

Index

- Adjoint method 156–7
 continuous 156
 discrete 156
- Aerofoil 42, 141–2, 149–51, 197–8
 see also *MATLAB* functions, *aerofoilcd.m*
- Aerospace design xv, 179
- Algorithmic differentiation 156, 165
 forward mode 156–7
 reverse mode 156–7
- ANOVA 6
- Automatic differentiation, *see* Algorithmic differentiation
- Auto-regressive 168
- Basis function(s) 45–51, 60, 63–5, 67–9, 75, 157–9,
 162, 164
 cubic 46, 103
 Gaussian 46–7, 49–50, 69, 158, 162
 inverse multiquadric 46
 linear 46
 multiquadric 46, 103
 thin plate spline 46–8, 103
 see also *Kernels*; *MATLAB* functions, *basis.m*
- Bayesian reasoning 34, 84
- Black box 3, 12, 33
- CFD (computational fluid dynamics) xv, xvi, 131,
 141, 167, 197, 198
 Euler xvi, 198
 potential flow xvi
 RANS (Reynolds-averaged Navier-Stokes) xvi
 see also *MATLAB* functions, *aerofoilcd.m*
- Cheap data 167, 169, 172–4
- Chi-squared distribution 97, 100–1
- Choleski factorization, *see* Matrix, Choleski factorization of
- Co-Kriging 167–7, 182, 195
 cost of 171
 covariance 168–9, 171
 error 172–5
 infill criteria when using 173
 likelihood 169–70
 MATLAB code for 170, 174
 model parameters 169–71, 174–6
 noise in 173
 one-variable demonstration of 173–6
 predictor 172
 regression 173
 see also *MATLAB* functions, *buildcokriging.m*;
 cokrigingpredictor.m; *likelihoodc.m*;
 likelihoodd.m
- Complexity 35, 47, 66, 71, 73
- Complex step approximation 156
- Conceptual design 3, 10
- Conditional likelihood, *see* Likelihood, conditional
- Confidence interval 100
- Confidence limit 98, 100
- Constraint(s) 117–39
 expected improvement with 125–31, 136–9,
 186–92
 function 118, 119, 121–2, 126–8
 Kriging model of 121–3
 level curve 118, 122–3, 130

- Constraint(s) (*Continued*)
MATLAB code for dealing with 129–30, 137–8
probability of improvement with
127–8
satisfaction by construction 117–18
see also MATLAB functions, *constrainedei.m*;
constrainedmultiei.m; Penalty functions
- Convergence
asymptotic 134
criteria 103–4, 123
to an optimum 82, 104
- Correlation 22, 51–4, 59, 64, 91, 94, 127, 143,
158–9, 161, 163, 170, 176
coefficient 37–8, 104
Gaussian 91
matrix 51, 56, 58–9, 68–9, 86, 143, 152, 159–60,
165, 169, 173
- Cost function, *see* Objective function
- Covariance 52, 172
matrix 52, 95, 168–9, 171–2
- Cross-validation
leave-one-out 36
see also Error, cross-validation
- Crowding 181
- Curse of dimensionality xvii, 4, 111
- Dot product 68
- Drag 5, 42, 118, 141, 197–8
see also MATLAB functions, *aerofoiled.m*
- Dual variables 67, 70
- Elementary effect 6–10, 12
- Empirical equations 167
- Error 35–9, 63, 118, 123, 126, 131, 144
computational 4
cross-validation 47
discretization 142, 197–8
experimental 4, 34, 63, 141
function (erf) 88, 90
generalization 47, 49, 54
human 5
modelling *see* prediction
MSE (mean squared) 36, 40, 84, 104, 122, 172
prediction 35–9, 48, 55, 66, 71, 84–5, 91, 93,
101–2, 122, 126, 130–1, 143–8, 152, 172–5,
186
random xvi, 5, 63
re-defined 146
RMSE (root mean squared) 37
subtractive cancellation 155–6
systematic 5
testing 37
truncation 155–6
- Exchange algorithm 28, 177
see also MATLAB functions, *subset.m*
- Expected improvement 89–92, 103, 146–9
constrained, *see* Constraint(s), expected
improvement with
convergence 92, 104, 106
failure of 91–2, 141–2, 144–5
graphical representation of 88
MATLAB code for 90
multi-objective, *see* Multi-objective, expected
improvement
weighted 102
see also MATLAB functions, *constrainedei.m*;
constrainedmultiei.m; *multiei.m* predictor.m
- Expensive
data 167, 169, 171, 173–6
response 3, 13, 77, 118, 121, 123, 168,
171, 195, 201
simulation xv, xvi, 4, 168, 180–1
- Experiment xv
computer xvi, 4–5, 33, 50, 55, 141, 144,
149, 192
physical xvi, 4–5, 33, 63, 141, 144, 149
- Exploitation, *see* Infill criteria, exploitation
- Exploration, *see* Infill criteria, exploration
- ϵ -insensitive loss function 66–7
- ϵ -tube 63, 65–6, 70, 74
- Feature space 68
- Finite differencing 155
- Floating point underflow 127, 148–9
- Full factorial 4, 13, 202
see also MATLAB functions, *fullfactorial.m*
- Gaussian
cumulative distribution function 183
pdf (probability density function) 88–90
process 5, 84, 92, 103–4, 126–7, 168, 182, 186
two-dimensional pdf 182
see also Basis function(s), Gaussian
- Generalization 40, 46–7, 49, 54, 66, 72
see also Error, generalization
- Geometry 104–6, 118, 131, 198, 203
- Geostatistics 75
- Gradient enhanced Kriging 157–65
MATLAB code for 159–61
predictor 161
- Gradient(s) 155–6
- Hessian enhanced Kriging 162–5
- Ill-conditioning, *see* Matrices, ill-conditioned
- Imputation 97, 133–5
- Infeasible designs, *see* Objective function, infeasibility
- Infill criteria 79–106
balanced exploitation/exploration 85–100, 102,
104, 124, 131, 139, 181, 186
conditional lower bound 97–100, 104

