left point (0,0) represents the strategy of never issuing a positive classification.

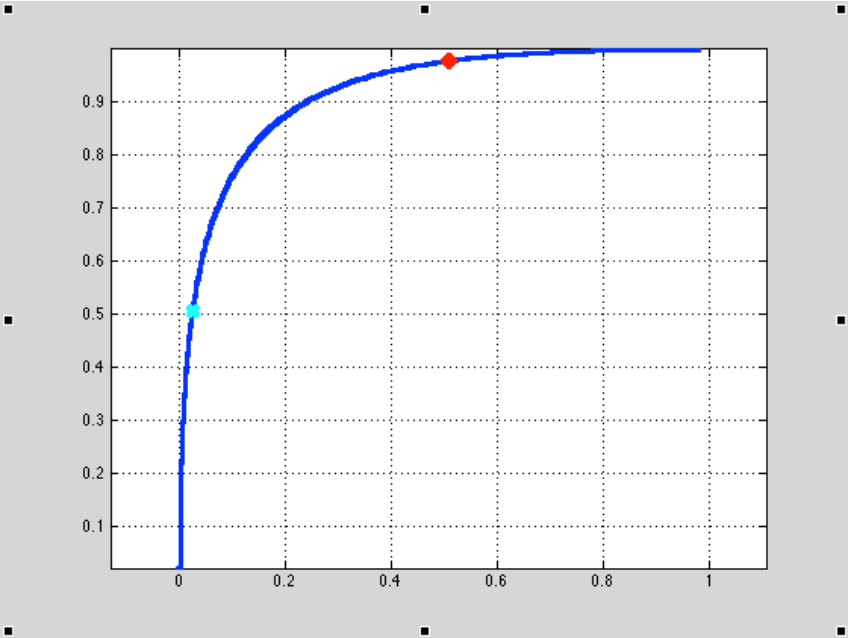
The opposite strategy is represented by the upper right point (1,1).

The point (0,1) represents perfect classification.

```
%two temperature distributions, healthy and sick
mu=36;
mu2=38;
sigma=1.0;
sigma2=1.0;
%sample it arround it's modes == peaks
X=linspace(mu-3,mu+3,201);
Y=linspace(mu2-3,mu2+3,201);
plot(X,normpdf(X,mu,sigma),'b',Y,normpdf(Y,mu2,sigma2),'g');grid on;
pause;
clf;
bounds=[34:0.02:40];%these are the values for boundaries
TN=normcdf(bounds,mu,sigma);% BLUE area
FP=1-TN;                    % ROSE area
FN=normcdf(bounds,mu2,sigma2);% CYAN area
TP=1-FN;                     % RED area
TPrate=TP./(TP+FN);% build percentage or rates
FPrate=FP./(FP+TN);%
plot(FPrate,TPrate);axis equal;grid on;%MY first ROC diagram
pause;
hold on
plot(FPrate(100),TPrate(100),'rd','LineWidth',3);% right in Raw,  is left in ROC
plot(FPrate(200),TPrate(200),'cx','LineWidth',3);%
Pause;
```

Results: normcdf, ROC by hand





Important Points in ROC space

Informally, one point in ROC space is **better** than another if it is to the **northwest** (TP rate is higher, FP rate is lower, or both) **of the first.**

Classifiers appearing on **the left hand-side of an ROC graph**, near the X axis, may be thought of as **conservative**: they make **positive classifications only with strong evidence** so they make few false positive errors, but they often have low true positive rates as well.

Classifiers on the **upper right-hand** side of an ROC graph may be thought of as **liberal.**

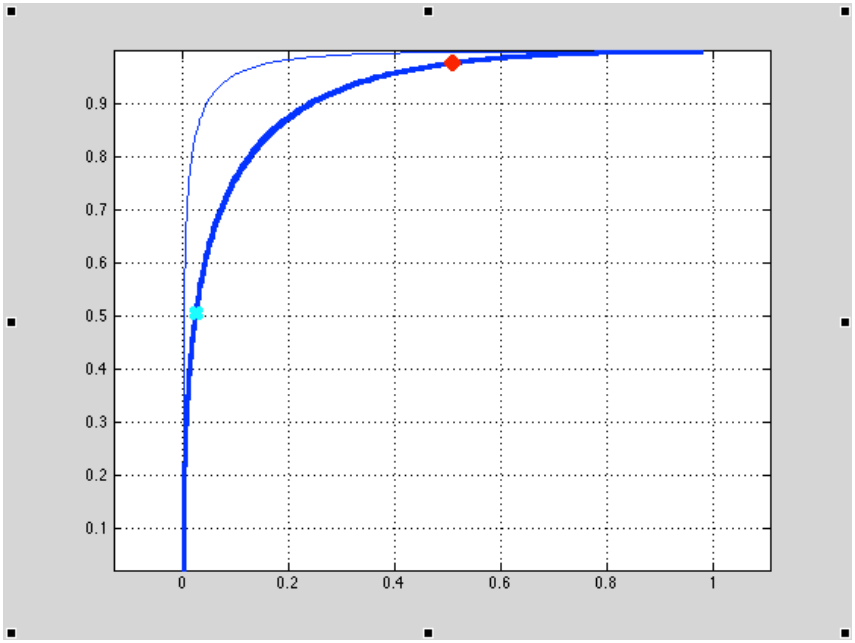
From:
ROC Graphs: Notes and Practical Considerations for Data Mining Researchers
Tom Fawcett,Intelligent Enterprise Technologies Laboratory, HP Laboratories Palo Alto,
slides from GIC'09

