

Geir Evensen

# Data Assimilation

The Ensemble Kalman Filter

Second Edition



---

## Contents

<b>List of symbols .....</b>	xvii
<b>1 Introduction .....</b>	1
<b>2 Statistical definitions .....</b>	5
2.1 Probability density function .....	5
2.2 Statistical moments .....	8
2.2.1 Expected value.....	8
2.2.2 Variance .....	8
2.2.3 Covariance .....	9
2.3 Working with samples from a distribution .....	9
2.3.1 Sample mean .....	9
2.3.2 Sample variance.....	10
2.3.3 Sample covariance .....	10
2.4 Statistics of random fields .....	10
2.4.1 Sample mean .....	10
2.4.2 Sample variance.....	10
2.4.3 Sample covariance .....	11
2.4.4 Correlation .....	11
2.5 Bias .....	11
2.6 Central limit theorem .....	12
<b>3 Analysis scheme .....</b>	13
3.1 Scalar case .....	13
3.1.1 State-space formulation .....	13
3.1.2 Bayesian formulation .....	15
3.2 Extension to spatial dimensions .....	16
3.2.1 Basic formulation .....	16
3.2.2 Euler–Lagrange equation .....	17
3.2.3 Representer solution .....	19
3.2.4 Representer matrix .....	20

3.2.5	Error estimate . . . . .	20
3.2.6	Uniqueness of the solution . . . . .	21
3.2.7	Minimization of the penalty function . . . . .	23
3.2.8	Prior and posterior value of the penalty function . . . . .	24
3.3	Discrete form . . . . .	24
<b>4</b>	<b>Sequential data assimilation . . . . .</b>	<b>27</b>
4.1	Linear Dynamics . . . . .	27
4.1.1	Kalman filter for a scalar case . . . . .	28
4.1.2	Kalman filter for a vector state . . . . .	29
4.1.3	Kalman filter with a linear advection equation . . . . .	29
4.2	Nonlinear dynamics . . . . .	32
4.2.1	Extended Kalman filter for the scalar case . . . . .	32
4.2.2	Extended Kalman filter in matrix form . . . . .	33
4.2.3	Example using the extended Kalman filter . . . . .	35
4.2.4	Extended Kalman filter for the mean . . . . .	36
4.2.5	Discussion . . . . .	37
4.3	Ensemble Kalman filter . . . . .	38
4.3.1	Representation of error statistics . . . . .	38
4.3.2	Prediction of error statistics . . . . .	39
4.3.3	Analysis scheme . . . . .	41
4.3.4	Discussion . . . . .	43
4.3.5	Example with a QG model . . . . .	44
<b>5</b>	<b>Variational inverse problems . . . . .</b>	<b>47</b>
5.1	Simple illustration . . . . .	47
5.2	Linear inverse problem . . . . .	50
5.2.1	Model and observations . . . . .	50
5.2.2	Measurement functional . . . . .	51
5.2.3	Comment on the measurement equation . . . . .	51
5.2.4	Statistical hypothesis . . . . .	52
5.2.5	Weak constraint variational formulation . . . . .	52
5.2.6	Extremum of the penalty function . . . . .	53
5.2.7	Euler–Lagrange equations . . . . .	53
5.2.8	Strong constraint approximation . . . . .	55
5.2.9	Solution by representer expansions . . . . .	55
5.3	Representer method with an Ekman model . . . . .	57
5.3.1	Inverse problem . . . . .	57
5.3.2	Variational formulation . . . . .	58
5.3.3	Euler–Lagrange equations . . . . .	59
5.3.4	Representer solution . . . . .	60
5.3.5	Example experiment . . . . .	60
5.3.6	Assimilation of real measurements . . . . .	64
5.4	Comments on the representer method . . . . .	67

