

# Contents

List of figures	ix
List of algorithms	xi
Notation	xiii
Preface	xv
<b>I Basic methods and algorithms for data assimilation</b>	<b>1</b>
<b>1 Introduction to data assimilation and inverse problems</b>	<b>3</b>
1.1 Introduction . . . . .	3
1.2 Uncertainty quantification and related concepts . . . . .	4
1.3 Basic concepts for inverse problems: Well- and ill-posedness . . . . .	6
1.4 Examples of direct and inverse problems . . . . .	7
1.5 DA methods . . . . .	11
1.6 Some practical aspects of DA and inverse problems . . . . .	22
1.7 To go further: Additional comments and references . . . . .	23
<b>2 Optimal control and variational data assimilation</b>	<b>25</b>
2.1 Introduction . . . . .	25
2.2 The calculus of variations . . . . .	26
2.3 Adjoint methods . . . . .	33
2.4 Variational DA . . . . .	50
2.5 Numerical examples . . . . .	67
<b>3 Statistical estimation and sequential data assimilation</b>	<b>71</b>
3.1 Introduction . . . . .	71
3.2 Statistical estimation theory . . . . .	75
3.3 Examples of Bayesian estimation . . . . .	83
3.4 Sequential DA and Kalman filters . . . . .	90
3.5 Implementation of the KF . . . . .	96
3.6 Nonlinearities and extensions of the KF . . . . .	99
3.7 Particle filters for geophysical applications . . . . .	100
3.8 Examples . . . . .	103

<b>II</b>	<b>Advanced methods and algorithms for data assimilation</b>	<b>119</b>
<b>4</b>	<b>Nudging methods</b>	<b>121</b>
4.1	Nudging . . . . .	122
4.2	Back-and-forth nudging . . . . .	126
<b>5</b>	<b>Reduced methods</b>	<b>133</b>
5.1	Overview of reduction methods . . . . .	133
5.2	Model reduction . . . . .	139
5.3	Filtering algorithm reduction . . . . .	142
5.4	Reduced methods for variational assimilation . . . . .	146
<b>6</b>	<b>The ensemble Kalman filter</b>	<b>153</b>
6.1	The reduced-rank square root filter . . . . .	154
6.2	The EnKF: Principle and classification . . . . .	156
6.3	The stochastic EnKF . . . . .	157
6.4	The deterministic EnKF . . . . .	162
6.5	Localization and inflation . . . . .	167
6.6	Numerical illustrations with the Lorenz-95 model . . . . .	172
6.7	Other important flavors of the EnKF . . . . .	174
6.8	The ensemble Kalman smoother . . . . .	189
6.9	A widespread and popular DA method . . . . .	193
<b>7</b>	<b>Ensemble variational methods</b>	<b>195</b>
7.1	The hybrid methods . . . . .	197
7.2	EDA . . . . .	202
7.3	4DEnVar . . . . .	203
7.4	The IEnKS . . . . .	207
<b>III</b>	<b>Applications and case studies</b>	<b>217</b>
<b>8</b>	<b>Applications in environmental sciences</b>	<b>219</b>
8.1	Physical oceanography . . . . .	219
8.2	Glaciology . . . . .	221
8.3	Fluid–biology coupling; marine biology . . . . .	226
8.4	Land surface modeling and agroecology . . . . .	229
8.5	Natural hazards . . . . .	231
<b>9</b>	<b>Applications in atmospheric sciences</b>	<b>237</b>
9.1	Numerical weather prediction . . . . .	237
9.2	Atmospheric constituents . . . . .	240
<b>10</b>	<b>Applications in geosciences</b>	<b>245</b>
10.1	Seismology and exploration geophysics . . . . .	245
10.2	Geomagnetism . . . . .	248
10.3	Geodynamics . . . . .	248
<b>11</b>	<b>Applications in medicine, biology, chemistry, and physical sciences</b>	<b>251</b>
11.1	Medicine . . . . .	251
11.2	Systems biology . . . . .	253