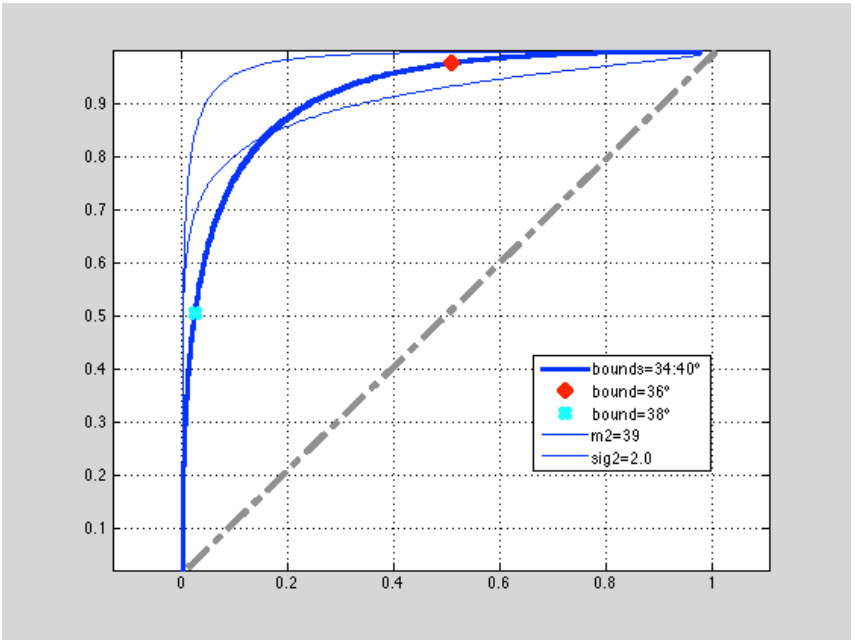
The **diagonal line y = x represents** the strategy of **randomly guessing** a class.

A random classier will produce an ROC point that slides back and forth on the diagonal based on the frequency with which it guesses the positive class. **In order to get away from this diagonal into the upper triangular region, the classifier must exploit some information in the data**.

Any classifier that appears in the **lower right triangle performs worse than random guessing**. This triangle is therefore usually empty in ROC graphs.

Results: 2nd ROC for mu2=39° 3rd ROC for sigma2=2.0





Eg.: Application to signals

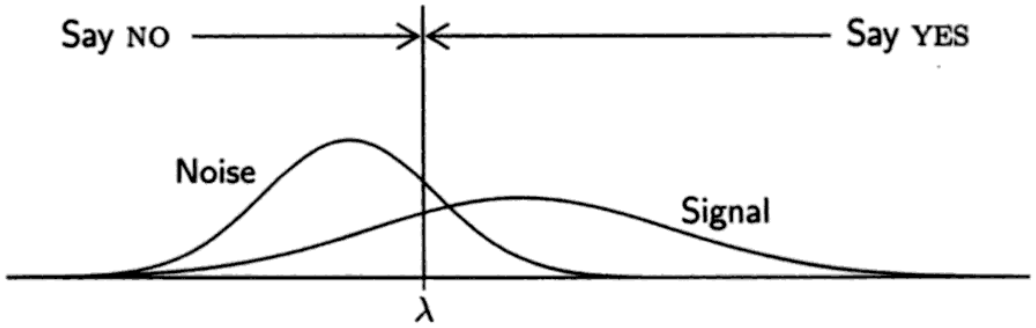


Figure 1.2: The signal and noise distributions of Figure 1.1 shown on a single axis with a decision criterion at the value λ.

$$X_n : \textit{random variable for noise trials, density } f_n(x)$$

$$X_s : \textit{random variable for signal trials, density } f_s(x)$$

$$\textit{false-alarm rate} : P_F = P(YES \mid noise) =$$

$$P(X > \lambda \mid noise) = P(X_n > \lambda) = \int_\lambda^\infty f_n(x)\,dx$$

$$= 1 - F_n(\lambda) \textit{ where } F_n \textit{ is Cummulative Distribution Function of } f_n$$

