

Directly and Efficiently Optimizing Prediction Error and AUC of Linear Classifiers

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Optimization and its Applications

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Introduction

Directly Optimizing Prediction Error

Directly Optimizing AUC

Numerical Analysis

Summary

Introduction

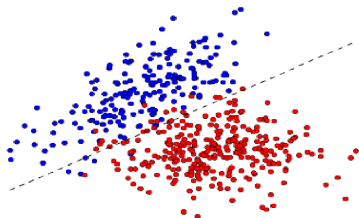
Directly Optimizing Prediction Error

Directly Optimizing AUC

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Summary

Supervised Learning Problem



- Given a finite sample data set $\mathcal{S}$ of n (input, label) pairs, e.g.,

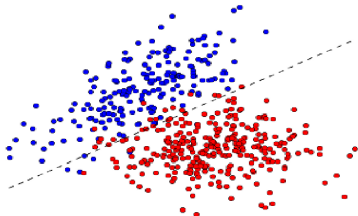
$$\mathcal{S} := \{(x_i, y_i) : i = 1, \dots, n\}, \text{ where } x_i \in \mathbb{R}^d \text{ and } y_i \in \{+1, -1\}.$$

- We are interested in **Binary Classification Problem** in supervised learning
- Binary Classification Problem $\Rightarrow$ **Discrete** valued output $+1$ or -1
- We are interested in **linear classifier** (predictor) $f(x; w) = w^T x$ so that

$$f : \mathcal{X} \rightarrow \mathcal{Y},$$

where $\mathcal{X}$ denote the space of input values and $\mathcal{Y}$ the space of output values.

Supervised Learning Problem



How good is this classifier?

- Prediction Error
- Area Under ROC Curve (AUC)

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Expected Risk (Prediction Error)

- In $\mathcal{S}$, each (x_i, y_i) is an i.i.d. observation of the random variables (X, Y) .
- (X, Y) has an unknown joint probability distribution $P_{X,Y}(x, y)$ over $\mathcal{X}$ and $\mathcal{Y}$.
- The *expected risk* associated with a linear classifier $f(x; w) = w^T x$ for **zero-one loss function** is defined as

$$\begin{aligned} R_{0-1}(f) &= \mathbb{E}_{\mathcal{X}, \mathcal{Y}} [\ell_{0-1}(f(X; w), Y)] \\ &= \int_{\mathcal{X}} \int_{\mathcal{Y}} P_{X,Y}(x, y) \ell_{0-1}(f(x; w), y) dy dx \end{aligned}$$

where

$$\ell_{0-1}(f(x; w), y) = \begin{cases} +1 & \text{if } y \cdot f(x; w) < 0, \\ 0 & \text{if } y \cdot f(x; w) \geq 0. \end{cases}$$

Empirical Risk Minimization

- The joint probability distribution $P_{X,Y}(x, y)$ is unknown
- The *empirical risk* of the linear classifier $f(x; w)$ for **zero-one loss function** over the finite training set $\mathcal{S}$ is of the interest, e.g.,

$$R_{0-1}(f; \mathcal{S}) = \frac{1}{n} \sum_{i=1}^n \ell_{0-1}(f(x_i; w), y_i).$$

Empirical Risk Minimization

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- Utilizing the **logistic regression loss function** instead of 0-1 loss function, results

$$R_{\log}(f; \mathcal{S}) = \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i \cdot f(x_i; w))),$$

- Practically

$$\min_{w \in \mathbb{R}^d} \left\{ F_{\log}(w) = \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i \cdot f(x_i; w))) + \lambda \|w\|^2 \right\}.$$

Alternative Interpretation of the Prediction Error

- We can interpret prediction error as a **probability value**:

$$\begin{aligned} F_{error}(w) &= R_{0-1}(f) \\ &= \mathbb{E}_{\mathcal{X}, \mathcal{Y}} [\ell_{0-1}(f(X; w), Y)] \\ &= P(Y \cdot w^T X < 0). \end{aligned}$$

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If the true values of the prior probabilities $P(Y = +1)$ and $P(Y = -1)$ are known or obtainable from a trivial calculation, then

Lemma 1

Expected risk can be interpreted in terms of the probability value, so that

$$\begin{aligned} F_{error}(w) &= P(Y \cdot w^T X < 0) \\ &= P(Z^+ \leq 0) P(Y = +1) + (1 - P(Z^- \leq 0)) P(Y = -1), \end{aligned}$$

where

$$Z^+ = w^T X^+, \quad \text{and} \quad Z^- = w^T X^-,$$

for X^+ and X^- as random variables from positive and negative classes, respectively.

