

Evaluating Learning Algorithms

The field of machine learning has matured to the point where many sophisticated learning approaches can be applied to practical applications. Thus it is of critical importance that researchers have the proper tools to evaluate learning approaches and understand the underlying issues.

This book examines various aspects of the evaluation process with an emphasis on classification algorithms. The authors describe several techniques for classifier performance assessment, error estimation and resampling, and obtaining statistical significance, as well as selecting appropriate domains for evaluation. They also present a unified evaluation framework and highlight how different components of evaluation are both significantly interrelated and interdependent. The techniques presented in the book are illustrated using R and WEKA, facilitating better practical insight as well as implementation.

Aimed at researchers in the theory and applications of machine learning, this book offers a solid basis for conducting performance evaluations of algorithms in practical settings.

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Evaluating Learning Algorithms

A Classification Perspective

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This book is dedicated to the memory of my father, Michel Japkowicz (1935–2008), who was my greatest supporter all throughout my studies and career, taking a great interest in any project of mine. He was aware of the fact that this book was being written, encouraged me to write it, and would be the proudest father on earth to see it in print today.

Nathalie

This book is dedicated to the loving memory of my father, Upendra Shah (1948–2006), who was my mentor in life. He taught me the importance of not falling for means but looking for meaning in life. He was also my greatest support through all times, good and bad. His memories are a constant source of inspiration and motivation. Here's to you Dad!

Mohak



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Preface

This book was started at Monash University (Melbourne, Australia) and Laval University (Quebec City, Canada) with the subsequent writing taking place at the University of Ottawa (Ottawa, Canada) and McGill University (Montreal, Canada). The main idea stemmed from the observation that while machine learning as a field is maturing, the importance of evaluation has not received due appreciation from the developers of learning systems. Although almost all studies make a case for the evaluation of the algorithms they present, we find that many (in fact a majority) demonstrate a limited understanding of the issues involved in proper evaluation, despite the best intention of their authors. We concede that optimal choices cannot always be made due to limiting circumstances, and trade-offs are inevitable. However, the methods adopted in many cases do not reflect attention to the details warranted by a proper evaluation approach (of course there are exceptions and we do not mean to generalize this observation).

Our aim here is not to present the readers with yet another recipe for evaluation that can replace the current default approach. Rather, we try to develop an understanding of and appreciation for the different concerns of importance in the practical application and deployment of learning systems. Once these concerns are well understood, the other pieces of the puzzle fall quickly in place since the researcher is not left shooting in the dark. A proper evaluation procedure consists of many components that should all be considered simultaneously so as to correctly address their interdependence and relatedness. We feel that the best (read most easily understood) manner to bring this holistic view of evaluation to the fore is in the classification setting. Nonetheless, most of the observations that we make with regard to the various evaluation components extend just as well to other learning settings and paradigms since the underlying evaluation principles and objectives are essentially the same.

Altogether, this book should be viewed not only as a tool designed to increase our understanding of the evaluation process in a shared manner, but also as a first



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step in the direction of stimulating a community-wide debate on the relevance and importance of the evaluation of learning algorithms.

Incorporating concepts from both machine learning and statistics proved to be a bit more involved than we had first imagined. The main challenge was to integrate the ideas together and present them in a coherent manner. Indeed, sometimes the same terms are used in the two fields to mean different quantities while at other times, the same quantities are referred to by multiple names and notations. We have tried to put some aspects under a unified scheme (of both terminology and notation) but have left others to their more conventional usage, just to make sure that the reader can relate these to other texts. For instance, while we have used α for the confidence parameter in the statistical significance testing, we have also, in some places, used the common notion of p-value to relate to other discussions. Similarly, both P and Pr frequently appear in probabilistic contexts. We have used both these terms, keeping in mind their common use as well as a better readability of the text. To achieve this, we have used Pr when referring to events or probabilities for discrete variables. For other cases, e.g., distributions over continuous variables and priors, we use P or other symbols, as indicated in the text. However, with some exceptions, most notations are used locally and explained in their proper context to avoid confusion.

We have tried to illustrate the various methods and tests presented in the book with the use of the freely available R statistical package and WEKA machine learning toolkit. Our code, however, is in no sense optimal. Our main aim here was to illustrate the concepts in the simplest possible manner so that even the least experienced programmers could apply the code easily in order to immediately utilize the tools presented in the book. We hope to post better optimized code on the book Web page in the near future.

While our names figure on the cover, we cannot claim complete credit for the work presented in this book. This work was made possible thanks to the support of many people. The deficiencies or errors, however, are solely due to us. We would now like to take some space to thank them and acknowledge their support, advice, and understanding.