Test for two simple Hyp‘s

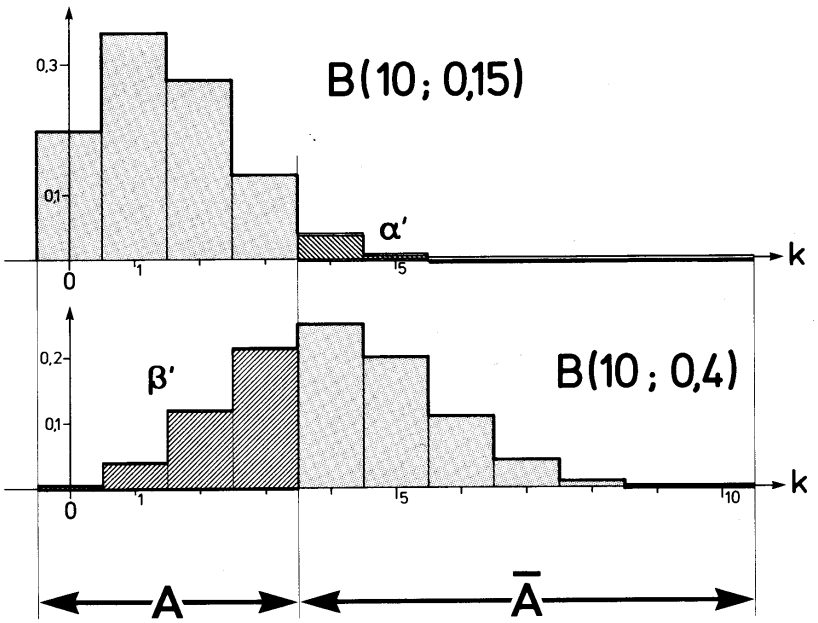


Fig. 339.1 Wahrscheinlichkeitsverteilung zur Hypothese 1 (Erste Qualität, oben) und Hypothese 2 (Zweite Qualität, unten) von Beispiel 1. grau: Wahrscheinlichkeit für ein richtiges Urteil. rot: Wahrscheinlichkeit für einen Fehler 1. Art bzw. 2. Art.

H_0: screws are defect according to B(10;0.15)

H_1: screws are defect according to B(10;0.4)

Till A : H_0 accepted (A == Annahmebereich)

Beyond A:H_0 assumed wrong, i.e. H_1 accepted

α = error of 1.st kind

β = error of 2.nd kind

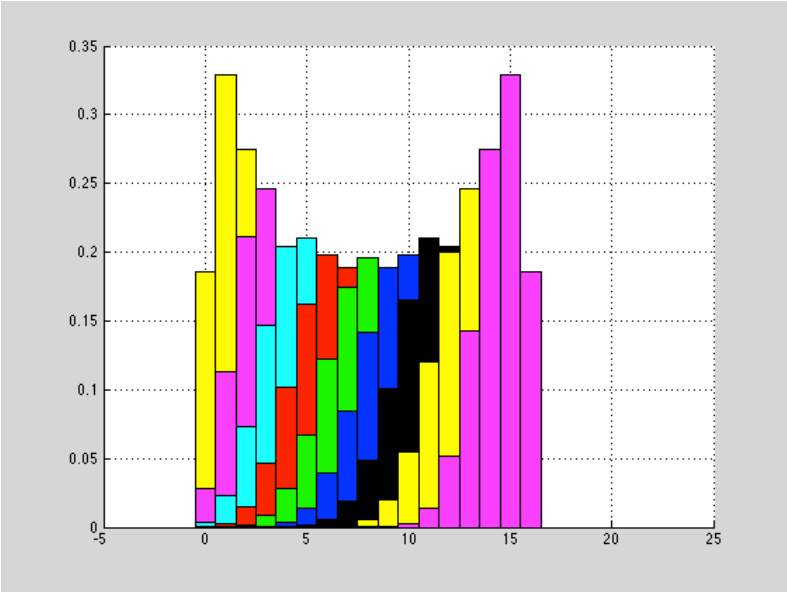
Sample Z=(0|1|1|1|0|0|1|1|1|0)

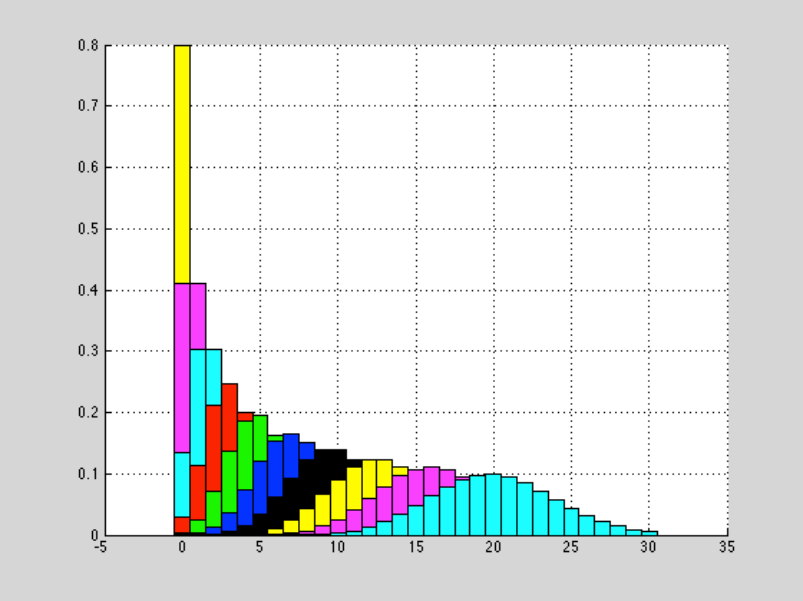
decision rule :

$$\delta_k : \begin{cases} Z \le k \Rightarrow decide\ for\ H_0 \\ Z > k \Rightarrow decide\ for\ H_1 \end{cases}$$

```
mycol=['y' 'm' 'c' 'r' 'g' 'b' 'k' 'y' 'm' 'c' 'r' 'g' 'b' 'k'];
hold on;trials=16;
for i=1:9
   p=0.1*i;
   bar1=bar(0:20,pdf('Binomial',0:20,trials,p));
   set(bar1,'BarWidth',1,'FaceColor',mycol(i));
end
```