- Suppose $(X_1, \dots, X_n)$ is a multivariate random variable.
- For a given mapping function $g(\cdot)$ we are interested in the c.d.f of

$$Z = g(X_1, \dots, X_n).$$

- If we define a region in space $\{\mathcal{X}_1 \times \dots \times \mathcal{X}_n\}$ such that $g(x_1, \dots, x_n) \leq z$, then we have

$$\begin{aligned} F_Z(z) &= P(Z \leq z) \\ &= P(g(X) \leq z) \\ &= P(\{x_1 \in \mathcal{X}_1, \dots, x_n \in \mathcal{X}_n : g(x_1, \dots, x_n) \leq z\}) \\ &= \int_{\{x_1 \in \mathcal{X}_1, \dots, x_n \in \mathcal{X}_n : g(x_1, \dots, x_n) \leq z\}} \dots \int f_{X_1, \dots, X_n}(x_1, \dots, x_n) dx_1 \dots dx_n. \end{aligned}$$

Assume

$$X^+ \sim \mathcal{N}(\mu^+, \Sigma^+) \quad \text{and} \quad X^- \sim \mathcal{N}(\mu^-, \Sigma^-).$$

Data with Normal Distribution

Assume

$$X^+ \sim \mathcal{N}(\mu^+, \Sigma^+) \quad \text{and} \quad X^- \sim \mathcal{N}(\mu^-, \Sigma^-).$$

Why Normal?

- The family of multivariate Normal distributions is **closed under linear transformations**.

Theorem 2 (Tong (1990))

If $X \sim \mathcal{N}(\mu, \Sigma)$ and $Z = CX + b$, where C is any given $m \times n$ real matrix and b is any $m \times 1$ real vector, then $Z \sim \mathcal{N}(C\mu + b, C\Sigma C^T)$.

- Normal Distribution has a **smooth c.d.f.**

Theorem 3

Suppose that

$$X^+ \sim \mathcal{N}(\mu^+, \Sigma^+) \quad \text{and} \quad X^- \sim \mathcal{N}(\mu^-, \Sigma^-).$$

Then,

$$F_{\text{error}}(w) = P(Y = +1) (1 - \phi(\mu_{Z+}/\sigma_{Z+})) + P(Y = -1) \phi(\mu_{Z-}/\sigma_{Z-}),$$

where

$$\mu_{Z+} = w^T \mu^+, \quad \sigma_{Z+} = \sqrt{w^T \Sigma^+ w}, \quad \text{and}$$

$$\mu_{Z-} = w^T \mu^-, \quad \sigma_{Z-} = \sqrt{w^T \Sigma^- w},$$

in which ϕ is the c.d.f of the standard normal distribution, e.g.,

$$\phi(x) = \int_{-\infty}^x \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}t^2) dt, \quad \text{for } \forall x \in \mathbb{R}.$$

Prediction Error as a Smooth Function

Theorem 3

Suppose that

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Prediction error is a smooth function of $w \Rightarrow$ we can compute the gradient and ...

