Nieuwsbrief no. 35
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Vereniging voor Ordinatie en Classificatie

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VOC-home page: http://www.voc.ac

VOC Fall Meeting
November 18, 2005
TNO, Utrechtseweg 48, Zeist

10.00 Welcome

10.30 John Gower - *Procrustes problems – An overview*

11.15 Garmt Dijksterhuis - *An application of Generalised Procrustes Analysis as a method to compare data sets collected by different methods*

12.00 Age Smilde - *Proteomics based clinical biomarkers: how to distinguish healthy from diseased? Introduction of the 'shoot-out'*

12.30 Lunch

13.30 *Proteomics based clinical biomarkers: how to distinguish healthy from diseased? The 'shoot-out' continued:*
- 13.30 Wies Akkermans - *Support vector machines*
- 13.45 Carina Rubingh - *Principal discriminant variates*
- 14.00 Suzanne Smit - *Principal components discriminant analysis*
- 14.15 Paul Eilers - *Penalized logistic regression*
- 14.30 Theo Reijmers - *Nearest shrunken centroids*
- 14.45 Margriet Hendriks - *Logit boost and discussion*

15.25 Tea

15.45 Michael Greenacre - *Tying up the loose ends of (simple) correspondence analysis*

16.45 Drinks

In dit nummer:

Van de voorzitter

De komende najaarsbijeenkomst wordt gehouden in Zeist bij TNO. Er ligt een goed programma voor met twee vermaarde buitenlandse sprekers. Michael Greenacre (UPF, Barcelona), één van 's werelds experts op het gebied van correspondentieanalyse, zal spreken over enige controverses van deze techniek. De tweede buitenlandse spreker, John Gower (Open University, Milton Keynes), zal samen met Garmt Dijksterhuis ingaan op Procrustesanalyse waarover zij onlangs een boek gepubliceerd hebben. De rest van de najaarsbijeenkomst wordt gewijd aan een praktische vergelijking van verschillende classificatietechnieken met het doel zieke patiënten te kunnen onderscheiden van gezonde personen. Voor meer details over de sprekers en hun presentaties, zie elders in deze nieuwsbrief. Al met al een mooi programma met aantrekkelijke sprekers. Ik hoop veel deelnemers te treffen op deze bijeenkomst.

Patrick Groenen, voorzitter VOC.

Reisbeurzen voor IFCS 2006 via het Chikio Hayashi Fund

In 2006 vindt het tweejaarlijkse IFCS-congres plaats in Ljubljana, Slovenië, van 25 tot en met 29 juli 2006 (zie http://vlado.fmf.uni-lj.si/info/ifcs06/). Het is bij uitstek een bijeenkomst waar VOC-onderzoek internationaal gepresenteerd kan worden. Ik verwacht dat ook deze keer er weer de mogelijkheid is voor jonge onderzoekers tot 35 jaar om mee te dingen naar een prijs uit het Chikio Hayashi Fund (voorheen de IFCS Travel Award). Deze prijs ondersteunt jonge onderzoekers om het IFCS congres in Ljubljana te kunnen bezoeken en hun werk daar te kunnen presenteren. Meestal gaat het om ongeveer $ 500 per vereniging. De precieze verdeelsleutel wordt bepaald door het IFCS Awards Committee.

Details van de procedure zijn op dit moment nog niet bekend, maar de procedure verloopt meestal volgens het onderstaande stramien. Waarschijnlijk dien je voor half maart (2006) een aanvraagformulier elektronisch aan mij op te sturen (groenen@few.eur.nl). Het formulier zal waarschijnlijk op de IFCS website (http://www.classification-society.org/) beschikbaar worden gesteld. Ik zal de aanvragen beoordelen op hun kwaliteit en de beste doorsturen aan het IFCS Awards Committee. Voorheen was begin mei de uitslag bekend. Zodra er meer details bekend zijn sturen we dit rond per e-mail. Ik hoop dat deze prijs onze jonge leden stimuleert om naar het IFCS-congres in Ljubljana af te reizen!

