Contents

\mathbf{R}	ules		ix			
Preface 2						
Prologue xv						
Mathematical Symbols xi						
1	Inti	oduction	1			
Ι	Ta	ngents and Gradients	13			
2	AF	ramework for Evaluating Functions	15			
	2.1	The Lighthouse Example	16			
	2.2	Three-Part Evaluation Procedures	18			
	2.3	Elemental Differentiability	23			
	2.4	Generalizations and Connections	25			
	2.5	Examples and Exercises	29			
3	Fun	damentals of Forward and Reverse	31			
	3.1	Forward Propagation of Tangents	32			
	3.2	Reverse Propagation of Gradients	37			
	3.3	Cheap Gradient Principle with Examples	44			
	3.4	Approximate Error Analysis	50			
	3.5	Summary and Discussion	52			
	3.6	Examples and Exercises	56			
4	Me	mory Issues and Complexity Bounds	61			
	4.1	Memory Allocation and Overwrites	61			
	4.2	Recording Prevalues on the Tape	64			
	4.3	Selective Saves and Restores	70			
	4.4	A Temporal Complexity Model	73			
	4.5	Complexity of Tangent Propagation	80			
	4.6	Complexity of Gradient Propagation	83			
	4.7	Examples and Exercises	88			

5	Rep	eating and Extending Reverse 92	L
	5.1	Adjoining Iterative Assignments	3
	5.2	Adjoints of Adjoints	5
	5.3	Tangents of Adjoints	3
	5.4	Complexity of Second-Order Adjoints	2
	5.5	Examples and Exercises	5
6	Imp	lementation and Software 10'	7
	6.1	Operator Overloading	0
	6.2	Source Transformation	0
	6.3	AD for Parallel Programs	9
	6.4	Summary and Outlook	8
	6.5	Examples and Exercises	9
II	Ja	acobians and Hessians 143	3
7	Spa	rse Forward and Reverse 14	5
	7.1	Quantifying Structure and Sparsity	7
	7.2	Sparse Derivative Propagation	1
	7.3	Sparse Second Derivatives	4
	7.4	Examples and Exercises	9
8	Exp	loiting Sparsity by Compression 16	1
	8.1	Curtis-Powell-Reid Seeding	4
	8.2	Newsam–Ramsdell Seeding	8
	8.3	Column Compression	1
	8.4	Combined Column and Row Compression	3
	8.5	Second Derivatives, Two-Sided Compression	6
	8.6	Summary	1
	8.7	Examples and Exercises	2
9	Goi	ng beyond Forward and Reverse 18	5
	9.1	Jacobians as Schur Complements	3
	9.2	Accumulation by Edge-Elimination	3
	9.3	Accumulation by Vertex-Elimination	J
	9.4	Face-Elimination on the Line-Graph	4
	9.5	NP-hardness via Ensemble Computation	7
	9.6	Summary and Outlook	9
	9.7	Examples and Exercises	9
10	Jaco	bian and Hessian Accumulation 21.	L
	10.1	Greedy and Other Heuristics	1
	10.2	Local Preaccumulations	U
	10.3	Scarcity and Vector Products	5
	10.4	Hessians and Their Computational Graph	6

10.5 Examples and Exercises	41
11 Observations on Efficiency 24	15
11.1 Ramification of the Rank-One Example	45
11.2 Remarks on Partial Separability	48
11.3 Advice on Problem Preparation	55
11.4 Examples and Exercises 29	57
	71
III Advances and Reversals 25	9
12 Reversal Schedules and Checkpointing 26	31
12.1 Reversal with Recording or Recalculation	62
12.2 Reversal of Call Trees	65
12.3 Reversals of Evolutions by Checkpointing	78
12.4 Parallel Reversal Schedules	95
12.5 Examples and Exercises 29	98
13 Taylor and Tensor Coefficients 29	}9
13.1 Higher-Order Derivative Vectors	00
13.2 Taylor Polynomial Propagation	03
13.3 Multivariate Tensor Evaluation	11
13.4 Higher-Order Gradients and Jacobians	17
13.5 Special Relations in Dynamical Systems	26
13.6 Summary and Outlook	32
13.7 Examples and Exercises 33	33
14 Differentiation without Differentiability 33	35
14.1 Another Look at the Lighthouse Example	37
14.2 Putting the Pieces Together	41
14.3 One-Sided Laurent Expansions	50
14.4 Summary and Conclusion	62
14.5 Examples and Exercises	63
15 Implicit and Iterative Differentiation 36	87
15 1 Besults of the Implicit Function Theorem 3	$\frac{70}{70}$
15.2 Iterations and the Nowton Scenario	$\frac{10}{75}$
15.2 Direct Design tive Decumencary	() 01
15.5 Direct Derivative necurrences	31 00
15.4 Adjoint Recurrences and Their Convergence	30 00
19.9 Second-Urder Adjomts	90 90
15.6 Summary and Outlook	93
15.7 Examples and Exercises	94
Epilogue 39	97