Introduction

Directly Optimizing Prediction Error

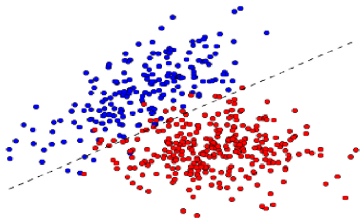
Directly Optimizing AUC

Numerical Analysis

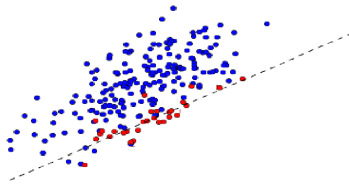
Summary

Learning From Imbalanced Data Sets

- Many real-world machine learning problems are dealing with imbalanced learning data



(a) Balanced data set



(b) Imbalanced data set

Receiver Operating Characteristic (ROC) Curve

- Sorted outputs based on descending value of $f(x; w) = w^T x$

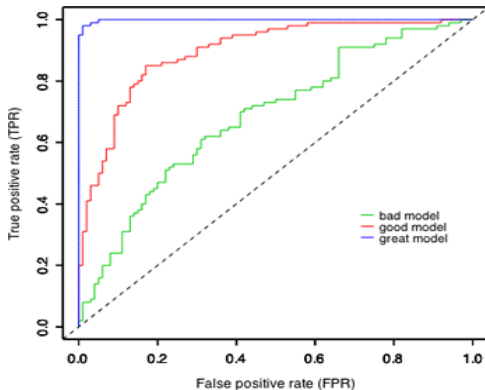


	Predicted Positive	Predicted Negative
Actual Positive	True Positive (TP)	False Negative (FN)
Actual Negative	False Positive (FP)	True Negative (TN)

- Various thresholds result in different True Positive Rate = $\frac{TP}{TP+FN}$ and False Positive Rate = $\frac{FP}{FP+TN}$.
- ROC curve presents the tradeoff between the TPR and the FPR, for all possible thresholds.

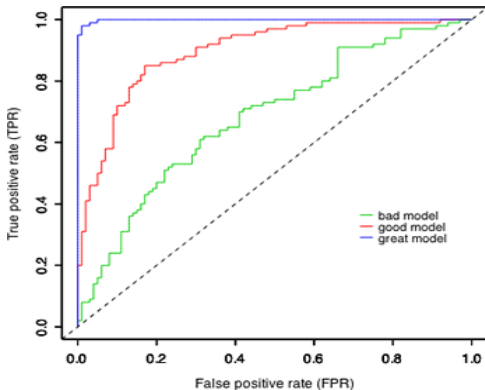
Area Under ROC Curve (AUC)

- How we can compare ROC curves?



Area Under ROC Curve (AUC)

- How we can compare ROC curves? Higher AUC $\implies$ Better classifier



An Unbiased Estimation of AUC Value

An unbiased estimation of the AUC value of a linear classifier can be obtained via Wilcoxon-Mann-Whitney (WMW) statistic result (*Mann and R. Whitney (1947)*), e.g.,

$$AUC(f; \mathcal{S}^+, \mathcal{S}^-) = \frac{\sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \mathbb{1} [f(x_i^+; w) > f(x_j^-; w)]}{n^+ \cdot n^-}.$$

where

$$\mathbb{1} [f(x_i^+; w) > f(x_j^-; w)] = \begin{cases} +1 & \text{if } f(x_i^+; w) > f(x_j^-; w), \\ 0 & \text{otherwise.} \end{cases}$$

in which $\mathcal{S} = \mathcal{S}^+ \cup \mathcal{S}^-$.

The indicator function $\mathbb{1}[\cdot]$ can be approximate with:

- Sigmoid surrogate function, *Yan et al. (2003)*,
- Pairwise exponential loss or pairwise logistic loss, *Rudin and Schapire (2009)*,
- Pairwise [hinge loss](#), *Steck (2007)*,

$$F_{\text{hinge}}(w) = \frac{\sum_{i=1}^{n^+} \sum_{j=1}^{n^-} \max \{0, 1 - (f(x_j^-; w) - f(x_i^+; w))\}}{n^+ \cdot n^-}.$$

Measuring AUC Statistically

- Let $\mathcal{X}^+$ and $\mathcal{X}^-$ denote the space of the positive and negative input values,
- Then x_i^+ is an i.i.d. observation of the random variable X^+ and x_j^- is an i.i.d. observation of the random variable X^- ,
- If the joint probability distribution $P_{X^+, X^-}(x^+, x^-)$ is known, the actual associated AUC value of a linear classifier $f(x; w) = w^T x$ is defined as

$$\begin{aligned} AUC(f) &= \mathbb{E}_{\mathcal{X}^+, \mathcal{X}^-} \left[\mathbb{1} \left[f(X^+; w) > f(X^-; w) \right] \right] \\ &= \int_{\mathcal{X}^+} \int_{\mathcal{X}^-} P_{X^+, X^-}(x^+, x^-) \mathbb{1} \left[f(x^+; w) > f(x^-; w) \right] dx^- dx^+. \end{aligned}$$