Patrick Groenen, voorzitter VOC.

Abstracts of the VOC Fall Meeting

John C. Gower (The Open University, Milton Keynes, U.K.): ***Procrustes Problems – An overview***

The basic two-sets Procrustes problem is to match given matrices $\mathbf{X}_1$, $\mathbf{X}_2$ via a transformation $\mathbf{X}_1\mathbf{T}$, where $\mathbf{T}$ is constrained in some specified way and has to be estimated. The matching may be by least-squares: $Min\|\mathbf{X}_1\mathbf{T} - \mathbf{X}_2\|^2$ or by maximising the inner-product $trace(\mathbf{X}_2'\mathbf{X}_1\mathbf{T})$ or by several other criteria. Typical constraints on $\mathbf{T}$ are that $\mathbf{T} = \mathbf{Q}$ (Orthogonal), $\mathbf{T} = \mathbf{P}$ (Projection), $\mathbf{T} = \mathbf{C}$ (Direction Cosines) but there are other possibilities. Variations include "two-sided Procrustes" $Min\|\mathbf{X}_1\mathbf{T}_1 - \mathbf{X}_2\mathbf{T}_2\|^2$ and "Double Procrustes" $Min\|\mathbf{T}_2\mathbf{X}_1\mathbf{T}_1 - \mathbf{X}_2\|^2$. Then, we may add isotropic scaling $Min\|s\mathbf{X}_1\mathbf{T} - \mathbf{X}_2\|^2$ or anisotropic scaling $Min\|\mathbf{S}\mathbf{X}_1\mathbf{T} - \mathbf{X}_2\|^2$ where $\mathbf{S}$ is an unknown diagonal scaling matrix which may appear in other positions too; alternatively $\mathbf{S}$ may be replaced by known weights, not necessarily diagonal.

Rather than two matrices, we may have Generalised Procrustes Analysis, where K matrices $\mathbf{X}_1,\mathbf{X}_2,\mathbf{X}_3,\ldots,\mathbf{X}_K$ are to be matched simultaneously. This may be regarded as a three-mode problem and has relationships with other three-mode Individual Scaling models and with Generalised Canonical Correlation.

I shall attempt to thread my way through this minefield; Garmt Dijksterhuis will discuss applications.

Professor John Gower graduated in Mathematical Statistics (with distinction) at the University of Manchester. He worked in applied multivariate analysis, particularly on classification problems and graphical methods for exposing structure in data involving observations on many variables. In the course of this work he developed several methods that are now widely used, including contributions to measures of similarity, classification methods, metric multidimensional scaling, Procrustes analysis, the analysis of asymmetry and, more recently, developing a unified theory of biplots.

He gained individual merit promotion in 1970 (equivalent to a personal chair in a university) and in 1984 became head of the Biomathematics Division, which included the Statistics and Computer Departments. Since retirement from Rothamsted in March 1990 at the mandatory age of 60 he has held several visiting appointments, notably in the Department of Data Theory of the University of Leiden (1991-1993) and, at the Universities of Dortmund and Salamanca. In 1994, he joined the Statistics Department of the Open University and in 1997 was awarded the title of Professor.

He has nearly 170 publications, including the first monograph on biplots - Gower, J. C. and Hand, D. J. (1996) *Biplots*, (Monographs on Statistics and Applied Probability, London: Chapman and Hall (277 pages)) and a monograph, with G.B. Dijksterhuis on *Procrustes Problems* 2004, Oxford University Press (247 pages).