<b>6</b>	<b>Nonlinear variational inverse problems . . . . .</b>	71
6.1	Extension to nonlinear dynamics . . . . .	71
6.1.1	Generalized inverse for the Lorenz equations . . . . .	72
6.1.2	Strong constraint assumption . . . . .	73
6.1.3	Solution of the weak constraint problem . . . . .	76
6.1.4	Minimization by the gradient descent method . . . . .	77
6.1.5	Minimization by genetic algorithms . . . . .	78
6.2	Example with the Lorenz equations . . . . .	82
6.2.1	Estimating the model error covariance . . . . .	82
6.2.2	Time correlation of the model error covariance . . . . .	83
6.2.3	Inversion experiments . . . . .	84
6.2.4	Discussion . . . . .	92
<b>7</b>	<b>Probabilistic formulation . . . . .</b>	95
7.1	Joint parameter and state estimation . . . . .	95
7.2	Model equations and measurements . . . . .	96
7.3	Bayesian formulation . . . . .	97
7.3.1	Discrete formulation . . . . .	98
7.3.2	Sequential processing of measurements . . . . .	99
7.4	Summary . . . . .	101
<b>8</b>	<b>Generalized Inverse . . . . .</b>	103
8.1	Generalized inverse formulation . . . . .	103
8.1.1	Prior density for the poorly known parameters . . . . .	103
8.1.2	Prior density for the initial conditions . . . . .	104
8.1.3	Prior density for the boundary conditions . . . . .	104
8.1.4	Prior density for the measurements . . . . .	105
8.1.5	Prior density for the model errors . . . . .	105
8.1.6	Conditional joint density . . . . .	107
8.2	Solution methods for the generalized inverse problem . . . . .	108
8.2.1	Generalized inverse for a scalar model . . . . .	108
8.2.2	Euler–Lagrange equations . . . . .	109
8.2.3	Iteration in $\alpha$ . . . . .	111
8.2.4	Strong constraint problem . . . . .	111
8.3	Parameter estimation in the Ekman flow model . . . . .	113
8.4	Summary . . . . .	117
<b>9</b>	<b>Ensemble methods . . . . .</b>	119
9.1	Introductory remarks . . . . .	119
9.2	Linear ensemble analysis update . . . . .	121
9.3	Ensemble representation of error statistics . . . . .	122
9.4	Ensemble representation for measurements . . . . .	124
9.5	Ensemble Smoother (ES) . . . . .	124
9.6	Ensemble Kalman Smoother (EnKS) . . . . .	126
9.7	Ensemble Kalman Filter (EnKF) . . . . .	129

9.7.1	EnKF with linear noise free model . . . . .	129
9.7.2	EnKS using EnKF as a prior . . . . .	130
9.8	Example with the Lorenz equations . . . . .	131
9.8.1	Description of experiments . . . . .	131
9.8.2	Assimilation Experiment . . . . .	132
9.9	Discussion . . . . .	137
<b>10</b>	<b>Statistical optimization . . . . .</b>	<b>139</b>
10.1	Definition of the minimization problem . . . . .	139
10.1.1	Parameters . . . . .	140
10.1.2	Model . . . . .	140
10.1.3	Measurements . . . . .	140
10.1.4	Cost function . . . . .	141
10.2	Bayesian formalism . . . . .	141
10.3	Solution by ensemble methods . . . . .	142
10.3.1	Variance minimizing solution . . . . .	144
10.3.2	EnKS solution . . . . .	144
10.4	Examples . . . . .	145
10.5	Discussion . . . . .	154
<b>11</b>	<b>Sampling strategies for the EnKF . . . . .</b>	<b>157</b>
11.1	Introduction . . . . .	157
11.2	Simulation of realizations . . . . .	158
11.2.1	Inverse Fourier transform . . . . .	159
11.2.2	Definition of Fourier spectrum . . . . .	159
11.2.3	Specification of covariance and variance . . . . .	160
11.3	Simulating correlated fields . . . . .	162
11.4	Improved sampling scheme . . . . .	163
11.4.1	Theoretical foundation . . . . .	164
11.4.2	Improved sampling algorithm . . . . .	165
11.4.3	Properties of the improved sampling . . . . .	166
11.5	Model and measurement noise . . . . .	168
11.6	Generation of a random orthogonal matrix . . . . .	169
11.7	Experiments . . . . .	169
11.7.1	Overview of experiments . . . . .	170
11.7.2	Impact from ensemble size . . . . .	172
11.7.3	Impact of improved sampling for the initial ensemble . .	173
11.7.4	Improved sampling of measurement perturbations . .	174
11.7.5	Evolution of ensemble singular spectra . . . . .	175
11.7.6	Summary . . . . .	176