---

11.3	Fluid dynamics . . . . .	254
11.4	Imaging and acoustics . . . . .	257
11.5	Mechanics . . . . .	259
11.6	Chemistry and chemical processes . . . . .	261
<b>12</b>	<b>Applications in human and social sciences</b>	<b>263</b>
12.1	Economics and finance . . . . .	263
12.2	Traffic control . . . . .	264
12.3	Urban planning . . . . .	265
	<b>Bibliography</b>	<b>267</b>
	<b>Index</b>	<b>303</b>



# List of figures

1	The big picture for DA methods and algorithms. . . . .	xvii
1.1	Ingredients of an inverse problem . . . . .	4
1.2	The deductive spiral of system science . . . . .	5
1.3	UQ for a random quantity . . . . .	5
1.4	Duffing's equation with small initial perturbations. . . . .	10
1.5	DA methods . . . . .	12
1.6	Sequential assimilation. . . . .	16
1.7	Sequential assimilation scheme for the KF. . . . .	17
2.1	A variety of local extrema . . . . .	26
2.2	Counterexamples for local extrema in $\mathbb{R}^2$ . . . . .	27
2.3	Curve $\eta(x)$ and admissible functions $y + \epsilon\eta(x)$ . . . . .	29
2.4	3D- and 4D-Var . . . . .	60
2.5	Simulation of the chaotic Lorenz-63 system of three equations. . . .	67
2.6	Assimilation of the Lorenz-63 equations by standard 4D-Var . . . . .	69
2.7	Assimilation of the Lorenz-63 equations by incremental 4D-Var . . . .	69
3.1	Scalar Gaussian distribution example of Bayes' law . . . . .	85
3.2	Scalar Gaussian distribution example of Bayes' law . . . . .	86
3.3	A Gaussian product example for forecasting temperature . . . . .	87
3.4	Bayesian estimation of noisy pendulum parameter . . . . .	88
3.5	Sequential assimilation trajectory . . . . .	91
3.6	Sequential assimilation scheme for the KF. . . . .	92
3.7	KF loop. . . . .	96
3.8	Analysis of the particle filter. . . . .	101
3.9	Particle filter applied to Lorenz model . . . . .	102
3.10	Estimating a constant by a KF: $R = 0.01$ . . . . .	109
3.11	Estimating a constant by a KF: $R = 1$ . . . . .	110
3.12	Estimating a constant by a KF: $R = 0.0001$ . . . . .	111
3.13	Estimating a constant by a KF: convergence . . . . .	112
3.14	Position estimation for constant-velocity dynamics. . . . .	115
3.15	Position estimation errors for constant-velocity dynamics. . . . .	116
3.16	Velocity estimation results for constant-velocity dynamics. . . . .	116
3.17	Extrapolation of position for constant-velocity dynamics. . . . .	117
3.18	Convergence of the KF . . . . .	117
4.1	Schematic representation of the nudging method. . . . .	121
4.2	Illustration of various nudging methods . . . . .	127