Garmt Dijksterhuis (Research institute Agrotechnology and Food Innovations, Wageningen University and Faculty of Economics, University of Groningen): *An application of Generalised Procrustes Analysis as a method to compare data sets collected by different methods*

A group of 207 subjects scored a set of associations to logos using brand personality items. This was done with the same set of 13 logos under the instructions that the logos belong to a particular product category. The exercise was repeated for four different product categories. In addition a set of 20 subjects sorted the logos into a number of groups, under no instruction at all, other than to freely group the logos. A Procrustes matching of the configurations of associations for the four product categories showed similar configurations of logos, so a group average configuration is representative for each of the four configurations. This group average is subsequently matched to the MDS configuration based on the free grouping. The match shows two significantly different configurations. We conjecture that the free grouping task taps a different process than the association scoring task. In the latter the subjects are guided by the meaning of the association items, in the former no interpretation is needed. The free grouping shows a more 'pure' perceptional result than the association task which always includes interpretation of verbal labels.

Garmt Dijksterhuis is a psychologist and methodologist. He studied theoretical and experimental psychology and psychology of perception at the University of Utrecht and wrote his Ph.D. dissertation at the department of Data Theory at the University of Leiden, in the Netherlands.

Garmt has written or co-authored over a hundred publications in sensory and consumer science, statistics and psychology. He is one of the founders of the sensometric society (www.sensometric.org) and is its current chair, a member of the editorial board of the journal Food Quality and Preference and chair of the sensory science branch of the Dutch marketing research association (MOA.nl).

Garmt taught courses in consumer and sensory science and methodology and related topics and has been a guest scientist at several universities and research institutes and an invited lecturer at many occasions. Currently he is employed as a senior scientist at the department Consumer and Market Insight of the research institute Agrotechnology and Food Innovations (Wageningen University and Research Centre), and as an associate professor at the Marketing department of the Faculty of Economics at the University of Groningen.
His main research interests are the psychology of perception and appreciation, and in particular the impact of the emotion-cognition controversy on choice behaviour and on research methodology.

Age Smilde[1], Carina Rubingh[2], Theo Reijmers[3,4], Wies Akkermans[5], Paul Eilers[6], Huub Hoefsloot[1], Suzanne Smit[1], Margriet Hendriks[7], Chris de Koster[8], Hans Aerts[9] ([1]Biosystems Data Analysis, Swammerdam Institute for Life Sciences, University of Amsterdam; [2]Analytical Sciences, TNO Quality of Life; [3]Groningen Bioinformatics Centre, University of Groningen; [4]Analytical Biosciences, Leiden/Amsterdam Centre for Drug Research, Leiden University; [5]Biometris, Wageningen University and Research Centre; [6]Department of Medical Statistics, Leiden University Medical Centre; [7]Metabolomics Centre, Academic Biomedical Centre, University of Utrecht; [8]Mass Spectrometry of Biomacromolecules, Swammerdam Institute for Life Sciences, University of Amsterdam; [9]Biochemistry, Amsterdam Medical Centre): *Proteomics based clinical biomarkers: how to distinguish healthy from diseased?*

Proteomics is a new genomics technique regarding the measurement of proteins in different samples, such as body fluids, tissue, cells, etc. One of the applications of proteomics is in obtaining insight in de development of diseases and of diagnosing diseases and their severity on the protein level. In our study a cohort of healthy persons is used as a control, and these are confronted with patients with Gaucher's disease. Of these two groups blood samples are available. These are measured with Surface Enhanced Laser Desorption Ionization Mass Spectrometry (SELDI-MS); a relatively new way of performing a proteomics measurement. Hence, the problem comes down to discriminating control versus diseased persons on the basis of their SELDI-MS spectra. These SELDI-MS spectra, however, generate an abundance of data: very many variables are measured for a single sample. This poses challenges to the subsequent data analysis. These challenges are: i) how to avoid overfitting, ii) which discrimination method to use, iii) how to perform variable selection, iv) how to assess the quality of the model and discrimination rule.

To answer some of the questions mentioned above we organized a 'shoot-out': every participant used his/her own favorite method on the same data set. A protocol was developed regarding the setup of the calculations (e.g. how to do the validation) in order to make the final results comparable. The methods used include: Nearest Shrunken Centroids, Principal Components Discriminant Analysis, Principal Discriminant Variates, LogitBoost, Penalized Logistic Regression and Support Vector Machines. All these methods were used and evaluated according to the previously developed protocol.

