A

Definition of Statistical Quantities

A.1 General Statistical Quantities

Let $\{x_i\}$, with $i = 1, \ldots, N$, be a given discrete time series of length N. $\{x_i\}$ is regarded as a finite sample from a continuous, infinite and stationary time series $x(t)$.

Mean

The true mean μ of $x(t)$ is estimated by the mean value $\overline{x}$ of $\{x_i\}$, which is defined by

$$\overline{x} = \frac{1}{N} \sum_{i=1}^{N} x_i \, . \tag{A.1}$$

Standard Deviation

The standard deviation $\sigma(x)$ of $x(t)$ is estimated by the standard deviation σ_x of the sample; hence,

$$\sigma_x = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (x_i - \overline{x})^2} \, , \tag{A.2}$$

where $\overline{x}$ denotes the mean according to (A.1). σ_x^2 will be referred to as variance.

Cross-correlation Coefficient

The cross-correlation measures the degree of linear dependence between two times series $x(t)$ and $y(t)$. It is defined by

$$r_{xy} = \frac{1}{\sigma_x \, \sigma_y} \frac{1}{N} \sum_{i=1}^{N} (x_i - \overline{x}) \, (y_i - \overline{y}) \ . \tag{A.3}$$

A.2 Error Measures

Error measures describe the average behaviour of deviations between predicted and measured values. The time series to be analysed is the difference between prediction, x_{pred}, and measurement, x_{meas}, i.e. the pointwise error at time i defined by

$$\epsilon_i = x_{\mathrm{pred,i}} - x_{\mathrm{meas,i}} \ . \tag{A.4}$$

Root Mean Square Error (rmse)

The root mean square error evaluates the squared difference between x_{pred} and x_{meas}; hence,

$$\mathrm{rmse} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(x_{\mathrm{pred,i}} - x_{\mathrm{meas,i}}\right)^2} = \sqrt{\overline{\epsilon^2}} \ . \tag{A.5}$$

Bias

The bias is the difference between the mean values of x_{pred} and x_{meas}, i.e.

$$\mathrm{bias} = \overline{x_{\mathrm{pred}}} - \overline{x_{\mathrm{meas}}} = \overline{\epsilon} \ . \tag{A.6}$$

Standard Deviation of Error (sde) and its Decomposition

The standard deviation of error is given by

$$\mathrm{sde} = \sigma(\epsilon) = \sqrt{\overline{\epsilon^2} - \overline{\epsilon}^2} \ . \tag{A.7}$$

By using simple algebra the variance of error, i.e. sde^2, can be split into two parts, namely the sdbias defined by the difference between the standard deviations of x_{pred} and x_{meas} and the dispersion, disp:

$$
\begin{aligned}
\mathrm{sde}^2 &= \sigma^2(\epsilon) \\
&= \overline{(\epsilon - \overline{\epsilon})^2} \\
&= \overline{\left(x_{\mathrm{pred}} - \overline{x_{\mathrm{pred}}} - (x_{\mathrm{meas}} - \overline{x_{\mathrm{meas}}})\right)^2} \\
&= \overline{(x_{\mathrm{pred}} - \overline{x_{\mathrm{pred}}})^2} + \overline{(x_{\mathrm{meas}} - \overline{x_{\mathrm{meas}}})^2} - 2\overline{(x_{\mathrm{pred}} - \overline{x_{\mathrm{pred}}})\,(x_{\mathrm{meas}} - \overline{x_{\mathrm{meas}}})} \\
&= \sigma^2(x_{\mathrm{pred}}) + \sigma^2(x_{\mathrm{meas}}) - 2\sigma(x_{\mathrm{pred}})\,\sigma(x_{\mathrm{meas}})\,r(x_{\mathrm{pred}}, x_{\mathrm{meas}}) \\
&= \big(\sigma^2(x_{\mathrm{pred}}) + \sigma^2(x_{\mathrm{meas}}) - 2\sigma(x_{\mathrm{pred}})\,\sigma(x_{\mathrm{meas}})\big) \\
&\qquad + 2\sigma(x_{\mathrm{pred}})\,\sigma(x_{\mathrm{meas}}) - 2\sigma(x_{\mathrm{pred}})\,\sigma(x_{\mathrm{meas}})\,r(x_{\mathrm{pred}}, x_{\mathrm{meas}}) \\
&= \underbrace{\left(\sigma(x_{\mathrm{pred}}) - \sigma(x_{\mathrm{meas}})\right)^2}_{\mathrm{sdbias}^2} + \underbrace{2\sigma(x_{\mathrm{pred}})\,\sigma(x_{\mathrm{meas}})(1 - r(x_{\mathrm{pred}}, x_{\mathrm{meas}}))}_{\mathrm{disp}^2}
\end{aligned}
\tag{A.8}
$$

