

## A

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### Definition of Statistical Quantities

#### A.1 General Statistical Quantities

Let  $\{x_i\}$ , with  $i = 1, \dots, N$ , 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  $\mu$  of  $x(t)$  is estimated by the mean value  $\bar{x}$  of  $\{x_i\}$ , which is defined by

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i . \quad (\text{A.1})$$

##### Standard Deviation

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

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

where  $\bar{x}$  denotes the mean according to (A.1).  $\sigma_x^2$  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

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

## 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,  $x_{\text{pred}}$ , and measurement,  $x_{\text{meas}}$ , i.e. the pointwise error at time  $i$  defined by

$$\epsilon_i = x_{\text{pred},i} - x_{\text{meas},i} . \quad (\text{A.4})$$

### Root Mean Square Error (rmse)

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

$$\text{rmse} = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_{\text{pred},i} - x_{\text{meas},i})^2} = \sqrt{\epsilon^2} . \quad (\text{A.5})$$

### Bias

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

$$\text{bias} = \overline{x_{\text{pred}}} - \overline{x_{\text{meas}}} = \bar{\epsilon} . \quad (\text{A.6})$$

### Standard Deviation of Error (sde) and its Decomposition

The standard deviation of error is given by

$$\text{sde} = \sigma(\epsilon) = \sqrt{\epsilon^2 - \bar{\epsilon}^2} . \quad (\text{A.7})$$

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

$$\begin{aligned}
\text{sde}^2 &= \sigma^2(\epsilon) \\
&= \overline{(\epsilon - \bar{\epsilon})^2} \\
&= \overline{(x_{\text{pred}} - \bar{x}_{\text{pred}} - (x_{\text{meas}} - \bar{x}_{\text{meas}}))^2} \\
&= \overline{(x_{\text{pred}} - \bar{x}_{\text{pred}})^2 + (x_{\text{meas}} - \bar{x}_{\text{meas}})^2 - 2(x_{\text{pred}} - \bar{x}_{\text{pred}})(x_{\text{meas}} - \bar{x}_{\text{meas}})} \\
&= \sigma^2(x_{\text{pred}}) + \sigma^2(x_{\text{meas}}) - 2\sigma(x_{\text{pred}})\sigma(x_{\text{meas}})r(x_{\text{pred}}, x_{\text{meas}}) \\
&= (\sigma^2(x_{\text{pred}}) + \sigma^2(x_{\text{meas}}) - 2\sigma(x_{\text{pred}})\sigma(x_{\text{meas}})) \\
&\quad + 2\sigma(x_{\text{pred}})\sigma(x_{\text{meas}}) - 2\sigma(x_{\text{pred}})\sigma(x_{\text{meas}})r(x_{\text{pred}}, x_{\text{meas}}) \\
&= \underbrace{(\sigma^2(x_{\text{pred}}) - \sigma^2(x_{\text{meas}}))}_{\text{sdbias}^2} + \underbrace{2\sigma(x_{\text{pred}})\sigma(x_{\text{meas}})(1 - r(x_{\text{pred}}, x_{\text{meas}}))}_{\text{disp}^2}
\end{aligned} \tag{A.8}$$

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

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

## B

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### 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  $\alpha$  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 $\chi^2$ Test

The  $\chi^2$  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  $\bar{x}$  and variance  $\sigma^2$ ”. The basic idea of the  $\chi^2$  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  $\Delta e$ . 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  $F(e_j) = \Phi((e_j - \bar{x})/\sigma)$  is the cumulated distribution function of a Gaussian distribution. Then the random variable