Lemma 4

We can interpret AUC value as a *probability value*:

$$\begin{aligned} F_{AUC}(w) &= 1 - AUC(f) \\ &= 1 - \mathbb{E}_{\mathcal{X}^+, \mathcal{X}^-} \left[\mathbb{1} \left[f(X^+; w) > f(X^-; w) \right] \right] \\ &= 1 - P(Z < 0), \end{aligned}$$

where

$$Z = w^T (X^- - X^+),$$

for X^+ and X^- as random variables from positive and negative classes, respectively.

Theorem 5

If two random variables X^+ and X^- have a joint multivariate normal distribution, such that

$$\begin{pmatrix} X^+ \\ X^- \end{pmatrix} \sim \mathcal{N}(\mu, \Sigma),$$

$$\text{where } \mu = \begin{pmatrix} \mu^+ \\ \mu^- \end{pmatrix} \quad \text{and} \quad \Sigma = \begin{pmatrix} \Sigma^{++} & \Sigma^{+-} \\ \Sigma^{-+} & \Sigma^{--} \end{pmatrix},$$

then the AUC function can be defined as

$$F_{AUC}(w) = 1 - \phi\left(\frac{\mu_Z}{\sigma_Z}\right),$$

where

$$\mu_Z = w^T (\mu^- - \mu^+) \quad \text{and}$$

$$\sigma_Z = \sqrt{w^T (\Sigma^{--} + \Sigma^{++} - \Sigma^{-+} - \Sigma^{+-}) w},$$

and is the c.d.f of the standard normal distribution.

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and is the c.d.f of the standard normal distribution.

AUC is a smooth function of $w \Rightarrow$ we can compute the gradient.

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Directly Optimizing AUC

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Computational Settings

- We have used *gradient descent with backtracking line search* as the optimization method.
- The algorithm is implemented in *Python 2.7.11* and computations are performed on the *COR@L computational cluster*.
- We have used both *artificial data sets* and *real data sets*.
- We used *five-fold cross-validation* with the *train-test* framework.

- Artificial data points with normal distribution are generated randomly.

Name	d	n	P^+	P^-	$out\%$
$data_1$	500	5000	0.05	0.95	0
$data_2$	500	5000	0.35	0.65	5
$data_3$	500	5000	0.5	0.5	10
$data_4$	1000	5000	0.15	0.85	0
$data_5$	1000	5000	0.4	0.6	5
$data_6$	1000	5000	0.5	0.5	10
$data_7$	2500	5000	0.1	0.9	0
$data_8$	2500	5000	0.35	0.65	5
$data_9$	2500	5000	0.5	0.5	10