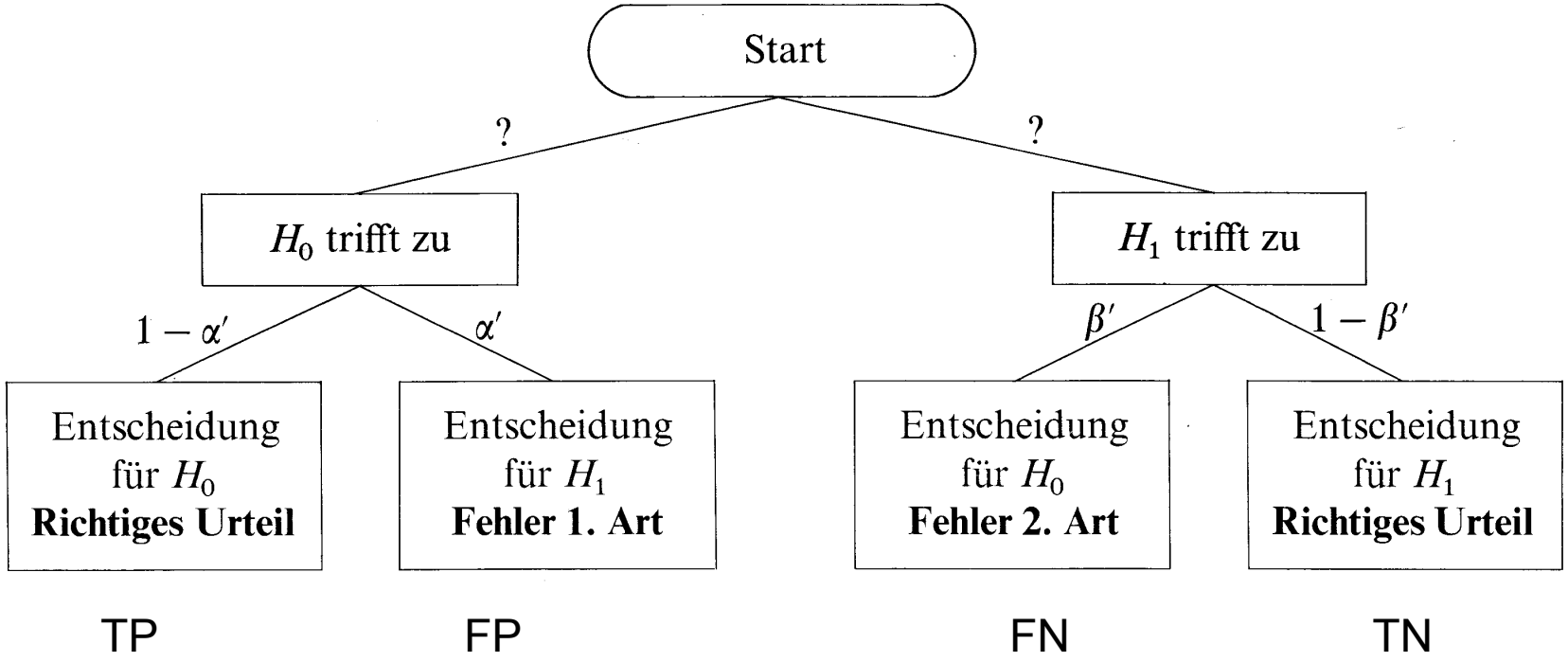
Binomial examples






```
p=0.2; hold on;
for i=1:10
   trials=i*i;
   bar1=bar(0:30,pdf('Binomial‘,0:30,trials,p));
   set(bar1,'BarWidth',1,'FaceColor',mycol(i));
end
```

H_0/H_1 Test with two simple Hyp's



Outline: Evaluating Hypotheses

[Read Ch. 5] Tom Mitchell: Machine Learning

[Recommended exercises: 5.2, 5.3, 5.4]

Error of a Sample versus true error

Confidence intervals for observed hypothesis error

Estimators

Binomial distribution, Normal distribution, Central Limit Theorem

Paired t tests

Comparing learning methods

Sampling

Consider learning the target function "people who plan to purchase new skis this year," given a sample of training data collected by surveying people as they arrive at a ski resort.

instance space X == space of all people (denoted by x). Each individual x may be described by features like e.g.: age, occupation, how many times they skied last year, etc.

Some (unknown) distribution D specifies for each person x the probability that x will be encountered as the next person arriving at the ski resort.

The target function *f: X -> {0,1}* classifies each x according to whether or not they plan to purchase skis this year.

We are interested in following two questions:

1. Given a hypothesis h and a data sample S containing n examples drawn at random according to the distribution D, what is the best estimate of the accuracy of h over future instances drawn from the same distribution?

2. What is the probable error in this accuracy estimate?

Two Definitions of Error

The true error of hypothesis h with respect to target function f and distribution D is the probability that h will misclassify an instance drawn at random according to D :

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[f(x) \neq h(x)]$$

The sample error of h with respect to target function f and data sample S is the proportion of examples that h misclassifies:

$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S} \delta(f(x) \neq h(x))$$

here $\delta(f(x) \neq h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise. (decision rule)

Q: How well does $error_S(h)$ estimate $error_D(h)$?