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

is defined which compares the empirically found frequencies,  $h_j$ , with the expected Gaussian probabilities,  $p_j$ . The variable  $\chi_s^2$  is approximately  $\chi^2$  distributed with  $k - 1$  degrees of freedom. A prerequisite for this approximation is  $N p_j \geq 5$ . The  $\chi^2$  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  $\alpha$  is selected. It implicitly defines the interval in which realisations of  $\chi_s^2$  according to (B.1) are rejected. Hence, the condition

$$F_{\chi^2}(\chi^2 \geq \chi_{\alpha, k-1}^2) = \alpha, \quad (\text{B.2})$$

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

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

$$\chi_s^2 \leq \chi_{\alpha, k-1}^2, \quad (\text{B.3})$$

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  $\chi^2$ -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

$$D = \max_j |P_j - H_j| \quad (\text{B.4})$$

where  $P_j = \Phi((x_j - \bar{x})/\sigma)$  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  $D_\alpha$  at the desired confidence level  $\alpha$  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

$$F = \frac{\text{explained variance}}{\text{unexplained variance}}. \quad (\text{B.5})$$

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  $i = 1, \dots, N_j$  and  $j = 1, \dots, r$ , denote the  $j$ th sample, e.g. in Sect. 9.3 the daily error values of one cluster; then  $\bar{x}^j$  is the sample mean.

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

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

The variance between the sample means is defined by

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

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

$$\bar{\bar{x}} = \frac{\sum_{j=1}^r N_j \bar{x}^j}{\sum_{j=1}^r N_j}. \quad (\text{B.8})$$

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

$$F = \frac{\sigma_m^2}{\sigma_p^2}. \quad (\text{B.9})$$

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,  $\sigma_m^2$ , will be larger compared with the within-sample variance,  $\sigma_p^2$ , 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  $\alpha$ , i.e. the probability that  $H_0$  is rejected though it is true, the critical value  $F_\alpha$  can be inferred from a tabulated  $F$  distribution with the suitable degree of freedom. If the condition

$$F \leq F_\alpha \quad (\text{B.10})$$

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:

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

where  $\mu_k - \mu_j$  is the difference between the true means of the two underlying populations,  $\bar{x}^k - \bar{x}^j$  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,  $\sigma_p^2$  is the pooled variance (B.6) and  $N_k, N_j$  are the sample sizes.

Thus, if the difference  $\bar{x}^k - \bar{x}^j$  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  $\bar{x}^k$  and  $\bar{x}^j$  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<sup>a</sup>

Cluster <sub><i>i</i></sub>	Cluster <sub><i>j</i></sub>	Difference of means <sub><i>ij</i></sub>	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

<sup>a</sup>The standard software SPSS has been used. “\*” denotes that the difference between the means is significant at the level  $\alpha = 0.05$ . Cluster<sub>*i*</sub> and cluster<sub>*j*</sub> 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<sup>a</sup>

Cluster <sub><i>i</i></sub>	Cluster <sub><i>j</i></sub>	Difference of means <sub><i>ij</i></sub>	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

<sup>a</sup>The standard software SPSS has been used. “\*” denotes that the difference between the means is significant at the level  $\alpha = 0.05$ . Cluster<sub>*i*</sub> and cluster<sub>*j*</sub> 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<sup>a</sup>

Cluster <sub><i>i</i></sub>	Cluster <sub><i>j</i></sub>	Difference of means <sub><i>ij</i></sub>	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 <sub><i>i</i></sub>	Cluster <sub><i>j</i></sub>	Difference of means <sub><i>ij</i></sub>	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

<sup>a</sup>The standard software SPSS has been used. “\*” denotes that the difference between the means is significant at the level  $\alpha = 0.05$ . Cluster<sub>*i*</sub> and cluster<sub>*j*</sub> 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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## Index

- adaptive estimation 11
- adaptive statistical methods 20
- adaptivity 13
- adiabatic expansion 33
- advection equation 70
- air pollution 138
- Aladin 10
- amplitude error 61, 63, 69, 70, 80
- arbitrary location 56
- Arpege 10
- atmospheric boundary layer 2, 8, 19
- atmospheric pressure 25, 33, 60, 138, 166, 167
- atmospheric stratification 32, 78, 89, 138
- auto-correlation 66, 88
- automatic classification 135
  