Using (A.5), (A.6), (A.7) and (A.8), the rmse can be written as

$$
\mathrm{rmse} = \sqrt{\mathrm{bias}^2 + \mathrm{sdbias}^2 + \mathrm{disp}^2}\ . \tag{A.9}
$$

B

Statistical Testing

The type of probability distribution of the variables plays an important role in the interpretation of the results, in particular in connection with confidence intervals. In some cases an assumption concerning the distribution of the variable in question can be made, e.g. the deviations between prediction and measurement are commonly expected to be normally distributed. Hypotheses of this kind can be tested with statistical methods. The idea is to formulate a hypothesis H_0, such as "$H_0 =$ A given sample $\{x_i\}$ is drawn from a distribution of type Y". Then a confidence level $1 - \alpha$ is set, where α is the probability of rejecting the hypothesis although it is true. The outcome of the test is either that H_0 is rejected or it is not rejected at the given confidence level. So the crucial point is that a statistical test cannot prove the hypothesis; i.e. even if the hypothesis is not falsified by the test, it can still be wrong. The value of these tests is to add some more confidence to the statement of the hypothesis.

B.1 The χ^2 Test

The χ^2 test is a popular form of hypothesis testing and is described in standard books on statistics, e.g. [121]. The test is used in this work as a so-called goodness-of-fit test to check whether a sample could have been drawn from a normal distribution. Hence, the null hypothesis is "$H_0 =$ The given random sample $\{x_i\}$ is drawn from a normal distribution with mean $\overline{x}$ and variance σ^2". The basic idea of the χ^2 test is to compare observed frequencies, h_j, with the theoretically expected probabilities, p_j, and provide criteria to decide if they show significant differences.

First of all, the N sample values $\{x_i\}$ are divided into k bins of equal width Δe. Let e_j be the upper boundary of bin j; then the theoretical probability, assuming that the distribution was Gaussian, is given by $p_j = F(e_j) - F(e_{j-1})$, where $F(e_j) = \Phi\left((e_j - \overline{x})/\sigma\right)$ is the cumulated distribution function of a Gaussian distribution. Then the random variable

$$\chi_s^2 = \sum_j^k \frac{(h_j - N\,p_j)^2}{N\,p_j} \tag{B.1}$$

is defined which compares the empirically found frequencies, h_j, with the expected Gaussian probabilities, p_j. The variable χ_s^2 is approximately χ^2 distributed with $k-1$ degrees of freedom. A prerequisite for this approximation is $Np_j \geq 5$. The χ^2 distribution is defined as the distribution of the sum of the squares of independent standard normal variables and its values are usually tabulated, e.g. in [121].

The probability of wrong rejection α is selected. It implicitly defines the interval in which realisations of χ_s^2 according to (B.1) are rejected. Hence, the condition

$$F_{\chi^2}(\chi^2 \geq \chi^2_{\alpha,k-1}) = \alpha \;, \tag{B.2}$$

where F_{χ^2} is the cumulated χ^2 distribution, gives a critical point, $\chi^2_{\alpha,k-1}$, and the probability to find values beyond this point is α. Typically, α is set to 0.10, 0.05 or 0.01 and is called the significance level. The corresponding values of $\chi^2_{\alpha,k-1}$ are tabulated.

After $\chi^2_{\alpha,k-1}$ is determined, the last step is to check whether the realisation of χ_s^2 is smaller than this critical point; i.e. if

$$\chi_s^2 \leq \chi^2_{\alpha,k-1} \;, \tag{B.3}$$

there is no objection to the assumption that the sample stems from a Gaussian distribution.

B.2 The Lilliefors Test

The Lilliefors test is also a goodness-of-fit test used to test a given distribution for normality. The test compares the empirical cumulative distribution of the sample $\{x_i\}$ with a normal cumulative distribution having the same mean and variance as $\{x_i\}$. Compared to the χ^2-test it has the advantage that the sample size is allowed to be relatively small.