4.3	Schematic representation of the BFN method. . . . .	128
5.1	Example of dimension reduction. . . . .	134
5.2	Incremental 4D-Var with reduced models. . . . .	149
5.3	Hybridization of the reduced 4D-Var and SEEK filter/smoothen algorithms. . . . .	151
6.1	Synthetic DA experiments with the anharmonic oscillator. . . . .	162
6.2	Schematic representation of the local update for EnKF . . . . .	168
6.3	Plot of the Gaspari–Cohn fifth-order piecewise rational function . .	169
6.4	Covariance localization . . . . .	170
6.5	Trajectory of a state of the Lorenz-95 model. . . . .	173
6.6	Average analysis RMSE for a deterministic EnKF (ETKF)—localization and inflation . . . . .	175
6.7	Average analysis RMSE of a deterministic EnKF (ETKF)—nonlinear observation . . . . .	181
6.8	Average analysis RMSE for a deterministic EnKF (ETKF)—optimal inflation . . . . .	188
6.9	Average analysis RMSE for a deterministic EnKF (ETKF)—ensemble size . . . . .	188
6.10	Schematic of the EnKS . . . . .	191
6.11	Analysis RMSE of the EnKS . . . . .	193
7.1	Synthetic DA experiments with the Lorenz-95 model . . . . .	196
7.2	Cycling of the SDA IEnKS . . . . .	210
7.3	Synthetic DA experiments with the Lorenz-95 model with IEnKS .	212
7.4	Chaining of the MDA IEnKS cycles. . . . .	214
7.5	Synthetic DA experiments with the Lorenz-95 model—comparison of localization strategies . . . . .	216
8.1	Illustration of DA in operational oceanography . . . . .	222
8.2	Illustration of DA for sea level rise and glaciology . . . . .	225
8.3	Illustration of DA in fish population ecology . . . . .	228
8.4	Illustration of DA in agronomy and crop modeling . . . . .	232
8.5	Illustration of DA for wildfire modeling and forecasting . . . . .	235
9.1	Anomaly correlation coefficient of the 500 hPa height forecasts for the extratropical northern hemisphere and southern hemisphere . .	239
9.2	Typical error growth following the empirical model (9.1). . . . .	239
9.3	Cesium-137 radioactive plume at ground level (activity concentrations in becquerel per cubic meter) emitted from the FDNPP in March 2011 . . . . .	242
9.4	Cesium-137 source term as inferred by inverse modeling . . . . .	243
9.5	Deposited cesium-137 (in kilobecquerel per square meter) measured (a) and hindcast (b) near the FDNPP . . . . .	243
11.1	Assimilation of medical data for the cardiovascular system . . . . .	252
11.2	Design cycle for aerodynamic shape optimization . . . . .	256
11.3	Physical setup for a geoacoustics inverse problem. . . . .	258
11.4	Kirchhoff imaging algorithm results for source localization . . . . .	260
11.5	A simple mechanical system . . . . .	261

# List of algorithms

1.1	Iterative 3D-Var (in its simplest form). . . . .	20
1.2	4D-Var in its basic form . . . . .	21
2.1	Iterative 3D-Var algorithm. . . . .	58
2.2	4D-Var . . . . .	61
4.1	BFN algorithm. . . . .	129
5.1	SEEK filter equations. . . . .	144
5.2	Incremental 4D-Var. . . . .	148
6.1	Algorithm of the EKF . . . . .	154
6.2	Algorithm for RRSQRT . . . . .	156
6.3	Algorithm for the (stochastic) EnKF . . . . .	160
6.4	Pseudocode for a complete cycle of the ETKF . . . . .	166
6.5	Pseudocode for a complete cycle of the MLEF, as a variant in ensemble subspace . . . . .	180
6.6	Pseudocode for a complete cycle of the EnKS in ensemble subspace. . . . .	192
7.1	A cycle of the lag-L/shift-S/SDA/bundle/Gauss-Newton IEnKS. . . . .	211
7.2	A cycle of the lag-L/shift-S/MDA/bundle/Gauss-Newton IEnKS. . . . .	214