List of Figures

List of Tables	403
Assumptions and Definitions	407
Propositions, Corollaries, and Lemmas	409
Bibliography	411
Index	433

Rules

0	Algorithmic differentiation does not incur truncation errors.	2
1	DIFFERENCE QUOTIENTS MAY SOMETIMES BE USEFUL TOO.	4
2	WHAT'S GOOD FOR FUNCTION VALUES IS GOOD FOR THEIR DERIVATIVES.	20
3	THE JACOBIAN-VECTOR AND JACOBIAN TRANSPOSED VECTOR PRODUCTS CALCULATED IN THE FORWARD AND REVERSE MODE, RESPECTIVELY, CORRESPOND TO THE EXACT VALUES FOR AN EVALUATION PROCEDURE WHOSE ELEMENTALS ARE PERTURBED AT THE LEVEL OF THE MACHINE PRECISION.	51
4	PRODUCTS OF TRANSPOSE-JACOBIANS WITH VECTORS ARE CHEAP, BUT THEIR TRACE IS AS EXPENSIVE AS THE WHOLE JA- COBIAN.	56
5	Adjoining can be performed line by line irrespective of dependencies and aliasing.	69
6	SAVE ONLY THE VALUES OF POWERS OR EXPONENTIALS AND THE ARGUMENTS OF OTHER NONLINEAR ELEMENTALS.	71
7	Additive tasks with bounded complexity on elementals are also bounded on composite functions.	79
8	Operation counts and random access memory require- ments for their gradients are bounded multiples of those for the functions.	88
9	The sequential access memory requirement of the basic reverse mode is proportional to the temporal complex- ity of the function.	88
10	NEVER GO BACK MORE THAN ONCE (AFTER ALL WEIGHT VEC- TORS ARE KNOWN).	92
11	INCREMENTAL ADJOINTS OF LINEAR PROCEDURES ARE REFLEX- IVE IRRESPECTIVE OF ALLOCATION.	98

- 12 DO AS MUCH AS POSSIBLE AT COMPILE-TIME, AS MUCH AS NEC- 139 ESSARY AT RUNTIME.
- 13 Face-elimination allows lower operations counts than 207 edge-elimination, which is in turn cheaper than vertexelimination.

- 14 Do not use greedy heuristics based on the Markowitz 218 degree for computing the Jacobians of final states with respect to initial states in evolutions.
- 15 LOCAL JACOBIANS SHOULD BE PREACCUMULATED IF THEIR 222 GENERIC RANK IS SIGNIFICANTLY SMALLER THAN THE NUMBER OF DERIVATIVE OR ADJOINT COMPONENTS BEING PROPAGATED GLOBALLY.
- 16 The calculation of gradients by nonincremental Reverse makes the corresponding computational graph symmetric, a property that should be exploited and maintained in accumulating Hessians.
- 17 The cheap gradient result does not yield cheap Jaco-247 bians as well.
- 18 Reverse beats forward only when the nonlinear width 255 is much larger than the nonlinear height.
- 19 JOINT REVERSALS SAVE MEMORY, SPLIT REVERSALS SAVE OP- 270 ERATIONS.
- 20 During call tree reversals all taping occurs in a Last- 275 IN-First-Out fashion.
- 21 The relative reversal cost (r) grows like the chain 286 length (l) raised to the reciprocal of the number of checkpoints available (c).
- 22 FORWARD DIFFERENTIATION CAN BE ENCAPSULATED IN TAYLOR 310 ARITHMETIC.
- 23 What works for first derivatives is fit to yield higher 326 derivatives by extension to Taylor Arithmetic.
- 24 WHEN PROGRAM BRANCHES APPLY ON OPEN SUBDOMAINS, AL- 343 GORITHMIC DIFFERENTIATION YIELDS USEFUL DERIVATIVES.
- 25 Functions given by evaluation procedures are almost 349 everywhere real analytic or stably undefined.
- 26 Fixed Point Iterations can and should be adjoined by 389 recording only single steps.