The test statistics of the Lilliefors test is defined as

$$D = \max_j |P_j - H_j| \tag{B.4}$$

where $P_j = \Phi\left((x_j - \overline{x})/\sigma\right)$ is the cumulative distribution of the normal standard distribution and H_j the empirical frequency of events with $x \leq x_j$. D according to (B.4) is tested against a critical value D_α at the desired confidence level α obtained from a table. If $D > D_\alpha$ the hypothesis that the distribution is normal will be rejected.

The known limitations of the Lilliefors test (which is similar to a test called Kolmogorov-Smirnov test) is that it tends to be more sensitive near the centre of the distribution than at the tails.

B.3 The *F* Test

In order to test whether several sample means show statistically significant differences the so-called *F* test is used (described, e.g., in [121]). The idea of this test is to compare the within variance among the members of one sample to the in-between variance among the means of the different samples. The variance between the sample means is "explained" by the fact that the samples might come from different populations, while the variance within one sample is "unexplained" in the sense that it is due to random fluctuations around the mean. Hence, the F test is based on evaluating the ratio

$$F = \frac{\text{explained variance}}{\text{unexplained variance}} \ . \tag{B.5}$$

Typically, the hypothesis to be tested is formulated as "$H_0 =$ The sample means belong to the same distribution."

To compare r different means derived from samples of unequal size the following notation is used: let $\{x_i^j\}$, with $i = 1, \ldots, N_j$ and $j = 1, \ldots, r$, denote the jth sample, e.g. in Sect. 9.3 the daily error values of one cluster; then $\overline{x}^j$ is the sample mean.

The average variance of the different samples from their respective mean values is called pooled variance and is defined by

$$\sigma_p^2 = \frac{\sum_{j=1}^{r} \sum_{i=1}^{N_j} (x_i^j - \overline{x}^j)^2}{\sum_{j=1}^{r} (N_j - 1)} \ . \tag{B.6}$$

The variance between the sample means is defined by

$$\sigma_m^2 = \frac{\sum_{j=1}^{r} N_j (\overline{x}^j - \overline{\overline{x}})^2}{r - 1} \ , \tag{B.7}$$

where $\overline{\overline{x}}$ denotes the mean of all x_i^j, i.e.

$$\overline{\overline{x}} = \frac{\sum_{j=1}^{r} N_j \overline{x}^j}{\sum_{j=1}^{r} N_j} \ . \tag{B.8}$$

Now the average within-variance of the individual samples is compared to the variance of the sample means defining the *F* ratio in (B.5) by

$$F = \frac{\sigma_m^2}{\sigma_p^2} \ . \tag{B.9}$$

The *F* ratio is determined for the given samples. If H_0 is true and the sample means are the same, then F is around 1. If the mean values are from different distributions and, hence, H_0 is not true, the variance among the mean values, σ_m^2, will be larger compared with the within-sample variance, σ_p^2, and F in (B.9) is expected to be greater than 1. The F distribution determines how large F is allowed to be under the assumption that H_0 is true. Hence, for a pre-defined significance level α, i.e. the probability that H_0 is rejected though it is true, the critical value F_α can be inferred from a tabulated F distribution with the suitable degree of freedom. If the condition

$$F \leq F_\alpha \tag{B.10}$$

holds, H_0 is not rejected.

Note that the hypothesis H_0 is "the means are equal" and, thus, if H_0 is rejected the alternative hypothesis H_1: "the means are NOT equal" is confirmed. However, this is only the first step because this test does not tell which pairs of mean values are different. This has to be tested by constructing simultaneous confidence intervals around each of the mean values. Using *Scheffe's multiple comparisons* [121] the differences between all pairs of sample means can be evaluated, and with 95% confidence the following statement is true for all sample pairs (k, j) simultaneously:

$$\mu_k - \mu_j = (\overline{x}^k - \overline{x}^j) \pm \sqrt{(r-1)\, F_{0.05}}\, \sigma_p \sqrt{\frac{1}{N_k} + \frac{1}{N_j}}\ , \tag{B.11}$$

where $\mu_k - \mu_j$ is the difference between the true means of the two underlying populations, $\overline{x}^k - \overline{x}^j$ is the difference between the sample means, r is the number of different samples, $F_{0.05}$ is the value of the F distribution at the significance level 0.05, σ_p^2 is the pooled variance (B.6) and N_k,N_j are the sample sizes.

Thus, if the difference $\overline{x}^k - \overline{x}^j$ exceeds the confidence range given by (B.11), the two samples $\{x_i^k\}$ and $\{x_i^j\}$ are believed to originate from two different distributions and the mean values $\overline{x}^k$ and $\overline{x}^j$ are regarded as significantly different.