# Notation

$\mathbb{R}^n$	state space
$\mathbb{R}^p$	observation space
$\mathbb{R}^m$	ensemble space, $i = 1, \dots, m$
$t_k$	time, $k = 1, \dots, K$
$\mathbf{I}$	identity matrix: $\mathbf{I}_n, \mathbf{I}_m, \mathbf{I}_p$
$\mathbf{x}$	vector
$\mathbf{x}^t$	true state vector
$\mathbf{x}^a$	analysis vector
$\mathbf{x}^b$	background vector
$\mathbf{x}^f$	forecast vector
$\mathbf{y}^o$	observation vector
$\epsilon^a$	analysis error
$\epsilon^b$	background error
$\epsilon^f$	forecast error
$\epsilon^o$	observation error
$\epsilon^q$	model error
$\mathbf{M}_k$	linear model operator: $\mathbf{x}_{k+1} = \mathbf{M}_{k+1} \mathbf{x}_k$ , with $\mathbf{M}_{k+1} = \mathbf{M}_{k+1:k}$ model from time step $k$ to time step $k+1$ ; $\mathcal{M}$ nonlinear model operator
$\mathbf{X}_a$	analysis perturbation matrix
$\mathbf{X}_f$	forecast perturbation matrix
$\mathbf{P}^f$	forecast error covariance matrix
$\mathbf{P}^a$	analysis error covariance matrix
$\mathbf{K}$	Kalman gain matrix
$\mathbf{B}$	background error covariance matrix
$\mathbf{H}$	linearized observation operator; $\mathcal{H}$ nonlinear observation operator
$\mathbf{Q}$	model error covariance matrix
$\mathbf{R}$	observation error covariance matrix
$\mathbf{d}$	innovation vector
$(j)$	iteration index of a variational assimilation (in parentheses).
$\mathbf{w}$	coefficients in ensemble space (ensemble transform)



# Preface

This book places data assimilation (DA) into the broader context of inverse problems and the theory, methods, and algorithms that are used for their solution. It strives to provide a framework and new insight into the inverse problem nature of DA—the book emphasizes “why” and not just “how.” We cover both statistical and variational approaches to DA (see Figure 1) and give an important place to the latest hybrid methods that combine the two. Since the methods and diagnostics are emphasized, readers will readily be able to apply them to their own, precise field of study. This will be greatly facilitated by numerous examples and diverse applications. The applications are taken from the following fields: geophysics and geophysical flows, environmental acoustics, medical imaging, mechanical and biomedical engineering, urban planning, economics, and finance.

In fact, this book is about *building bridges*—bridges between inverse problems and DA, bridges between variational and statistical approaches, bridges between statistics and inverse problems. These bridges will enable you to cross valleys and moats, thus avoiding the dangers that are most likely/possibly lurking down there. These bridges will allow you to fetch/go and get/retrieve different approaches and better understanding of the vast, and sometimes insular, domains of DA and inverse problems, stochastic and deterministic approaches, and direct and inverse problems. We claim that by assembling these, by reconciling these, we will be better armed to confront and tackle the grand societal challenges of today, broadly defined as “global change” issues—such as climate change, disaster prediction and mitigation, and nondestructive and noninvasive testing and imaging.

The aim of the book is thus to provide a comprehensive guide for advanced undergraduate and early graduate students and for practicing researchers and engineers engaged in (partial) differential equation-based DA, inverse problems, optimization, and optimal control—we will emphasize the close relationships among all of these. The reader will be presented with a statistical approach and a variational approach and will find pointers to all the numerical methods needed for either. Of course, the applications will furnish many case studies.

The book favours a continuous (infinite-dimensional) approach to the underlying inverse problems, and we do not make the distinction between continuous and discrete problems—every continuous problem, after discretization, yields a discrete (finite-dimensional) problem. Moreover, continuous problems admit a far richer and more extensive mathematical theory, and though DA (via the Kalman filter (KF)) is *in fine* a discrete approach, the variational analysis will be performed on the continuous model. Discrete inverse problems (finite dimensional) are very well presented in a number of excellent books, such as those of Lewis et al. [2006], Vogel [2002], and Hansen [2010], the latter of which has a strong emphasis on regularization methods.

Some advanced calculus and tools from linear algebra, real analysis, and numerical analysis are required in the presentation. We introduce and use Hadamard's well-posedness theory to explain and understand both *why things work* and *why they go wrong*. Throughout the book, we observe a maximum of mathematical rigor but with a minimum of formalism. This rigor is extremely important in practice, since it enables us to eliminate possible sources of error in the algorithmic and numerical implementations.