Estimate a binomial p **IS SAME** as estimate the $error_D(h)$

Estimate p from random sample of coin tosses	Estimate $error_D(h)$ from random sample of instances
single toss	draw single random instance i from D.
probability p that a coin toss yields head up	i is misclassified by h
r heads over n tosses = r/n	$error_S(h)$

General setting for Binom. distr.

1. There is a base, or underlying, experiment (e.g., toss of the coin) whose outcome can be described by a random variable, say Y. The random variable Y can take on only two possible values (e.g., $Y = 1$ if heads, $Y = 0$ if tails).
2. The probability that $Y = 1$ on any single trial of the underlying experiment is given by some constant p, independent of the outcome of any other experiment. The probability that $Y = 0$ is therefore $(1 - p)$. Typically, p is not known in advance, and the problem is to estimate it.
3. A series of n independent trials of the underlying experiment is performed (e.g., n independent coin tosses), producing the sequence of independent, identically distributed random variables $Y_1, Y_2, \ldots, Y_n$. Let R denote the number of trials for which $Y_i = 1$ in this series of n experiments:
$$R \equiv \sum_{i=1}^{n} Y_i$$
4. The probability that the random variable R will take on a specific value r (e.g., the probability of observing exactly r heads) is given by the Binomial distribution
$$\Pr(R = r) = \binom{n}{r} p^r (1-p)^{n-r}$$

   A plot of this probability distribution is shown on slide 69.

Problems when Estimating Error

1. Bias:
   If ***s*** is training set, $error_S(h)$ is optimistically biased
   $$bias = E[error_S(h)] - error_D(h)$$
   For unbiased estimate, ***h*** and ***S*** must be chosen independently
2. Variance:
   Even with unbiased ***S***, $error_S(h)$ may still vary from $error_D(h)$

Example

Hypothesis h misclassifies 12 of the 40 examples in *S*

$$error_S(h) = \frac{12}{40} = 0.30$$

What is $error_D(h)$?

Estimators

Experiment:

1. *choose sample* S *of size* n *according to distribution* D
2. *measure* $error_S(h)$

$error_S(h)$ is a random variable (why?)

(i.e., the result of a random experiment)

$error_S(h)$ is an unbiased estimator for $error_D(h)$

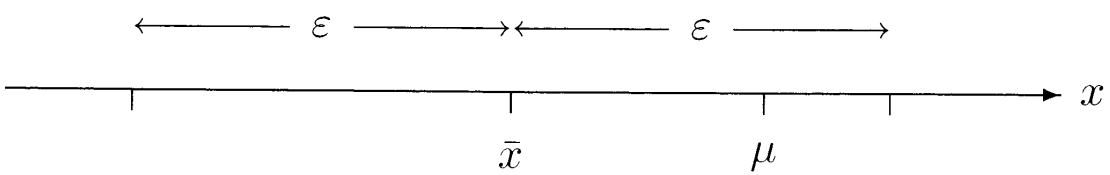
given the observed $error_S(h)$ what can we conclude about $error_D(h)$?

Confidence Intervals

If

S contains *n* examples, drawn independently of *h* and each other,

and *n* >= *30*



then

with approximately 95% probability,

$error_D(h)$ lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Theorem

Confidence Intervals

If

S contains *n* examples, drawn independently of *h* and each other,

and *n* >= *30*

then

with approximately N% probability, $error_D(h)$ lies in interval

N%	z_N
50%	0.67
68%	1.00
80%	1.28
90%	1.64
95%	1.96
99%	2.58

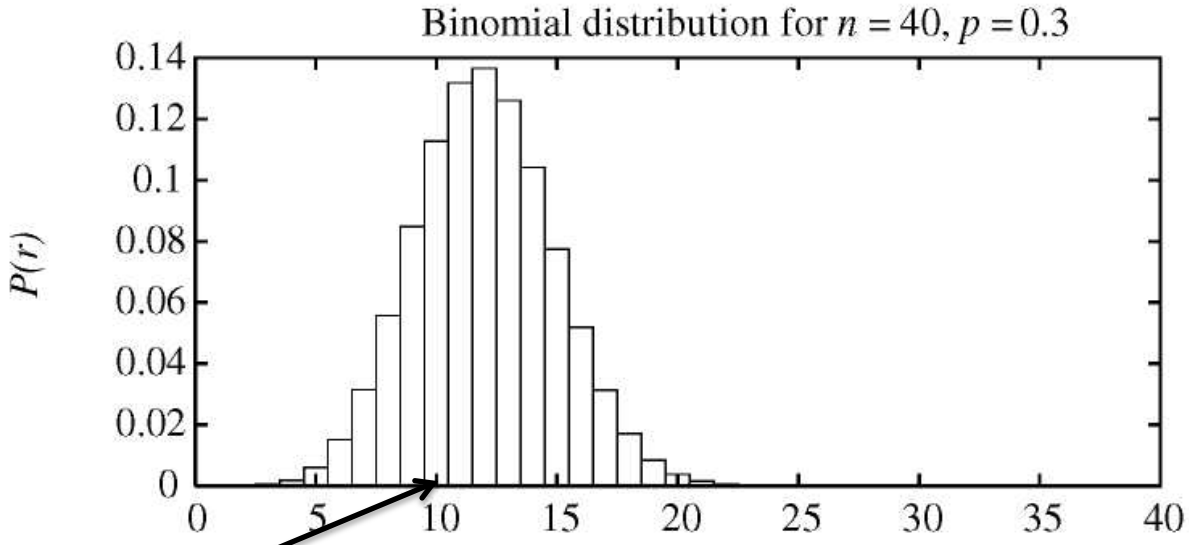
(Table 5.1)