B.4 *F* Test Results from Sect. 9.3

Table B.1. *F* ratios (B.9) of investigated stations (see Sect. 9.3)

	Number of clusters	Linkage type	*F* ratio
Fehmarn	6	Complete	7.73
	6	Ward's	5.65
Hilkenbrook	7	Complete	6.23

Table B.2. Results of Scheffe's multiple comparison for daily rmse for Fehmarn clustering with complete linkage[a]

Cluster$_i$	Cluster$_j$	Difference of means$_{ij}$	Significance	Lower boundary	Upper boundary
1	2	−0.0709	1.000	−0.7788	0.6371
	3	0.4120	0.063	−0.0119	0.8360
	4	0.7619(*)	0.001	0.2061	1.3176
	5	−0.0875	0.999	−0.7433	0.5682
	6	0.4930(*)	0.011	0.0690	0.9169
2	1	0.0709	1.000	−0.6371	0.7788
	3	0.4829	0.297	−0.1702	1.1360
	4	0.8327(*)	0.017	0.0873	1.5782
	5	−0.0167	1.000	−0.8394	0.8060
	6	0.5638	0.141	−0.0893	1.2170
3	1	−0.4120	0.063	−0.8360	0.0119
	2	−0.4829	0.297	−1.1360	0.1702
	4	0.3498	0.323	−0.1341	0.8338
	5	−0.4996	0.167	−1.0957	0.0965
	6	0.0809	0.983	−0.2433	0.4051
4	1	−0.7619(*)	0.001	−1.3176	−0.2061
	2	−0.8327(*)	0.017	−1.5782	−0.0873
	3	−0.3498	0.323	−0.8338	0.1341
	5	−0.8494(*)	0.006	−1.5455	−0.1534
	6	−0.2689	0.630	−0.7529	0.2151
5	1	0.0875	0.999	−0.5682	0.7433
	2	0.0167	1.000	−0.8060	0.8394
	3	0.4996	0.167	−0.0965	1.0957
	4	0.8494(*)	0.006	0.1534	1.5455
	6	0.5805	0.062	−0.0156	1.1766
6	1	−0.4930(*)	0.011	−0.9169	−0.0690
	2	−0.5638	0.141	−1.2170	0.0893
	3	−0.0809	0.983	−0.4051	0.2433
	4	0.2689	0.630	−0.2151	0.7529
	5	−0.5805	0.062	−1.1766	0.0156

[a]The standard software SPSS has been used. "*" denotes that the difference between the means is significant at the level $\alpha = 0.05$. Cluster$_i$ and cluster$_j$ refer to the cluster numbers used in Sect. 9.3. If "significance" is smaller than $\alpha = 0.05$, the mean values of the two clusters i and j are regarded as significantly different. Lower boundary and upper boundary refer to the boundaries of the 95% confidence interval given by B.11. This interval does not contain the origin if the clusters are significantly different.

Table B.3. Results of Scheffe's multiple comparison for daily rmse, for Fehmarn with Ward's linkage[a]

Cluster$_i$	Cluster$_j$	Difference of means$_{ij}$	Significance	Lower boundary	Upper boundary
1	2	0.1725	0.959	−0.3920	0.7369
	3	−0.2504	0.757	−0.7669	0.2662
	4	−0.0253	1.000	−0.5898	0.5391
	5	−0.3974	0.592	−1.087	0.2926
	6	−0.4223	0.206	−0.9474	0.1029
2	1	−0.1725	0.959	−0.7369	0.3920
	3	−0.4228(*)	0.048	−0.8439	−0.0017
	4	−0.1978	0.861	−0.6764	0.2809
	5	−0.5699	0.097	−1.191	0.0519
	6	−0.5947(*)	0.001	−1.026	−0.1631
3	1	0.2504	0.757	−0.2662	0.7669
	2	0.4228(*)	0.048	0.0017	0.8439
	4	0.2250	0.670	−0.1961	0.6462
	5	−0.1471	0.982	−0.7258	0.4316
	6	−0.1719	0.782	−0.5387	0.1949
4	1	0.0253	1.000	−0.5391	0.5898
	2	0.1978	0.861	−0.2809	0.6764
	3	−0.2250	0.670	−0.6462	0.1961
	5	−0.3721	0.549	−0.9939	0.2497
	6	−0.3969	0.095	−0.8286	0.0347
5	1	0.3974	0.592	−0.2926	1.0875
	2	0.5699	0.097	−0.0519	1.1917
	3	0.1471	0.982	−0.4316	0.7258
	4	0.3721	0.549	−0.2497	0.9939
	6	−0.0248	1.000	−0.6112	0.5616
6	1	0.4223	0.206	−0.1029	0.9474
	2	0.5947(*)	0.001	0.1631	1.0264
	3	0.1719	0.782	−0.1949	0.5387
	4	0.3969	0.095	−0.0347	0.8286
	5	0.0248	1.000	−0.5616	0.6112