- convergence of 103–4
- error based 84–5
- expected improvement, *see* Expected improvement
- exploitation 78–84, 103–4, 192
- exploration 78–9, 84–5, 104, 176
- goal seeking 93–6, 104–6
- hybrid 102
- MATLAB* code for 86–8, 90, 94–6, 98–100, 105
- parallel 101–2
- prediction based 79–84
- probability of improvement, *see* Probability of improvement
- statistical lower bound 86–7
- see also MATLAB* functions, *condlikelihood.m*;
 - constrainedei.m*; *constrainedmultiei.m*; *lb.m*;
 - multiei.m*; *predictor.m*; *regpredictor.m*;
 - reintcondlikelihood.m*; *reintpredictor.m*
- Inner product 68
- Interpolation 39, 46, 50, 142–3, 146
- Jones, Donald R. xii–xiv, 59, 79, 93, 97
- Karush–Kuhn–Tucker conditions 70
- Kernel(s)
 - Gaussian 65
 - homogeneous polynomial 68
 - inhomogeneous polynomial 68
 - Kriging 68
 - linear 68
 - Mercer 68
 - trick 67
 - see also* Basis function(s)
- Krige, Danie G. 50–1
- Krigeage, *see* Kriging
- Kriging
 - blind 76
 - correlation 51
 - interpolation 50
 - MATLAB* code for 56–8, 61–2
 - model parameters 52–9
 - predictor 60
 - regression 143–4
 - variable screening with 53–4
 - variance 55
 - see also MATLAB* functions, *likelihood.m*; *pred.m*;
 - predictor.m*
- Lagrange multipliers 66, 73
- Lagrangian 66, 73
- Latin hypercube 15–23, 30
 - see also MATLAB* functions, *bestlh.m*; *rlh.m*
- Latin square 15
- Learning
 - instance based 34
 - reinforcement 102
 - supervised 34
- Lift 42, 118, 198
- Likelihood 35
 - concentrated ln-likelihood function 55, 170, 172
 - conditional 93–4, 96–9, 101, 105, 149, 151, 152
 - function 55
 - ln-likelihood function 36, 55, 59
 - MATLAB* code for calculating 56–7, 152
 - MATLAB* code for MLE 58
 - MLE (maximum likelihood estimate) 35–6, 40, 54–60, 144, 161, 163, 169, 171–2, 174
 - ratio test 97–100
 - see also MATLAB* functions, *condlikelihood.m*;
 - likelihood.m*; *likelihoodc.m*; *likelihoodd.m*;
 - likelihoodratiotest.m*; *regcondlikelihood.m*;
 - reintcondlikelihood.m*
- Linear model 18, 35, 64
- LU decomposition, *see* Matrix, LU decomposition of
- Machine overflow 119
- Maclaurin series 149
- MAD 157
- Markov property 168–9
- Matheron, G. 50
- MATLAB* functions
 - aerofoilcd.m* 148, 150–1, 197
 - area.m* 199
 - arearatioconstraint.m* 188, 190, 199
 - bendingconstraint.m* 188, 190, 199
 - bending.m* 188, 190, 199
 - bestlh.m* 26, 58
 - branimfailures.m* 134–5
 - branim.m* 58, 62, 196
 - bucklingconstraint.m* 188, 190, 199
 - buildcokriging.m* 174
 - cheaponevar.m* 195
 - chol.m* 56, 152
 - cokrigingpredictor.m* 174
 - condlikelihood.m* 94, 99
 - constrainedei.m* 129, 138
 - constrainedmultiei.m* 186, 188, 190
 - deflectionconstraint.m* 188, 190, 199
 - dome.m* 47–8, 114–15
 - fminbnd.m* 72
 - fminsearch.m* 78
 - fullfactorial.m* 13–14
 - ga.m* 78
 - intersections.m* 105, 203
 - jd.m* 18, 20, 21
 - lb.m* 86
 - liftsurf.w.m* 10
 - likelihoodc.m* 169, 174