Optimizing $F_{error}(w)$ vs. $F_{log}(w)$ on Artificial Data

Data	$F_{error}(w)$ Minimization		$F_{error}(w)$ Minimization		$F_{log}(w)$ Minimization	
	Exact moments		Approximate moments			
	Accuracy $\pm$ std	Time (s)	Accuracy $\pm$ std	Time (s)	Accuracy $\pm$ std	Time (s)
$data_1$	0.9965 $\pm$ 0.0008	0.25	0.9907 $\pm$ 0.0014	1.04	0.9897 $\pm$ 0.0018	3.86
$data_2$	0.9905 $\pm$ 0.0023	0.26	0.9806 $\pm$ 0.0032	0.86	0.9557 $\pm$ 0.0049	13.72
$data_3$	0.9884 $\pm$ 0.0030	0.03	0.9745 $\pm$ 0.0037	1.28	0.9537 $\pm$ 0.0048	15.79
$data_4$	0.9935 $\pm$ 0.0017	0.63	0.9791 $\pm$ 0.0034	5.51	0.9782 $\pm$ 0.0031	10.03
$data_5$	0.9899 $\pm$ 0.0026	5.68	0.9716 $\pm$ 0.0048	10.86	0.9424 $\pm$ 0.0055	28.29
$data_6$	0.9904 $\pm$ 0.0017	0.83	0.9670 $\pm$ 0.0058	5.18	0.9291 $\pm$ 0.0076	25.47
$data_7$	0.9945 $\pm$ 0.0019	4.79	0.9786 $\pm$ 0.0028	32.75	0.9697 $\pm$ 0.0031	43.20
$data_8$	0.9901 $\pm$ 0.0013	9.96	0.9290 $\pm$ 0.0045	119.64	0.9263 $\pm$ 0.0069	104.94
$data_9$	0.9899 $\pm$ 0.0028	1.02	0.9249 $\pm$ 0.0096	68.91	0.9264 $\pm$ 0.0067	123.85

Real Data Sets Information

These data sets can be downloaded from LIBSVM website ¹ and UCI machine learning repository ².

Name	AC	d	n	P^+	P^-
fourclass	$[-1, 1]$, real	2	862	0.35	0.65
svmguide1	$[-1, 1]$, real	4	3089	0.35	0.65
diabetes	$[-1, 1]$, real	8	768	0.35	0.65
shuttle	$[-1, 1]$, real	9	43500	0.22	0.78
vowel	$[-6, 6]$, int	10	528	0.09	0.91
magic04	$[-1, 1]$, real	10	19020	0.35	0.65
poker	$[1, 13]$, int	11	25010	0.02	0.98
letter	$[0, 15]$, int	16	20000	0.04	0.96
segment	$[-1, 1]$, real	19	210	0.14	0.86
svmguide3	$[-1, 1]$, real	22	1243	0.23	0.77
ijcnn1	$[-1, 1]$, real	22	35000	0.1	0.9
german	$[-1, 1]$, real	24	1000	0.3	0.7
landsat satellite	$[27, 157]$, int	36	4435	0.09	0.91
sonar	$[-1, 1]$, real	60	208	0.5	0.5
a9a	binary	123	32561	0.24	0.76
w8a	binary	300	49749	0.02	0.98
mnist	$[0, 1]$, real	782	100000	0.1	0.9
colon-cancer	$[-1, 1]$, real	2000	62	0.35	0.65
gisette	$[-1, 1]$, real	5000	6000	0.49	0.51

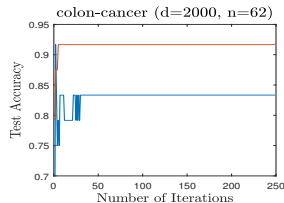
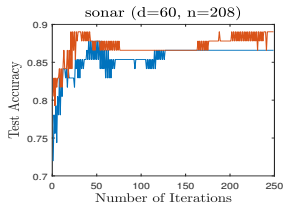
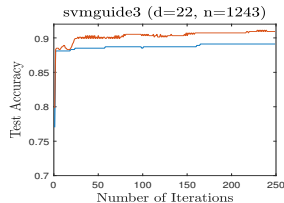
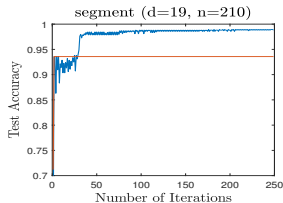
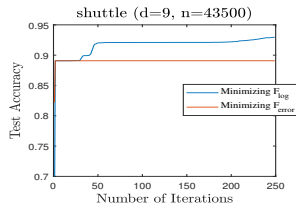
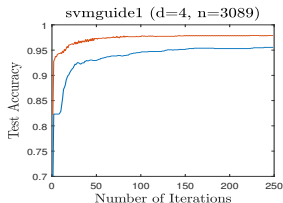
¹<https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html>