- balance 4, 5, 24, 36, 163, 177, 179
- balancing power 5
- Bessel function 49, 50
- Bessel series 50
- between-cluster variance 142
- boundary conditions 4, 19, 49
- boundary layer VII, 2, 8, 17, 19–21, 23, 24, 26, 29, 31, 39, 41, 42, 47, 52, 78, 91, 101, 103, 180, 203
- bulk gradient 103
- buoyancy 19, 31, 32, 34, 35, 38, 44, 45, 78, 92
- BZ-model 48
  
- Cabouw 57, 92, 94
- CENER 20
- certified power curve 16, 22, 131, 133, 180
- channelling effects 47, 165, 166
- chaotic properties 136
- classification 92, 135–138, 140, 142, 143, 148, 149, 154, 155, 157, 158, 160, 161, 164–167, 180
- climatological mean 43, 68, 88
- climatology 3, 135, 137, 148, 166, 179, 180
- cluster analysis 20, 138, 140, 144, 148, 149, 166
- cluster distance 141, 149, 150
- complete linkage method 141
- complex terrain 15, 19, 47, 48, 74, 78, 79, 82, 86, 89, 167, 179
- computational grid 8, 55, 56
- conditional pdf 115–123, 125–127, 132
- confidence interval 62, 64, 66, 68, 70, 75, 79, 125, 126, 158, 159, 187, 190–192, 194
- conservation of mass 19, 23, 26
- conservation of momentum 25
- continuity equation 26
- conventional power plants 1, 3, 4, 6, 7
- cooling 33, 44
- Coriolis force 24, 25, 36, 37
- cost-efficient energy supply 4

- coupling 24, 25, 36–38, 43, 44, 78, 92, 94, 109
- covariance matrix 139
- cross-correlation 61, 69, 70, 72, 73, 80, 86, 87, 90, 97–101, 105, 107, 111, 172, 173, 175, 177, 178, 183
- cup anemometer 55
- cut-in speed 68, 117
- cylindrical polar coordinates 49
- daily forecast error 163, 167
- data matrix 139, 140, 144, 148
- day ahead 6
- daytime 44, 78, 82, 107, 109, 110, 113, 114
- decomposition 27, 69, 70, 72, 75, 80, 81, 86, 89
- degree of freedom 190
- Denmark V, 5, 10, 11
- detailed roughness description 2
- diagnostic level 56
- Diagnostic models 21
- direction dependent 21, 39, 43, 108
- dispersion 70, 72, 73, 80, 81, 87–90, 184
- distribution of distance 175
- diurnal variation 78
- diurnal cycle 32, 44, 109, 111, 114
- Diurnal variation 78, 89
- diurnal variation 15, 78, 80, 82, 89, 110, 111, 114, 145, 147
- dry adiabatic temperature gradient 33
- dry gas constant 60
- dynamic viscosity 25
- ECMWF 136
- economic value 6
- effective non-linearity factor 81, 87
- eigenmode 138–140, 148
- eigenvalue 139, 144, 145, 148
- eigenvector 137, 139, 140
- Ekman layer 23, 31
- electricity V, VI, 1, 3–7, 169, 179
- ELSAM 11
- ELTRA 11
- empirical pdf 126
- energy market 4
- energy supplier 1
- ensemble of wind farms 169, 177
- equations of motion 2, 8, 18, 20, 23, 26, 37, 47, 49, 55, 56, 136
- equidistant bin 120
- error characteristic 68
- error source 69, 128, 133, 180
- estimation procedure 11
- European Weather Service 9
- European Wind Atlas 21, 37, 41, 48
- evaluation 3, 68, 144
- EWEA 1
- extreme situation 163
- F test 143, 158, 163, 189
- Fitnah 19, 47
- flat terrain 74, 78, 79, 82, 83, 86, 89, 91, 108, 111, 177
- flow distortion 58, 66, 165, 166
- flow effect 19, 25
- fluctuation V, 1, 3, 6, 26–30, 32, 34, 38, 56, 70, 75, 79, 86, 90, 169, 189
- forecast accuracy 62, 114, 121
- forecast error 2, 3, 6, 21, 39, 61, 64, 67, 72, 80, 81, 89, 90, 115, 126, 130, 135, 138, 142, 144, 148, 150, 158–161, 163–167, 169, 170, 172, 173, 176
- forecast situation 115, 116, 132, 180
- forecasting system 2, 20, 61
- forgetting factor 13–15
- Fourier series 50
- friction velocity 31, 32, 36, 37, 42, 47
- frontal system 138
- Gaussian 15, 61, 64, 65, 67, 90, 115–122, 127, 132, 133, 187, 188
- geostrophic drag law 37, 41, 43
- geostrophic wind 23–25, 36, 37, 41, 94
- Gesima 47
- global model 9, 56
- Globalmodell 10
- gradient method 45
- gravitational constant 60
- gravity 25, 36