MATLAB functions (*Continued*)

likelihood.m 170, 174
 likelihood.m 56, 58
 likelihoodratiotest.m 98, 100
 mmlhs.m 27
 mm.m 19, 23
 mmphi.m 21–3, 26, 29
 mmsort.m 22–3, 27
 multiei.m 186–7
 nested4.m 114–16
 onevar.m 195
 pcolor.m 113
 perturb.m 25–6, 29
 phisort.m 22–3
 polynomial.m 41–3
 predictor.m 99, 129–30, 135,
 186–7
 pred.m 62
 predrbf.m 47–8, 116
 quadprog.m 68, 70
 randorient.m 7–8
 rbf.m 47–8
 regcondlikelihood.m 149, 151
 reglikelihood.m 144, 148–51
 regpredictor.m 144, 151
 reintcondlikelihood.m 151
 reintpredictor.m 146, 148
 rlh.m 17, 27
 screeningplan.m 8
 screeningplot.m 9
 shearconstraint.m 188, 190, 199
 subset.m 28
 svd.m 152
 tileplot.m 113–14
 wing.m 12, 113

Matrix

Cholesky factorization of 42, 47, 56, 58,
 86, 152
 see also *MATLAB* functions, chol.m
 Gram 46, 49
 ill-conditioned 47, 142, 144, 152
 inversion of 56, 171
 LU decomposition of 46, 56, 152
 (non-)positive definite 46, 48, 56, 68
 (non-)singular 56, 60
 partitioned inverse 59, 60, 172
 sampling 7, 12
 SVD (singular value decomposition) of
 152
 see also *MATLAB* functions, svd.m
 Vandermonde 40

Mesh sensitivity 63

Missing at random 132

Missing data xvi, 131–6

MATLAB code for dealing with 134–5

Missingness 132

Morris, M.D. 6–7, 18, 21, 23, 25

Multi-objective(s) 179–92

 expected improvement 184, 186, 199

 GA (genetic algorithm) 181

MATLAB code for 186–90

 optimization 179–81

 probability of improvement 182–4

 probability of improvement centroid 184–6

 surrogate assisted GA 181

see also *MATLAB* functions, constrainedmultiei.m;
 multiei.m; Pareto

Multiple design objectives

see also Multi-objective(s)

Needle(s) in a haystack 34

Nested dimensions plot 114–16

MATLAB code for 114

see also *MATLAB* functions, nested4.m

Niching 181

Noise 5, 34, 141, 152

 in computer experiments 5, 42, 44, 142, 144, 146,
 195, 197

 filtering 141

 over-fitting 35, 40, 49, 141

 in physical experiments 5, 144

 regressing 49

see also Kriging, regression; Regression; SVR

 trends in data with 141–3, 146

 underfitting 141

Nowacki beam 186, 198–200

NSGA-II 181

Objective function (s)

 automated calculation of 132–3

 gradient(s) of 155

see also Algorithmic differentiation; Adjoint
 method

 infeasibility 119, 134, 136

 multiple, *see* Multiple design objectives

 sensitivities, *see* Objective function(s),
 gradient(s)