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

$error_S(h)$ is a (binomial) Random Variable

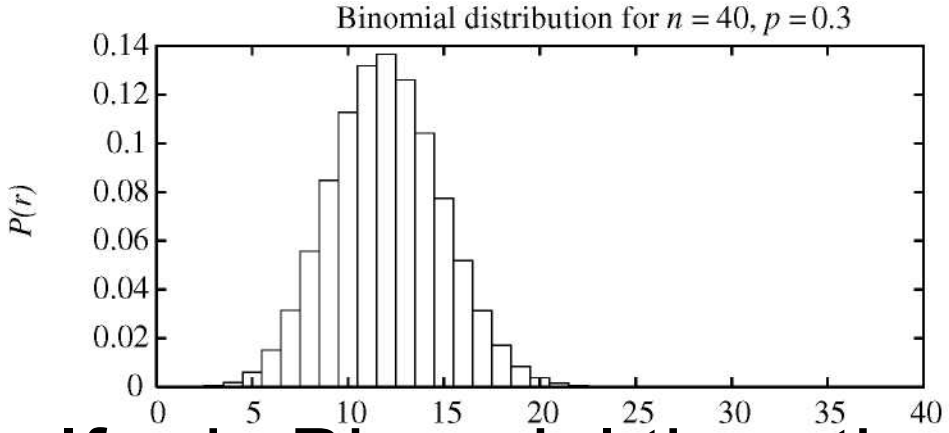
Rerun the experiment with different randomly drawn S (of size n)

Probability of observing r misclassified examples:



$$P(r) = \frac{n!}{r!(n-r)!} error_{\mathcal{D}}(h)^r (1 - error_{\mathcal{D}}(h))^{n-r}$$

Binomial Probability Distribution



$$P(r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}$$

If X is Binomial then the probability $Pr(X=r)$ of r heads in n coin flips, is given by $P(r)$

Expected, or mean value of X, $E[X]$, is :

$$E[X] \equiv \sum_{i=0}^{n} iP(i) = np$$

Variance of X is :

$$Var(X) \equiv E[(X - E[X])^2]$$
$$= np(1-p)$$

Standard deviation of X, σ_X, is :

$$\sigma_X \equiv \sqrt{E[(X - E[X])^2]}$$
$$= \sqrt{np(1-p)}$$

Now: Normal Distribution approximates Binomial distr. !!!

$error_S(h)$ follows a **Binomial distribution**, with a mean that is

$\mu_{errorS}(h) = error_D(h)$

and standard deviation:

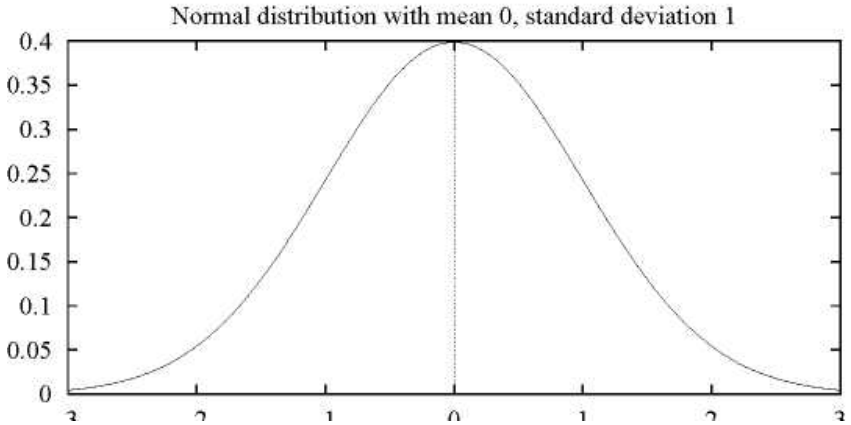
$$\sigma_{error_S(h)} = \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

approximate this by a **Normal distribution** with estimated mean and variance:

$\mu_{errorS}(h)$

and estimated standard deviation:

$$\sigma_{error_S(h)} \approx \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$