In a series of presentations, the results of this 'shoot-out' will be presented. First, the background of Gaucher's disease and of SELDI-MS will be shortly sketched, followed by the setup of the comparison. Then, in short presentations, each team member will present his/her method and the result. The series will be closed by an overall presentation of the results. Differences and agreements will be discussed.

Michael Greenacre (Departament d'Economia i Empresa, Universitat Pompeu Fabra, Barcelona): ***Tying up the loose ends of (simple) correspondence analysis***

Although correspondence analysis is now widely available in computer software packages and applied in a variety of contexts, notably the social and environmental sciences, there are still some misconceptions about this method as well as unresolved issues which remain controversial to this day. In this seminar we hope to settle several of these matters, namely (i) the way CA measures variance in a two-way table, (ii) the influence, or rather lack of influence, of outliers in CA maps, (iii) the issue of the scaling of maps and their interpretation, and (iv) whether or not to rotate the CA solution. Two examples are used as illustrations of the theory, one from linguistics and the other from marine biology.

Michael Greenacre is Professor of Statistics at the Universitat Pompeu Fabra, Barcelona. His main research interests are in multivariate data analysis in the social and environmental sciences, especially the analysis of categorical data. He has published two books on correspondence analysis and co-edited three volumes on the analysis and visualization of categorical data. Apart from his university teaching he has taught short courses internationally, on correspondence analysis in the social sciences and multivariate analysis for environmental biologists.

Registration for the VOC Fall Meeting:

Attendance is free and open to anyone interested, but registration is mandatory (via email to Marieke Timmerman, m.e.timmerman@rug.nl, before Thursday November 10). The lunch is to be paid cash at the meeting. When registering, please indicate whether you would like to join lunch.

Boekbespreking

Analyzing Categorical Data. Jeffrey S. Simonoff. Springer (2003).

The goal of this book is, as the writer states in the Preface, to present categorical data analysis based on a strong regression foundation. This explains why (after a minimal Introduction) the first two chapters present gaussian model building and model criticism in some detail. The next chapter introduces categorical data and their distributions (binomial, Poisson, negative binomial, beta binomial) in situations without covariates. Then follows a long chapter on regression models, parametric and non-parametric, for count data. A lot of attention is paid to overdispersion, which is a good thing, because overdisperison is ubiquitous. Two-way tables, with and without structure (like ordered categories and symmetry) are discussed in the next two chapters, followed by one on multidimensional tables. The final two chapters are about binary data and about multiple category data.

This is a practical book. Many interesting data sets are presented and the analysis is concerned with realistic questions. Theory of the generalized linear model (GLM), the central model in this book, is presented in handsome portions, specialized to the specific type of data in each chapter. All data sets (over 80 of them) can be obtained at a website (http://pages.stern.nyu.edu/~jsimonof/AnalCatData). There you will also find a large S+/R script that enables you to repeat the analyses in the book on your own computer. I often find it very illuminating to walk through an analysis step by step and see that you obtain the same results as published in a book or paper, especially when I plan to use a new type of model for my own data.

Personally I'm very charmed by the ample attention given to detection and modelling overdispersion (and underdispersion). In real life counts seldom follow a Poisson (or binomial) distribution, because of (latent) clustering or unmeasured covariates. It can do little harm for the estimation of expected values, but confidence intervals based on Poisson (binomial) assumption can be far too optimistic. The data examples are analysed in detail and realistic modelling alternatives are presented. Surprisingly, from an author who wrote a book on smoothing, semi-parametric methods get very little attention. This is not the book for learning about generalized additive models and related methods. The book has over 200 exercises, a mix of theoretical questions and proposals to analyse additional data sets. Solutions are not given, but according to the web site, they are available for instructors, on request. In short, if you want an easy going book introduction to modern parametric modelling of categorical data, you will find this book interesting and useful.