Ockham's Razor 66

Optimization 78

 complex method for 78

 conjugate gradient 78

 constrained 66, 73, 99, 113, 117–21, 136–9,
 186–92

see also Constraint(s)

 direct 78

 dual variable 68

 GA (genetic algorithm) for 78

 gradient based 78, 119, 155

 Hooke and Jeeves method for 78

 jump-started 133

 managing surrogate based 102–4

- multi-objective 179–81
 - Newton method for 78
 - Pareto 179–81
 - quasi-Newton method for 78
 - simplex method for 78
 - simulated annealing method for 78
 - stalled 79, 144–5, 149
 - see also* *MATLAB* functions, `fminbnd.m`;
`fminsearch.m`; `ga.m`
- Orthogonal array(s) 30
- Overfitting 34–5, 40, 141

- Parallel computing 101
- Parameter estimation 35–7, 40, 45–7, 49, 73–5, 92, 165
 - see also* Likelihood, MLE
- Parameterization 131, 201
- Pareto
 - front 139, 180–2, 184, 186, 190–2, 199, 201–2
 - optimality 179
 - optimization 179–81
 - set 179–84, 186
- Penalty functions 118–26
 - expected improvement with 126
 - external (*also* exterior) 119–22
 - interior 119–20, 122
 - one-pass 121, 126
- Polynomial 35, 40
 - MATLAB* code for 41–2
- Primal variables 67, 73
- Probability of improvement 88–9
 - constrained, *see* Constraint(s), probability of improvement with
 - convergence 89, 104
 - failure of 91
 - graphical representation of 88
 - MATLAB* code for 88
 - multi-objective, *see* Multi-objective(s), probability of improvement
 - see also* *MATLAB* functions, `predictor.m`

- Quadratic 35
 - programming 68–9
 - see also* *MATLAB* functions, `quadprog.m`
 - surrogate 78
 - see also* Polynomial

- Radial basis function(s), *see* Basis function(s)
- Random
 - field 51, 168
 - orientation 7–10, 12
 - variable 51–2, 85, 88, 128
 - vector 51–2

- Regression
 - constant 143–4, 146, 152
 - Kriging 143–5
 - least-squares 36, 40, 49
 - MATLAB* code for 148, 150–1
 - polynomial 79
 - radial basis function 49
 - re-sampling when using 146
 - support vector, *see* SVR
 - see also* *MATLAB* functions, `regcondlikelihood.m`;
`reglikelihood.m`; `regpredictor.m`; Polynomial, Re-interpolation
- Regularization parameter 49
 - see also* Regression, constant
- Reinforcement learning 102
- Re-interpolation 146–51
 - conditional likelihood 149
 - error 146
 - MATLAB* code for 148, 150–1
 - predictor 146
 - see also* *MATLAB* functions, `reintcondlikelihood.m`;
`reintpredictor.m`
- Repeatability 5

- Sacks, J. 50, 84
- Saddle point 67, 73
- Saturation 39
- Scalar product 68
- Screening 5–13, 33, 54
 - MATLAB* code for 7–9
 - see also* *MATLAB* functions, `screeningplan.m`;
`screeningplot.m`
- Search, *see* Optimization
- Slack variables 66, 70–1, 73
- Sobol sequence(s) 30
- Stochastic process 5, 51, 168
- Stopping criteria, *see* Convergence, criteria
- SUMT (Sequential unconstrained minimization technique) 119–20
- Surrogate modelling process xv–xviii, 3, 33, 77, 102
- SVD (singular value decomposition), *see* Matrices, SVD (singular value decomposition) of
- SVM (support vector machine) 63–4
- SVR (support vector regression) 63–75
 - Discontinuity 53, 119
 - MATLAB* code for 69–71, 74
 - ν -SVR 73–5

- Taxonomy 6, 78–9, 103
- Test function
 - Branin 57, 62–3, 161, 196
 - constrained Branin 121–36, 196–7

Test function (*Continued*)

- Dome 114
- multi-fidelity 173
- with noise 142, 197–8
- one-variable 195
- see also* *MATLAB* functions, `branin.m`;
 `braninfailures.m`; `cheaponevar.m`; `dome.m`;
 `onevar.m`
- Tileplot 113
- MATLAB* code for 113
- see also* *MATLAB* functions, `tileplot.m`

Under-fitting 141

Update, *see* Infill criteria

Variable

- interactions 6–7, 11–12, 54
- screening 5–13, 33, 54
- Vibration isolator 104–6, 202–3
- see also* *MATLAB* functions, `intersections.m`
- Visualization 102, 104, 111–16
- see also* *MATLAB* functions, `nested4.m`;
 `screeningplot.m`; `tileplot.m`