- Greenpeace 1
- grid cell 8, 41, 55, 79, 89
- grid domain 19
- grid operator 1
- Grosswetterlage 137
- ground level 44, 45, 49, 60
- heat capacity 32, 34, 78, 180
- heat flux 32, 34, 43–45, 47
- hierarchical 140
- high grid penetration 4, 5
- high-pressure 3, 135, 136, 147, 152–161, 163, 165, 166
- hill 20, 21, 47, 79, 89, 144, 165, 166
- HIRLAM 15, 20, 21, 64
- horizontal momentum 24, 29–31, 37, 44, 93
- hub height 3, 8, 17, 39, 82, 89, 91, 95, 107, 109, 111, 113, 114, 120, 179
- hydrostatic 19, 105
- IBL 41–43
- individual correction 98
- individual site 61, 74, 86, 172
- initial condition 9, 48, 88, 136
- installed wind power capacity 1
- integration of wind energy 1
- internal boundary layer 41, 42, 180
- inverse distance 56
- inversion 44, 82
- irrotational 49
- ISSET VIII, 15, 20
- isobar 24, 36
- Jackson and Hunt 48
- joint distribution 116, 117
- k-step prediction 14
- kinematic viscosity 28, 29
- Laplace equation 49
- large synoptic pressure system 36
- large-scale weather map 135, 144, 152, 154, 166
- least-squares estimation 11
- limit distribution 175
- linear regression 11, 39, 71, 72, 81, 87, 90, 121, 124, 132
- linear transformation 61, 70–73, 81, 90, 98
- linkage method 141, 149, 203
- load profile 4
- local effect 89, 165–167
- local refinement 2, 11, 20, 21, 82, 90
- local thermal effect 105
- local wind condition 23, 87, 181
- LocalPred 15
- logarithmic profile 32, 35, 48, 51, 91, 96, 98, 100, 101, 113
- logarithmic wind profile 2, 3, 32, 40, 41, 43, 56, 79, 81, 113
- Lokalmmodell 10
- look-up table 20, 50
- lower atmosphere 3, 25, 29, 38, 43, 91
- lower boundary layer 78, 91, 101, 103
- main run 56
- manual method 137
- marine boundary layer 180
- marine boundary layer 52
- MASS 6 20
- mass-consistent model 19, 20
- matching relation 43
- MATLAB 144
- meso-scale 15, 19, 20, 43, 47, 79, 89, 179, 181
- meteorological mast 57
- micro-scale 18, 19
- mixing length 28–30, 38
- model level 56
- model output statistic 70
- molecular friction 25, 36
- molecular viscosity 25, 28, 38
- momentum transport 31, 49, 50, 78, 94, 109
- Monin–Obukhov theory 2, 3, 23, 32, 57, 95, 98, 101, 113
- MORE-CARE 17
- multi-dimensional power curve 16
- Navier–Stokes 28