[a]The standard software SPSS has been used. "*" denotes that the difference between the means is significant at the level $\alpha = 0.05$. Cluster$_i$ and cluster$_j$ refer to the cluster numbers used in Sect. 9.3. If "significance" is smaller than $\alpha = 0.05$, the mean values of the two clusters i and j are regarded as significantly different. Lower boundary and upper boundary refer to the boundaries of the 95% confidence interval given by B.11. This interval does not contain the origin if the clusters are significantly different.

Table B.4. Results of Scheffe's multiple comparison for daily rmse for Hilkenbrook with complete linkage[a]

Cluster_i	Cluster_j	Difference of means_{ij}	Significance	Lower boundary	Upper boundary
1	2	−0.2309	0.372	−0.5544	0.0925
	3	−0.1616	0.964	−0.6443	0.3212
	4	−0.2806(*)	0.035	−0.5509	−0.0104
	5	−0.2365	0.852	−0.7561	0.2831
	6	−0.7372(*)	0.000	−1.1838	−0.2906
	7	−0.2088	0.580	−0.5516	0.1341
2	1	0.2309	0.372	−0.0925	0.5544
	3	0.0694	1.000	−0.4218	0.5605
	4	−0.0497	0.999	−0.3347	0.2353
	5	−0.0055	1.000	−0.5330	0.5219
	6	−0.5063(*)	0.017	−0.9619	−0.0506
	7	0.0222	1.000	−0.3324	0.3767
3	1	0.1616	0.964	−0.3212	0.6443
	2	−0.0694	1.000	−0.5605	0.4218
	4	−0.1191	0.990	−0.5769	0.3388
	5	−0.0749	1.000	−0.7126	0.5628
	6	−0.5756	0.053	−1.1553	0.0041
	7	−0.0472	1.000	−0.5513	0.4569
4	1	0.2806(*)	0.035	0.0104	0.5509
	2	0.0497	0.999	−0.2353	0.3347
	3	0.1191	0.990	−0.3388	0.5769
	5	0.0442	1.000	−0.4525	0.5408
	6	−0.4566(*)	0.021	−0.8761	−0.0370
	7	0.0719	0.994	−0.2349	0.3787
5	1	0.2365	0.852	−0.2831	0.7561
	2	0.0055	1.000	−0.5219	0.5330
	3	0.0749	1.000	−0.5628	0.7126
	4	−0.0442	1.000	−0.5408	0.4525
	6	−0.5007	0.203	−1.1115	0.1100
	7	0.0277	1.000	−0.5118	0.5672
6	1	0.7372(*)	0.000	0.2906	1.1838
	2	0.5063(*)	0.017	0.0506	0.9619
	3	0.5756	0.053	−0.0041	1.1553
	4	0.4566(*)	0.021	0.0370	0.8761
	5	0.5007	0.203	−0.1100	1.1115
	7	0.5284(*)	0.014	0.0588	0.9980

(*cont.*)

Table B.4. Contd.

Cluster$_i$	Cluster$_j$	Difference of means$_{ij}$	Significance	Lower boundary	Upper boundary
7	1	0.2088	0.580	−0.1341	0.5516
	2	−0.0222	1.000	−0.3767	0.3324
	3	0.0472	1.000	−0.4569	0.5513
	4	−0.0719	0.994	−0.3787	0.2349
	5	−0.0277	1.000	−0.5672	0.5118
	6	−0.5284(*)	0.014	−0.9980	−0.0588

[a]The standard software SPSS has been used. "*" denotes that the difference between the means is significant at the level $\alpha = 0.05$. Cluster$_i$ and cluster$_j$ refer to the cluster numbers used in Sect. 9.3. If "significance" is smaller than $\alpha = 0.05$, the mean values of the two clusters i and j are regarded as significantly different. Lower boundary and upper boundary refer to the boundaries of the 95% confidence interval given by B.11. This interval does not contain the origin if the clusters are significantly different

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