We would like to thank all our colleagues at the various institutions that hosted us while this book was in progress. They helped us form and develop our ideas on evaluation and stimulate our thoughts on various aspects of the problem, either directly or indirectly. These include: Peter Tischer, Ingrid Zuckerman, and Yuval Marom at Monash; Mario Marchand, Jacques Corbeil, and Francois Laviolette at Laval; Stan Matwin and Marcel Turcotte at the University of Ottawa; Chris Drummond and Peter Turney at the University of Ottawa and the National Research Council of Canada; Tal Arbel, D. Louis Collins, Doina Precup, and Douglas L. Arnold at McGill; the graduate students and postdoctoral Fellows William Klement, Guichong Li, Lisa Gaudette, Alex Kouznetsov, and Shiven Sharma at the University at Ottawa; Heidar Pirzadeh and Sara Shanian at Laval; and Dante De Nigris and Simon Francis at McGill. William, Alex,



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Nathalie would also like to thank her husband, Norrin Ripsman, for sharing his experience with writing and publishing books. His advice on dealing with presses and preparing our material was particularly helpful. On a more personal note, she appreciated him for being there every step of the way, especially at times when the goal seemed so far away. Her daughter Shira also deserves great thanks for being the excellent girl that she is and bearing with her Mum's work all along. The baby-to-be, now lovely little Dafna, showed tremendous patience



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(in both her fetal and infant states), which made it possible for Nathalie to continue working on the project prior to and after her birth. Nathalie's father, Michel Japkowicz, and her mother, Suzanne Japkowicz, have also always been an unconditional source of loving support and understanding. Without their constant interest in her work, she would not be where she is today. Nathalie is also grateful to her in-laws, Toba and Michael Ripsman, for being every bit as supportive as her own parents during the project and beyond.

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Finally, we heartily apologize to friends and colleagues whose names may have been inadvertently missed in our acknowledgments.

Nathalie Japkowicz and Mohak Shah Ottawa and Montreal 2010



Acronyms

2D	two-dimensional	Inf	infimum
3D	three-dimensional	KDD	Knowledge Discovery in
ALL	acute lymphoblastic		Databases (Archive)
	leukemia	KL	Kullback-Leibler
AML	acute myloid leukemia	KS	Kolmogorov-Smirnov
ANOVA	analysis of variance	LOO	leave-one-out
ARI	adjusted Rand index	MAP	maximum a posteriori
AUC	area under the (ROC)	MDS	multidimensional scaling
	curve	MRI	Magnetic Resonance
Bin	Binomial (distribution)		Imaging
BIR	Bayesian information	NEC	normalized expected
	reward		cost
CD	critical difference	NHST	null hypothesis statistical
CDF	cumulative distribution		testing
	function	NPV	negative predictive value
CTBT	Comprehensive Nuclear	PAC	probably approximately
	Test Ban Treaty		correct
CV	cross-validation	PPV	positive predictive value
DEA	data envelopment analysis	PR	precision-recall
DET	Detection Error Trade-Off	RMSE	root-mean-square error
ERM	empirical risk minimization	ROC	receiver operating
exp	exponential		characteristic (curve)
HSD	honestly significant	ROCCH	ROC convex hull
	difference	ROCR	ROC in R package
IBSR	Internet Brain	SAR	metric combining squared
	Segmentation Repository		error (S), accuracy (A),
iff	if and only if		and ROC area (R)
i.i.d.	independently and	SAUC	scored AUC
	identically distributed	SCM	set covering machine



xvi	Acronyms			
SIM	simple and intuitive	SVM	support vector machine	
511.1	measure	UCI	University of California,	
SRM	structural risk		Irvine	
	minimization	VC	Vapnik-Chervonenkis	
SS	sums of squares	w.r.t.	with regard to	
Algorithms				
1nn	1-nearest-neighbor	NN	nearest neighbor	
ADA	AdaBoost using decision	RF	random forest	
	trees	RIP	Ripper	
C45	decision tree (c4.5)	SCM	set covering machine	
NB	naive Bayes	SVM	support vector machine	

Algorithms are set in small caps to distinguish them from acronyms.

Acronyms used in tables and math

CI	confidence interval	LR	likelihood ratio
FN	false negative	Pr	probability
FP	false positive	TN	true negative
FPR	false-positive rate	TP	true positive
IR	information reward	TPR	true-positive rate

These are not acronyms, although sometimes TPR and FPR will appear as such. Authors' preferences were followed in this case.