Normal Probability Distribution

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

The probability that *X* will fall into the interval (a,b) is given by =>

$$\int_a^b p(x)dx$$

Expected, or mean value of *X*, *E[X]*, is

=> $E[X] = \mu$

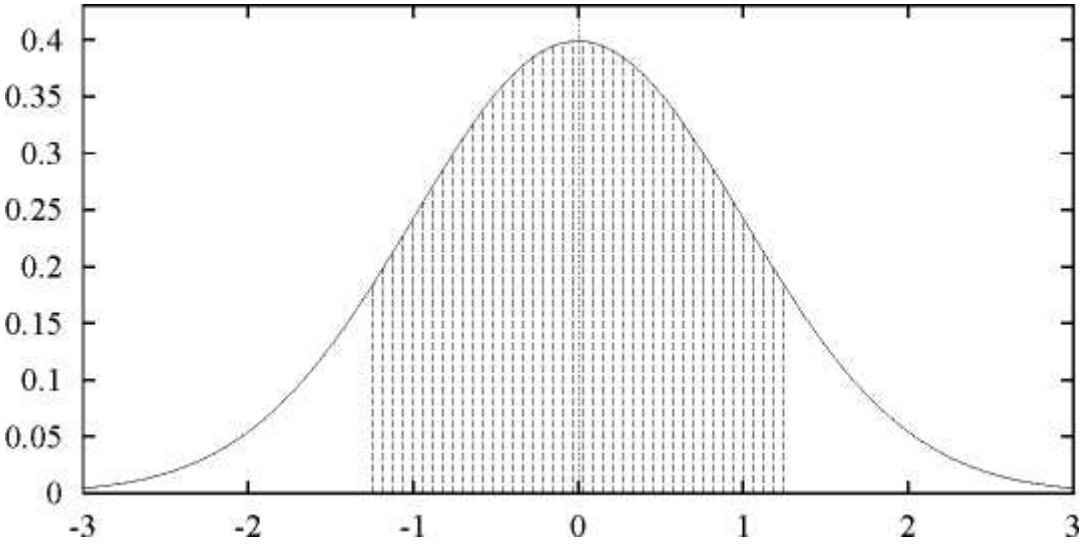
Variance of *X* is

=> $Var(X) = \sigma^2$

Standard deviation of *X*, σ_X, is

$\Rightarrow \sigma_X = \sigma$

Normal Probability Distribution



80% of area (probability) lies in $\mu \pm 1.28\sigma$

N% of area (probability) lies in $\mu \pm z_N\sigma$

$N\%$:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.58

Confidence Intervals, More Correctly

If

S contains *n* examples,
drawn independently of *h* and each other
and *n* > *30*

then

with approximately 95% prob., $error_S(h)$ lies in the interval

$$error_{\mathcal{D}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1-error_{\mathcal{D}}(h))}{n}}$$

equivalently, $error_D(h)$ lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1-error_{\mathcal{D}}(h))}{n}}$$

which is approximately

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

Central Limit Theorem

Consider a set of independent, identically distributed random variables $Y_1,..,Y_n$ all governed by an arbitrary probability distribution with mean μ and finite variance σ^2. Define the sample mean, $\bar{Y} \equiv \frac{1}{n} \sum_{i=1}^{n} Y_i$

As $n \rightarrow oo$, the distribution governing $\bar{Y}$ approaches a Normal distribution, with mean μ and variance σ^2/n.

Calculating Confidence Intervals

1. Pick parameter p to estimate:
   e.g. $error_D(h)$
2. Choose an estimator:
   e.g. $error_S(h)$
3. Determine probability distribution that governs the estimator:
   $error_S(h)$ is governed by Binomial Distribution, which in turn is approximated by a Normal Distribution (if n >= 30)
4. Find the interval (θ_L, θ_U), such that $N\%$ of probability mass falls in this interval:
   i.e. use table of z_N values

Difference Between Hypotheses

Test h_1 on sample S_1, test h_2 on S_2 (Section 5.5)

1. Pick parameter to estimate

$$d \equiv error_D(h_1) - error_D(h_2)$$

2. Choose an estimator

$$\hat{d} \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$$

3. Determine probability distribution that governs estimator

$$\sigma_{\hat{d}} \approx \sqrt{\frac{error_{S_1}(h_1)(1-error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1-error_{S_2}(h_2))}{n_2}}$$

4. Find interval (L,U) such that N% of probability mass falls in the interval

$$\hat{d} \pm z_N \sqrt{\frac{error_{S_1}(h_1)(1-error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1-error_{S_2}(h_2))}{n_2}}$$

Paired *t* test to compare h_A, h_B

Partition data into k disjoint test sets T_1, T_2,...,T_k of equal size, where this size is at least 30.

For i from 1 to k, do

$$\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$$

Return the value δ, where

$$\bar{\delta} \equiv \frac{1}{k}\sum_{i=1}^{k}\delta_i$$

N% confidence interval estimate for d:

$$\bar{\delta} \pm t_{N,k-1}\, s_{\bar{\delta}} \qquad (5.17)$$

$$s_{\bar{\delta}} = \sqrt{\frac{1}{k(k-1)}\sum_{i=1}^{k}(\delta_i - \bar{\delta})^2}$$

Note: δ_i are approximately Normally distributed

	Confidence level N			
	90%	95%	98%	99%
$\nu = 2$	2.92	4.30	6.96	9.92
$\nu = 5$	2.02	2.57	3.36	4.03
$\nu = 10$	1.81	2.23	2.76	3.17
$\nu = 20$	1.72	2.09	2.53	2.84
$\nu = 30$	1.70	2.04	2.46	2.75
$\nu = 120$	1.66	1.98	2.36	2.62
$\nu = \infty$	1.64	1.96	2.33	2.58

Comparing learning algorithms L_A and L_B

What we'd like to estimate:

$$E_{S \subset D}[error_D(L_A(S)) - error_D(L_B(S))]$$

where L(S) is the hypothesis output by learner L using training set S

i.e., the expected difference in true error between hypotheses output by learners L_A and L_B, when trained using randomly selected training sets S drawn according to distribution D.