²<http://archive.ics.uci.edu/ml/>

Optimizing $F_{error}(w)$ vs. $F_{log}(w)$ on Real Data

Data	$F_{error}(w)$ Minimization		$F_{log}(w)$ Minimization	
	Accuracy $\pm$ std	Time (s)	Accuracy $\pm$ std	Time (s)
fourclass	0.8782 $\pm$ 0.0162	0.02	0.8800 $\pm$ 0.0147	0.12
svmguide1	0.9735 $\pm$ 0.0047	0.42	0.9506 $\pm$ 0.0070	0.28
diabetes	0.8832 $\pm$ 0.0186	1.04	0.8839 $\pm$ 0.0193	0.13
shuttle	0.8920 $\pm$ 0.0015	0.01	0.9301 $\pm$ 0.0019	4.05
vowel	0.9809 $\pm$ 0.0112	0.91	0.9826 $\pm$ 0.0088	0.11
magic04	0.8867 $\pm$ 0.0044	0.66	0.8925 $\pm$ 0.0041	1.75
poker	0.9897 $\pm$ 0.0008	0.17	0.9897 $\pm$ 0.0008	10.96
letter	0.9816 $\pm$ 0.0015	0.01	0.9894 $\pm$ 0.0009	4.51
segment	0.9316 $\pm$ 0.0212	0.17	0.9915 $\pm$ 0.0101	0.36
svmguide3	0.9118 $\pm$ 0.0136	0.39	0.8951 $\pm$ 0.0102	0.17
ijcnn1	0.9512 $\pm$ 0.0011	0.01	0.9518 $\pm$ 0.0011	4.90
german	0.8780 $\pm$ 0.0125	1.09	0.8826 $\pm$ 0.0159	0.62
landsat satellite	0.9532 $\pm$ 0.0032	0.01	0.9501 $\pm$ 0.0049	3.30
sonar	0.8926 $\pm$ 0.0292	0.49	0.8774 $\pm$ 0.0380	0.92
a9a	0.9193 $\pm$ 0.0021	0.98	0.9233 $\pm$ 0.0020	11.45
w8a	0.9851 $\pm$ 0.0005	0.36	0.9876 $\pm$ 0.004	24.16
mnist	0.9909 $\pm$ 0.0004	3.79	0.9938 $\pm$ 0.0004	136.83
colon-cancer	0.9364 $\pm$ 0.0394	15.92	0.8646 $\pm$ 0.0555	1.20
gisette	0.9782 $\pm$ 0.0025	310.72	0.9706 $\pm$ 0.0036	136.71

Optimizing $F_{error}(w)$ vs. $F_{log}(w)$ on Real Data



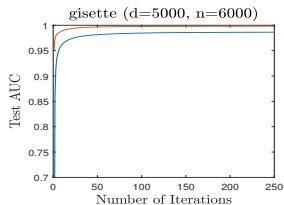
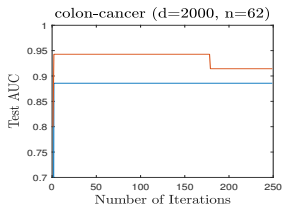
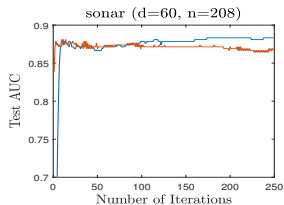
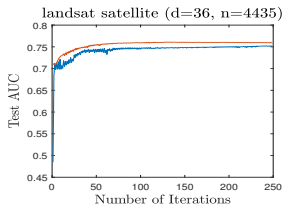
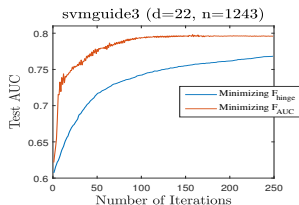
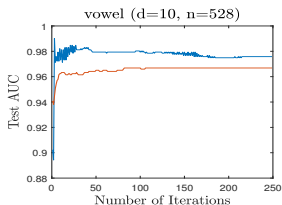
Optimizing $F_{AUC}(w)$ vs. $F_{hinge}(w)$ on Artificial Data