<b>12 Model errors . . . . .</b>	177
12.1 Simulation of model errors . . . . .	177
12.1.1 Determination of $\rho$ . . . . .	177
12.1.2 Physical model . . . . .	178
12.1.3 Variance growth due to the stochastic forcing . . . . .	178
12.1.4 Updating model noise using measurements . . . . .	182
12.2 Scalar model . . . . .	182
12.3 Variational inverse problem . . . . .	183
12.3.1 Prior statistics . . . . .	183
12.3.2 Penalty function . . . . .	184
12.3.3 Euler–Lagrange equations . . . . .	184
12.3.4 Iteration of parameter . . . . .	185
12.3.5 Solution by representer expansions . . . . .	185
12.3.6 Variance growth due to model errors . . . . .	186
12.4 Formulation as a stochastic model . . . . .	187
12.5 Examples . . . . .	187
12.5.1 Case A0 . . . . .	188
12.5.2 Case A1 . . . . .	191
12.5.3 Case B . . . . .	191
12.5.4 Case C . . . . .	194
12.5.5 Discussion . . . . .	195
<b>13 Square Root Analysis schemes . . . . .</b>	197
13.1 Square root algorithm for the EnKF analysis . . . . .	197
13.1.1 Updating the ensemble mean . . . . .	198
13.1.2 Updating the ensemble perturbations . . . . .	198
13.1.3 Properties of the square root scheme . . . . .	200
13.1.4 Final update equation . . . . .	203
13.1.5 Analysis update using a single measurement . . . . .	204
13.1.6 Analysis update using a diagonal $C_{\epsilon\epsilon}$ . . . . .	205
13.2 Experiments . . . . .	205
13.2.1 Overview of experiments . . . . .	206
13.2.2 Impact of the square root analysis algorithm . . . . .	207
<b>14 Rank issues . . . . .</b>	211
14.1 Pseudo inverse of $\mathbf{C}$ . . . . .	211
14.1.1 Pseudo inverse . . . . .	212
14.1.2 Interpretation . . . . .	213
14.1.3 Analysis schemes using the pseudo inverse of $\mathbf{C}$ . . . . .	213
14.1.4 Example . . . . .	214
14.2 Efficient subspace pseudo inversion . . . . .	216
14.2.1 Derivation of the subspace pseudo inverse . . . . .	217
14.2.2 Analysis schemes based on the subspace pseudo inverse . . . . .	220
14.2.3 An interpretation of the subspace pseudo inversion . . . . .	221
14.3 Subspace inversion using a low-rank $C_{\epsilon\epsilon}$ . . . . .	222

14.3.1	Derivation of the pseudo inverse . . . . .	223
14.3.2	Analysis schemes using a low-rank $C_{\epsilon\epsilon}$ . . . . .	224
14.4	Implementation of the analysis schemes . . . . .	225
14.5	Rank issues related to the use of a low-rank $C_{\epsilon\epsilon}$ . . . . .	226
14.6	Experiments with $m \gg N$ . . . . .	228
14.7	Validity of analysis equation . . . . .	233
14.8	Summary . . . . .	235
15	<b>Spurious correlations, localization, and inflation</b> . . . . .	237
15.1	Spurious correlations . . . . .	237
15.2	Inflation . . . . .	239
15.3	An adaptive covariance inflation method . . . . .	240
15.4	Localization . . . . .	241
15.5	Adaptive localization methods . . . . .	242
15.6	A localization and inflation example . . . . .	243
16	<b>An ocean prediction system</b> . . . . .	255
16.1	Introduction . . . . .	255
16.2	System configuration and EnKF implementation . . . . .	256
16.3	Nested regional models . . . . .	259
16.4	Summary . . . . .	260
17	<b>Estimation in an oil reservoir simulator</b> . . . . .	263
17.1	Introduction . . . . .	263
17.2	Experiment . . . . .	265
17.2.1	Parameterization . . . . .	266
17.2.2	State vector . . . . .	267
17.3	Results . . . . .	269
17.4	Summary . . . . .	272
A	<b>Other EnKF issues</b> . . . . .	273
A.1	Nonlinear measurements in the EnKF . . . . .	273
A.2	Assimilation of non-synoptic measurements . . . . .	275
A.3	Time difference data . . . . .	276
A.4	Ensemble Optimal Interpolation (EnOI) . . . . .	277
B	<b>Crononogical listing of EnKF publications</b> . . . . .	279
B.1	Applications of the EnKF . . . . .	279
B.2	Other ensemble based filters . . . . .	290
B.3	Ensemble smoothers . . . . .	290
B.4	Ensemble methods for parameter estimation . . . . .	291
B.5	Nonlinear filters and smoothers . . . . .	291
<b>References</b>	. . . . .	293
<b>Index</b>	. . . . .	305