

Section headings

1 Of maps and monkeys: an introduction to the maximum entropy method

G. J. Daniell

1.1	Introduction	1
1.2	The general philosophy of data processing	2
1.3	Data processing strategies	3
1.3.1	A: The case $N < K$: inconsistent data and experimental errors	3
1.3.2	B: The case $N > K$: insufficient data and inverse theory	6
1.3.3	C: The case $N = K$ and unstable problems	8
1.3.4	D: The case $N = \infty$	8
1.4	The Bayesian approach to the $N > K$ case: maximum entropy	9
1.5	Maximum entropy in practice	11
1.6	Understanding maximum entropy solutions	11
1.7	An example	13
1.8	Return to the general philosophy of data processing	17

2 Fundamentals of MaxEnt in data analysis

J. Skilling

2.1	Introduction	19
2.2	Probability calculus	20
2.3	Image reconstruction	24
2.4	The probability of an image	26
2.5	The quantitative assessment of theories	31
2.6	Deconvolution of Poisson data	33
2.7	Conclusions	39

3 Maximum entropy and nuclear magnetic resonance

P. J. Hore	
3.1 Introduction	41
3.2 Nuclear magnetic resonance	41
3.3 Conventional data processing	43
3.4 Maximum entropy	45
3.5 Problems	48
3.5.1 Sensitivity	48
3.5.2 Resolution	50
3.5.3 Truncation	53
3.5.4 Dispersion lineshapes	56
3.6 Examples	58
3.6.1 Rotating frame imaging	60
3.6.2 Chemical shift correlation	63
3.7 A different approach	66
3.8 Conclusions	68

4 Enhanced information recovery in spectroscopy using the maximum entropy method

S. Davies, K. J. Packer, A. Baruya and A. I. Grant

4.1 Introduction	73
4.2 Background	74
4.3 The maximum entropy method (MaxEnt)	76
4.4 Applications	79
4.4.1 Raman spectroscopy	80
4.4.2 Fourier transform nuclear magnetic resonance spectroscopy (FT-NMR)	89
4.5 The Wright–Belton approach	99
4.5.1 Mathematical outline	99
4.5.2 Results	102
4.6 Conclusions	105

5 Maximum entropy and plasma physics

G. A. Cottrell

5.1 Introduction	109
5.1.1 Overview of controlled thermonuclear fusion	111
5.1.2 Overview of the tokamak	112
5.2 Illustration of the maximum entropy method	114

5.2.1	Measurement of electron density	114
5.2.2	The discrete Abel inversion	116
5.2.3	The maximum entropy method	117
5.2.4	Results of Abel inversion	118
5.3	Spectroscopic deconvolution	122
5.3.1	Zeeman splitting of emission lines in a tokamak	122
5.3.2	Deconvolution of instrumental blurring with MaxEnt	123
5.4	Fourier transform spectroscopy	125
5.4.1	Measurement of electron cyclotron emission from a tokamak plasma	125
5.4.2	The autocorrelation function	126
5.4.3	Autocalibration with MaxEnt	128
5.5	Two-dimensional tomography	130
5.5.1	Neutral beam tomography	130
5.5.2	Solution and autocalibration with MaxEnt	133
5.6	Conclusions	136

6 Macroirreversibility and microreversibility reconciled: the second law

A. J. M. Garrett

6.1	Introduction: the problem	139
6.2	Probability	143
6.3	Probability assignment under linear constraints	148
6.4	Predictive statistical mechanics	153
6.5	Ergodic theory is irrelevant	158
6.6	Conclusions	158
6.A	Appendix: Other views of probability	159
6.B	Appendix: Bayes' theorem; continuous spaces and measure; improper priors	163
6.C	Appendix: Kinetic theory	167

7 Some misconceptions about entropy

S. F. Gull

7.1	Introduction	171
7.2	Entropy in thermodynamics and statistical mechanics	172
7.3	Inference: the ground rules	173
7.3.1	Bayes' theorem	173
7.3.2	Maximum entropy	174
7.3.3	Inference and statistical mechanics	174

7.4	Gibbs versus Boltzmann entropies	175
7.4.1	That awful H -theorem	177
7.4.2	The second law of thermodynamics	177
7.4.3	The theoretical second law	178
7.5	Non-equilibrium phenomena	179
7.5.1	Time asymmetry in physics	179
7.5.2	Brownian motion	180
7.6	Uncertainty versus fluctuations	184
7.7	Conclusion	185

8 The X-ray crystallographic phase problem

G. Bricogne

8.1	Introduction	188
8.2	Overview	189
8.2.1	Preamble	189
8.2.2	The phase problem	190
8.2.3	Atomicity and the random atom model	191
8.2.4	The basic idea	191
8.2.5	The basic shortcoming	192
8.2.6	Consequences	192
8.2.7	The maximum entropy method	192
8.2.8	A tree-directed multisolution strategy	193
8.2.9	Calculation of joint probabilities	193
8.2.10	Maximum entropy extrapolation	194
8.2.11	Calculation of conditional probabilities	194
8.2.12	Likelihood and likelihood ratio	195
8.2.13	Comparison with conventional direct methods	195
8.3	Analytical methods of probability theory	196
8.3.1	Convolution of probability densities	196
8.3.2	Characteristic functions	197
8.3.3	Moment-generating functions	197
8.3.4	Cumulant-generating functions	198
8.3.5	Asymptotic expansions and limit theorems	198
8.3.6	The saddlepoint approximation	200
8.4	The statistical theory of phase determination	201
8.4.1	Vectors of trigonometric structure factor expressions	202
8.4.2	Probability distributions of random atoms and moment-generating functions	202
8.4.3	The joint probability distribution of structure factors	203
8.4.4	Overcoming the limitations of the Edgeworth series	203
8.5	The maximum entropy method	205

8.5.1	The context of information theory	205
8.5.2	Definition and meaning of entropy	205
8.5.3	The maximum entropy criterion	206
8.5.4	The maximum entropy formalism	207
8.5.5	The crystallographic maximum entropy formalism	209
8.6	The saddlepoint method	210
8.6.1	Relation between the maximum entropy method and the saddlepoint method	211
8.7	Summary	212