Data	$F_{AUC}(w)$ Minimization		$F_{AUC}(w)$ Minimization		$F_{hinge}(w)$ Minimization	
	Exact moments		Approximate moments			
	AUC $\pm$ std	Time (s)	AUC $\pm$ std	Time (s)	AUC $\pm$ std	Time (s)
$data_1$	0.9972 $\pm$ 0.0014	0.01	0.9941 $\pm$ 0.0027	0.23	0.9790 $\pm$ 0.0089	5.39
$data_2$	0.9963 $\pm$ 0.0016	0.01	0.9956 $\pm$ 0.0018	0.22	0.9634 $\pm$ 0.0056	159.23
$data_3$	0.9965 $\pm$ 0.0015	0.01	0.9959 $\pm$ 0.0018	0.24	0.9766 $\pm$ 0.0041	317.44
$data_4$	0.9957 $\pm$ 0.0018	0.02	0.9933 $\pm$ 0.0022	0.83	0.9782 $\pm$ 0.0054	23.36
$data_5$	0.9962 $\pm$ 0.0011	0.02	0.9951 $\pm$ 0.0013	0.80	0.9589 $\pm$ 0.0068	110.26
$data_6$	0.9962 $\pm$ 0.0013	0.02	0.9949 $\pm$ 0.0015	0.82	0.9470 $\pm$ 0.0086	275.06
$data_7$	0.9965 $\pm$ 0.0021	0.08	0.9874 $\pm$ 0.0034	4.61	0.9587 $\pm$ 0.0092	28.31
$data_8$	0.9966 $\pm$ 0.0008	0.07	0.9929 $\pm$ 0.0017	4.54	0.9514 $\pm$ 0.0051	104.16
$data_9$	0.9962 $\pm$ 0.0014	0.08	0.9932 $\pm$ 0.0020	4.54	0.9463 $\pm$ 0.0085	157.62

Optimizing $F_{AUC}(w)$ vs. $F_{hinge}(w)$ on Real Data

Data	$F_{AUC}(w)$ Minimization		$F_{hinge}(w)$ Minimization	
	AUC± std	Time (s)	AUC ± std	Time (s)
fourclass	0.8362±0.0312	0.01	0.8362±0.0311	6.81
svmguide1	0.9717±0.0065	0.06	0.9863±0.0037	35.09
diabetes	0.8311±0.0311	0.03	0.8308±0.0327	12.48
shuttle	0.9872±0.0013	0.11	0.9861±0.0017	2907.84
vowel	0.9585±0.0333	0.12	0.9765 ±0.0208	2.64
magic04	0.8382±0.0071	0.11	0.8419±0.0071	1391.29
poker	0.5054±0.0224	0.11	0.5069±0.0223	1104.56
letter	0.9830±0.0029	0.12	0.9883±0.0023	121.49
segment	0.9948±0.0035	0.21	0.9992±0.0012	4.23
svmguide3	0.8013 ±0.0420	0.34	0.7877±0.0432	23.89
ijcnn1	0.9269±0.0036	0.08	0.9287±0.0037	2675.67
german	0.7938±0.0292	0.14	0.7919±0.0294	32.63
landsat satellite	0.7587 ±0.0160	0.43	0.7458±0.0159	193.46
sonar	0.8214±0.0729	0.88	0.8456 ±0.0567	2.15
a9a	0.9004±0.0039	0.92	0.9027±0.0037	15667.87
w8a	0.9636±0.0055	0.54	0.9643±0.0057	5353.23
mnist	0.9943±0.0009	0.64	0.9933±0.0009	28410.2393
colon-cancer	0.8942 ±0.1242	2.50	0.8796±0.1055	0.05
gisette	0.9957 ±0.0015	31.32	0.9858±0.0029	3280.38

Optimizing $F_{AUC}(w)$ vs. $F_{hinge}(w)$ on Real Data



Introduction

Directly Optimizing Prediction Error

Directly Optimizing AUC

Numerical Analysis

Summary

- We proposed some conditions under which the expected error and AUC are smooth functions.
- Any gradient-based optimization method can be applied to directly optimize these functions.
- These new proposed approaches work efficiently without perturbing the unknown distribution of the real data sets.
- Studying data distributions may lead to new efficient approaches.

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Thanks for your attention!