- Navier–Stokes equation 19, 25–27
- negative load 4, 5
- nesting 19, 20
- neutral stratification 36, 96
- Newtonian fluid 25, 28
- nighttime 44, 78, 82, 109, 110
- noise sensitivity 13
- non hydrostatic 19, 105
- non-Gaussian 67
- non-linear power curve 90
- non-parametrical Lilliefors test 64
- nonlinear power curve 3, 61, 68, 115, 180
- normal distribution 64–66, 121–123, 187
- numerical grid 8, 50, 181
- numerical integration 55
- numerical model 18, 20, 26, 47, 48
- NWP 2, 7–9, 11, 17, 19–21, 23, 39, 41, 43, 44, 56, 57, 64, 78, 79, 82, 87–90, 105, 107, 109, 111, 113, 120, 135, 136, 165, 177, 181
- offset 70
- offshore 52, 78, 132, 179, 180
- on-site condition 8, 17, 41, 74, 89, 165
- online monitoring 15
- online operation 13
- orographic effect 2, 21, 49, 108, 144, 165
- orography 21, 39, 74, 79, 89, 165, 166
- orthogonal basis 50, 148
- orthonormal basis 139
- overestimation 62, 79, 82, 86, 89, 97, 109
- parameterisation 15
- persistence 21, 68, 69, 87, 88
- phase error 61–63, 69, 70, 79–81, 85, 87, 89, 143
- phase space 139–141, 148, 149
- physical approach VII, 15, 21, 39
- physical parameterisation 15
- physical prediction system 2, 17, 22
- physical system 2, 8, 10, 21, 22
- point prediction 56, 66
- pointwise error 62, 64, 172, 184
- pointwise prediction error 62, 172
- poor man's ensemble forecast 136
- post-processing 70
- potential flow 49, 50
- potential temperature 33, 36, 92
- Prandtl layer 31, 37
- predictability 105, 113, 165, 167
- predictable V, 136
- prediction accuracy 3, 6, 22, 61, 68, 70, 73, 74, 81, 106, 107
- prediction uncertainty VII, 3, 131, 135, 177
- Prediktor 21
- pressure gradient 24, 25, 138, 153, 155, 159, 160
- principal component analysis 135, 137, 166
- probability 62, 64, 68, 115–119, 132, 136, 187, 188, 190
- rated power 63, 67, 81, 82, 109, 117, 127, 128, 131
- reconstruction procedure 119, 126, 127
- reference model 88
- reference system 68, 69, 87, 88
- regional prediction 170–173
- regional smoothing effect 3, 177
- renewable energy VI, 1, 6
- representative site 16, 21, 40, 179
- Reynolds averaging 26
- Richardson number 33, 34, 38, 45, 46
- risk index 136
- rotational speed of the earth 25, 37
- roughness 2, 11, 19, 21, 22, 31, 37, 39–43, 58, 79, 89, 95, 96, 101, 113, 144, 180, 204
- roughness change 50
- roughness length 50, 101
- saturation level 173, 175, 177
- SCADA 17
- scheduling scheme 7
- Scheffe's multiple comparison 143, 190–193
- sde 70, 75, 79, 80, 86, 107, 113, 121, 126, 129–131, 184
- sea breeze 8