But, given limited data D_0, what is a good estimator?

We could partition D_0 into training set S and training set T_0, and measure

$$error_{T_0}(L_A(S_0)) - error_{T_0}(L_B(S_0))$$

even better, repeat this many times and average the results (next slide)

Comparing learning algorithms L_A and L_B

1. Partition data D_0 into k disjoint test sets $T_1, T_2, \ldots, T_k$, of equal size, where this size is at least 30.
2. For i from 1 to k, do

   use T_i for the test set, and the remaining data for training set S_i

   $S_i \leftarrow \{D_0 - T_i\}$

   $h_A \leftarrow L_A(S_i)$

   $h_B \leftarrow L_B(S_i)$

   $\delta_i \leftarrow error_{Ti}(h_A) - error_{Ti}(h_B)$
3. Return the value $\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$

Comparing learning algorithms L_A and L_B

Notice we'd like to use the paired t test on δ to obtain a confidence interval

but not really correct, because the training sets in this algorithm are not independent (they overlap!)

more correct to view algorithm as producing an estimate of

$$E_{S \subset D_0}[error_D(L_A(S)) - error_D(L_B(S))] \quad (5.16)$$

instead of

$$E_{S \subset D}[error_D(L_A(S)) - error_D(L_B(S))] \quad (5.14)$$

but even this approximation is better than no comparison

Summary

Statistical theory provides a basis for estimating the true error ($error_D(h)$) of a hypothesis h, based on its observed error ($error_S(h)$) over a sample S of data. For example, if A is a discrete-valued hypothesis and the data sample S contains n > 30 examples drawn independently of h and of one another, then the N% confidence interval for $error_D(h)$ is approximately

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

where values for z_N are given in Table 5.1.

In general, the problem of estimating confidence intervals is approached by identifying the parameter to be estimated (e.g., $error_D(h)$) and an estimator (e.g., $error_S(h)$) for this quantity. Because the estimator is a random variable (e.g., $error_S(h)$ depends on the random sample S, it can be characterized by the probability distribution that governs its value. Confidence intervals can then be calculated by determining the interval that contains the desired probability mass under this distribution.

One possible cause of errors in estimating hypothesis accuracy is estimation bias. If Y is an estimator for some parameter p, the estimation bias of Y is the difference between p and the expected value of Y. For example, if S is the training data used to formulate hypothesis h, then $error_S(h)$ gives an optimistically biased estimate of the true error $error_D(h)$

Summary

A second cause of estimation error is variance in the estimate. Even with an unbiased estimator, the observed value of the estimator is likely to vary from one experiment to another. The variance σ^2 of the distribution governing the estimator characterizes how widely this estimate is likely to vary from the correct value. This variance decreases as the size of the data sample is increased.

Comparing the relative effectiveness of two learning algorithms is an estimation problem that is relatively easy when data and time are unlimited, but more difficult when these resources are limited. One possible approach described in this chapter is to run the learning algorithms on different subsets of the available data, testing the learned hypotheses on the remaining data, then averaging the results of these experiments.

In most cases considered here, deriving confidence intervals involves making a number of assumptions and approximations. For example, the above confidence interval for $error_D(h)$ involved approximating a Binomial distribution by a Normal distribution, approximating the variance of this distribution, and assuming instances are generated by a fixed, unchanging probability distribution. While intervals based on such approximations are only approximate confidence intervals, they nevertheless provide useful guidance for designing and interpreting experimental results in machine learning.

EXERCISES (5 out of 8)

1. Suppose you test a hypothesis h and find that it commits $r = 300$ errors on a sample S of $n = 1000$ randomly drawn test examples. What is the standard deviation is $error_S(h)$? How does this compare to the standard deviation in the example at the end of Section 5.3.4?
2. Consider a learned hypothesis, h, for some Boolean concept. When h is tested on a set of 100 examples, it classifies 83 correctly. What is the standard deviation and the 95% confidence interval for the true error rate for $Error_D(h)$?
3. Suppose hypothesis h commits $r = 10$ errors over a sample of $n = 65$ independently drawn examples. What is the 90% confidence interval (two-sided) for the true error rate? What is the 95% one-sided interval (i.e., what is the upper bound U such that $error_D(h) <= U$ with 95% confidence)? What is the 90% one-sided interval?
4. You are about to test a hypothesis h whose $error_D(h)$ is known to be in the range between 0.2 and 0.6. What is the minimum number of examples you must collect to assure that the width of the two-sided 95% confidence interval will be smaller than 0.1?
5. Give general expressions for the upper and lower one-sided $N\%$ confidence intervals for the difference in errors between two hypotheses tested on different samples of data. Hint: Modify the expression given in Section 5.5.
6. Explain why the confidence interval estimate given in Equation (5.17) applies to estimating the quantity in Equation (5.16), and not the quantity in Equation (5.14).
7. proof E[X] for binomial == np
8. Prove: for binomial Var(X) = np(1-p)