Paul Eilers

Agenda

11 - 13 January 2006. Lima, Peru. Fifth International Symposium on Business and Industrial Statistics (ISBIS5). http://kitchen.stat.vt.edu/isbis5/

13 - 14 January 2006. Gainesville, Florida, USA. University of Florida Eighth Annual Winter Workshop on Frontiers of Theoretical Statistics. http://www.stat.ufl.edu/symposium/2006/theory/index.html

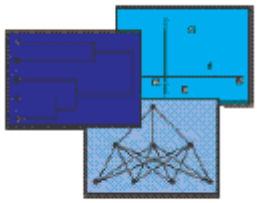
16 - 18 January 2006. Honolulu, Hawaii. 5th Annual Hawaii International Conference on Statistics,

Mathematics and related Fields. http://www.hicstatistics.org/

8 - 10 March 2006. Berlin, Germany. 30th Annual Conference of the German Classification Society. http://www.wiwiss.fu-berlin.de/lenz/gfkl2006/

GfKl 2006

30th Annual Conference of the German Classification Society (GfKl)



Advances in Data Analysis

March 8 - 10, 2006

Free University of Berlin

30 April - 2 May 2006. Manhattan, Kansas, USA. 18th Annual Kansas State University Conference on Applied Statistics in Agriculture. http://www.k-state.edu/stats/agstat.conference/

10 - 13 May 2006. Piscataway, New Jersey, USA. 2006 Annual Meeting of the Classification Society of North America. http://www.classification-society.org/csna/csna06.html

28 - 31 May 2006. London, Ontario, Canada. 34th Annual Meeting of the Statistical Society of Canada. http://www.ssc.ca/2006/index_e.html

28 May - 1 June 2006. Veldhoven, the Netherlands. Fourth International Chemometrics Research Meeting. http://www.icrm.info/

ICRM 2006

4th INTERNATIONAL CHEMOMETRICS RESEARCH MEETING

May 28th - June 1st, 2006, Veldhoven, the Netherlands

The Dutch Chemometric Society invites you to the 4th International Chemometrics Research Meeting, held May 28th - June 1st, 2006 in Veldhoven, the Netherlands. This meeting is organized under the auspices of the Royal Netherlands Chemical Society. The International Chemometrics Research Meeting aims at bringing together researchers active in the field of chemometrics.

Following the successful earlier meetings in 1994, 1998, and 2002 the format of the conference will be such that lectures reflect the current state-of-the-art in chemometrics and will be a starting point for extended discussions and exchanges of views.

29 - 31 May 2006. Limassol, Cyprus. International Conference on Statistical Models for Biomedical and Technical Systems. http://www.ucy.ac.cy/biostat2006/

5 - 9 June 2006. Smolenice Castle, Slovakia. 5th International Conference on Probability and Statistics, PROBASTAT 2006. http://aiolos.um.savba.sk/~viktor/probastat.html

7 - 9 June 2006. Knoxville, Tennessee, USA. Joint Research Conference 2006 on Statistics in Quality, Industry, and Technology (JRC 2006). http://web.utk.edu/~leon/JRC2006/

14 - 17 June 2006. Montreal, Canada. 71st Annual Meeting of the Psychometric Society (IMPS2006). http://www.psychometrika.org/meeting/2006/index.html

14 - 17 June 2006. Storrs, Connecticut, USA. ICSA 2006 Applied Statistics Symposium. http://www.icsa.org/

12 - 14 July 2006. Colchester, UK. International Conference: Methodology of Longitudinal Surveys (MOLS). http://www.iser.essex.ac.uk/ulsc/mols2006/