In summary, this is really a PDE-based book on inverse and DA modeling—readers interested in the specific application to meteorology or oceanography should additionally consult other sources, such as Lewis et al. [2006] and Evensen [2009]. Those who require a more mathematical approach to inverse problems are referred to Kirsch [1996] and Kaipio and Somersalo [2005], and for DA to the recent monographs of Law et al. [2015] and Reich and Cotter [2015].

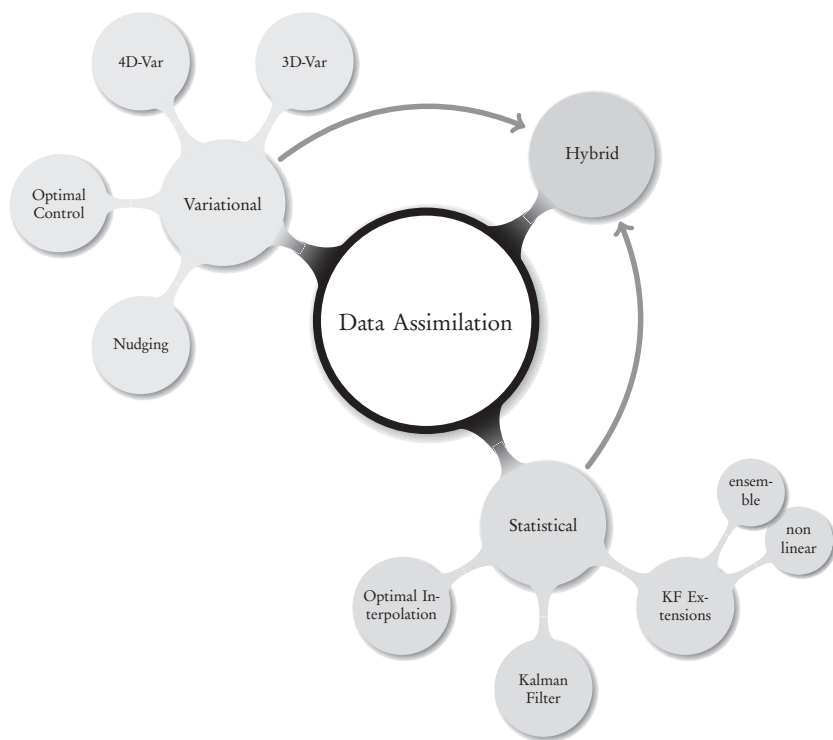
Proposed pathways through the book are as follows (this depends on the level of the reader):

- The “debutant” reader is encouraged to study the first chapter in depth, since it will provide a basic understanding and the means to choose the most appropriate approach (variational or statistical).
- The experienced reader can jump directly to Chapter 2 or Chapter 3 according to the chosen or best-adapted approach.
- All readers are encouraged to initially skim through the examples and applications sections of Part III to be sure of the best match to their type of problem (by seeing what kind of problem is the closest to their own)—these can then be returned to later, after having mastered the basic methods and algorithms of Part I or eventually the advanced ones of Part II.
- For the most recent approaches, the reader or practitioner is referred to Part II and in particular to Chapters 4 and 7.

The authors would like to acknowledge their colleagues and students who accompanied, motivated, and inspired this book. MB thanks Alberto Carrassi, Jean-Matthieu Haussaire, Anthony Fillion, Victor Winiarek, Alban Farchi, and Sammy Metref. MN thanks Elise Arnaud, Arthur Vidard, Eric Blayo, and Claire Lauvernet. MA thanks in particular the CIMPA<sup>1</sup> and the Universidad Simon Bolivar in Caracas, Venezuela (where the idea for this book was born), for their hospitality. We thank the CIRM<sup>2</sup> for allowing us to spend two intensive weeks finalizing (in optimal conditions) the manuscript.

<sup>1</sup>Centre International de Mathématiques Pures et Appliquées, Nice, France.

<sup>2</sup>Centre International de Rencontres Mathématiques, Marseille, France.



**Figure 1.** *The big picture for DA methods and algorithms.*