- self-calibrating 11, 15
- sensible heat flux 45
- sensor carrying boom 57
- shadowing effect 2, 21, 39, 50, 53, 57, 107
- short-term prediction 2, 7, 17, 43
- signal to noise ratio 174
- significance level 64, 66, 188, 190
- similarity 69
- single site 3, 169–173, 176, 177
- singular perturbation method 37
- situation dependent assessment 3, 132
- skill score 68
- small perturbation 48
- smoothing effect 3, 40, 169, 170, 177, 179, 180, 206
- solar irradiation 19, 44, 78
- sonic anemometer 45
- spatial average 55, 56
- spatial correlation function 169
- spatial refinement 17, 41
- spatial resolution 8–10, 18–20, 23, 39, 56
- speed-up effect 47, 165, 166
- spot market 6
- stability parameter 98, 111
- stability classes 91, 92, 94
- stability correction 56, 101, 103, 105, 107, 109, 111, 113
- stability parameter 34, 45, 91, 96, 98, 103, 109
- stable high-pressure 3, 153
- stable stratification 91–95, 98, 103, 105, 109
- standard deviation 64–66, 69, 70, 72, 74, 75, 79–82, 86, 87, 89, 98, 100, 101, 105, 107, 111, 115, 118–122, 125–127, 129, 132, 139, 171, 172, 183, 184
- state of the art 179
- stationary situation 95, 98
- statistical approach 7, 17
- statistical behaviour 3, 8, 61, 66, 73, 74
- statistical correction 21, 39, 70
- statistical distribution 62, 67, 91, 95, 107, 132
- statistical error measure 68, 69, 71, 75, 97
- statistical significance 143
- statistical system 2, 8, 10, 11, 15, 22, 39
- statistical test 64, 121, 122, 129, 158, 187
- stochastic process 11
- sub-grid scale 8
- subspace 139, 140
- surface layer VI, 23, 31, 35–37, 44, 94, 100, 109, 113
- surface pressure 60, 139, 144
- surface roughness 21, 22, 31, 39, 40, 42, 43, 89, 144, 180
- surface temperature 60
- synoptic climatology 3, 135, 137, 166, 180
- synoptic scale 56, 60
- synoptic weather system 8
- systematic forecast error 39
- Taylor expansion 118, 129
- temperature difference 43, 45, 47, 96, 103–107, 111, 113, 138
- temporal evolution 62, 71, 135, 145
- temporal mean 69
- terrain type 31, 78, 79, 82, 89
- test case 3, 74
- thermal correction 2, 3, 35, 95–97, 100, 101, 104, 109, 110, 113
- thermal effect VII, 19, 25, 26, 31, 32, 38, 100, 105, 205
- thermal stratification 2, 3, 15, 21, 23, 32–34, 37–39, 43, 45, 47, 82, 89, 91, 94, 96, 98, 99, 101, 105, 107, 109, 111, 113, 114
- thermally corrected profile 97, 98, 101
- thermally corrected wind profile 44
- thermally induced turbulence 45
- time-delay embedding 139
- time-varying parameter 13, 15
- topographic structure 47
- total variance 144, 145
- training period 16
- transmission system operator 4, 169, 179
- TSO 4–6, 11, 15, 39
- turbulence VII, 8, 18, 19, 25, 27–29, 31–34, 38, 45, 49, 56, 207
- turbulent fluctuation 27, 28, 32

- turbulent mixing 25, 38, 43, 44, 92
- turbulent momentum flux 31, 38
- turbulent momentum transport 31, 49, 50, 109
- turbulent motion 27
- uncertainty VII, 3, 21, 62, 98, 107, 116, 131, 133, 135, 136, 167, 177, 179, 180, 206
- unconditional error distribution 117
- uncorrelated source 174
- underestimation 62, 79, 86, 89, 97–99
- Unified Model 10
- University of Oldenburg 2, 21, 39
- unstable stratification 93, 103, 105, 109
- up-scaling 21, 40, 179
- UTC 56, 87, 136, 138, 139, 167
- value of wind energy 3
- variance of the error 69, 143, 184
- velocity gradient 25, 30, 34, 35, 38, 92
- verification VI, 73, 127, 171
- vertical heat flux at the surface 34
- vertical velocity gradient 30, 34
- vertical wind profile 23, 25, 31, 32, 37, 41, 91, 101
- visual inspection 61, 64, 139
- von Karman constant 31, 37
- wake effect 51, 52, 180
- WAsP 19, 20
- weather situation 136, 148, 155
- weather classes 135, 137, 140, 144, 150, 152–154, 157, 160, 165, 167
- weather condition 3, 135, 142, 148, 160, 166, 177
- weather situation 3, 135–138, 150, 151, 154–159, 161, 163–167
- Weibull distribution 75, 120
- weighting factor 16
- wind shear 31, 45
- within-cluster variance 142, 143
- WMEP measurement data 62, 64
- WPMS 15, 16, 20
- WPPT 11, 14, 15