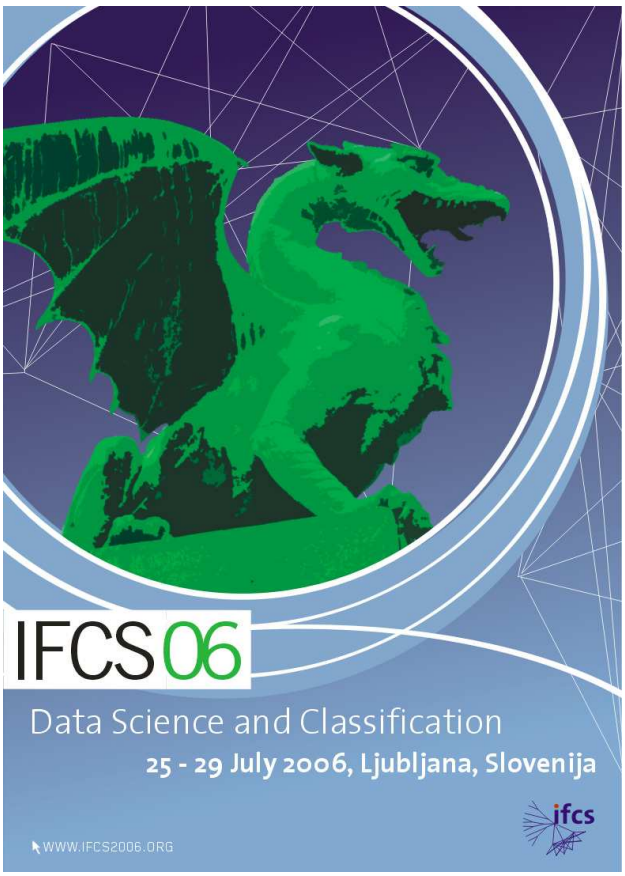
13 - 17 July 2006. Istanbul, Turkey. The 2006 Meeting of the Society for Social Choice and Welfare. http://scw2006.bilgi.edu.tr/

16 - 21 July 2006. Montréal, Québec, Canada. XXIII International Biometric Conference. http://www.ibc2006.org/

17 - 21 July 2006. Paris, France. 31st Conference on Stochastic Processes and their Applications. http://www.proba.jussieu.fr/pageperso/spa06/

24 - 28 July 2006. Torun, Poland. XXVI European Meeting of Statisticians. http://www.ems2006.umk.pl/

25 - 29 July 2006. Ljubljana, Slovenia. IFCS 2006 Conference: Data Science and Classification. http://vlado.fmf.uni-lj.si/info/ifcs06/



2 - 4 August 2006. Ås, Norway. 8th Sensometrics Meeting: Imagine the senses. http://www.sensometric.org/pages/meet.htm

6 - 10 August 2006. Seattle, Washington, USA. 2006 Joint Statistical Meetings. http://www.amstat.org/meetings/jsm/2006/

28 August - 1 September, 2006. Rome, Italy. Compstat 2006. http://w3.uniroma1.it/compstat2006/

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Routebeschrijving

http://www.tno.nl/kwaliteit_van_leven/wie_we_zijn/contact/locatie_zeist/

TNO | Knowledge for business

Utrechtseweg 48
Zeist

BY PUBLIC TRANSPORT

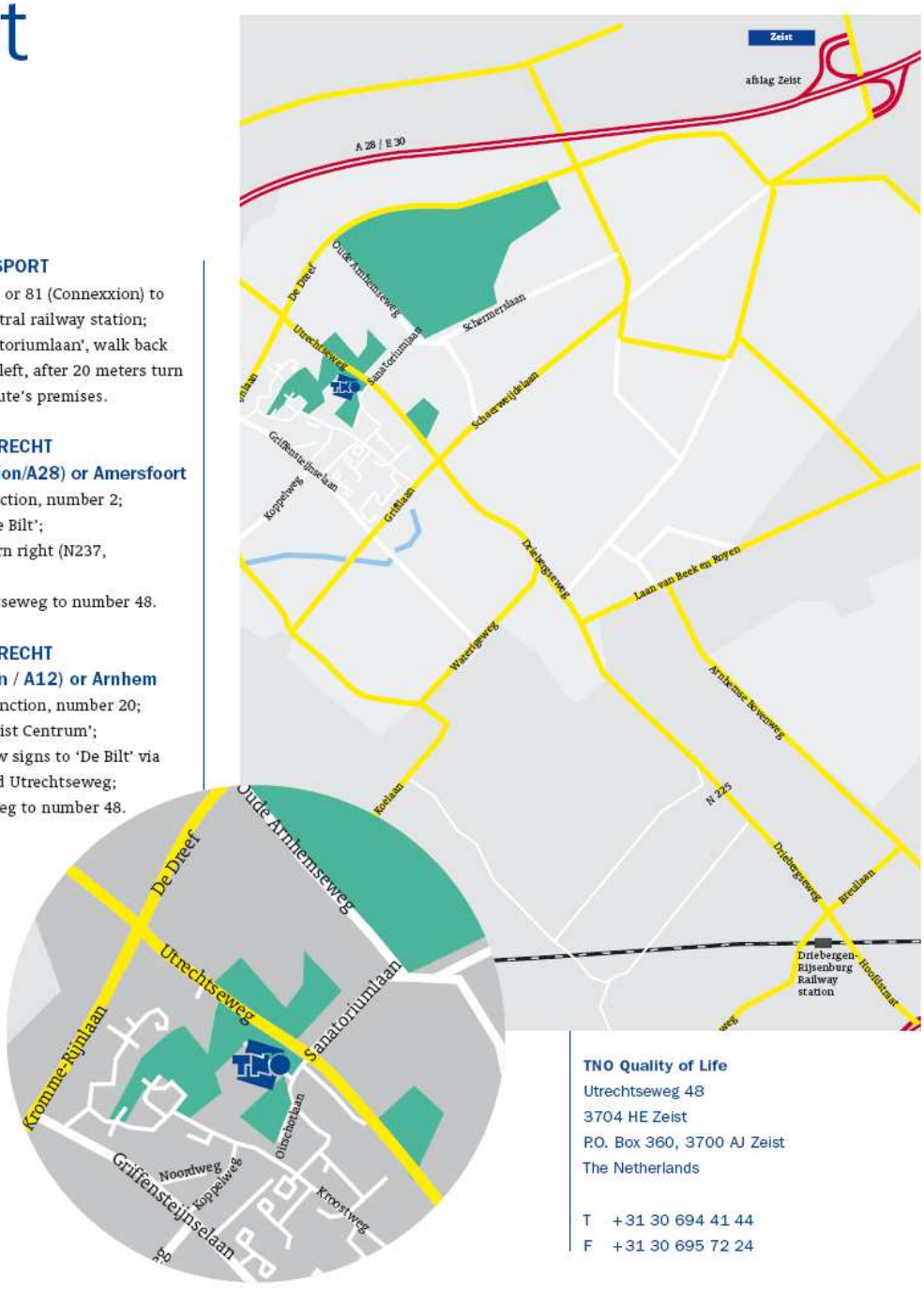
Take bus number 50 or 81 (Connexxion) to Zeist at Utrecht Central railway station; Get out at the 'Sanatoriumlaan', walk back 30 meters and turn left, after 20 meters turn right into the Institute's premises.

BY CAR FROM UTRECHT (Rijnsweerd junction/A28) or Amersfoort

- Take De Uithof junction, number 2;
- Follow signs to 'De Bilt';
- At traffic lights turn right (N237, Utrechtseweg);
- Follow the Utrechtseweg to number 48.

BY CAR FROM UTRECHT (Lunetten junction / A12) or Arnhem

- Take Driebergen junction, number 20;
- Follow signs to 'Zeist Centrum';
- In the center follow signs to 'De Bilt' via de Dorpsstraat and Utrechtseweg;
- Follow Utrechtseweg to number 48.



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