Learning to Benchmark

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Benchmarks and benchmarking

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1. Meta-learning
2. Performance benchmarks
3. Empirical information divergence estimation
4. Ensemble divergence estimators
5. Applications
6. Summary

Predicting classification performance

The problem of predicting fundamental performance limits has long history:

- Optimal design of experiments - Gergonne[1], Smith[2], Lindley[3]

[1] J.D. Gergonne (1815), Application de la méthode des moindre quarrés a l'interpolation des suites. Annales de Mathématiques Pures et Appliquées. 5:242-252

[2] K. Smith (1918), "On the standard deviations of adjusted ... Biometrika 12:1-85.

[3] D. V. Lindley (1956). On a measure of information provided by an experiment. Annals of Math Stat., 27(4):986-1005.

Predicting performance

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- Optimal design of experiments - Gergonne[1], Smith[2], Lindley[3]
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- Model selection - Akaike[7], Stein[8], Donoho[9].

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[7] Akaike, H. (1974). A new look at the statistical model identification. IEEE T. Autom. control, 19(6):716-723.

[8] C.M Stein (1981), Estimation of the mean of a multivariate normal distribution. Annals of Statistics, 9(6):1135-1151.

[9] D.L. Donoho and I.M. Johnstone (1995). Adapting to unknown smoothness via wavelet shrinkage. J. Amer Stat. Assoc, 90(432):1200-1224.

Learning performance limits by empirical estimation of Bayes error bound

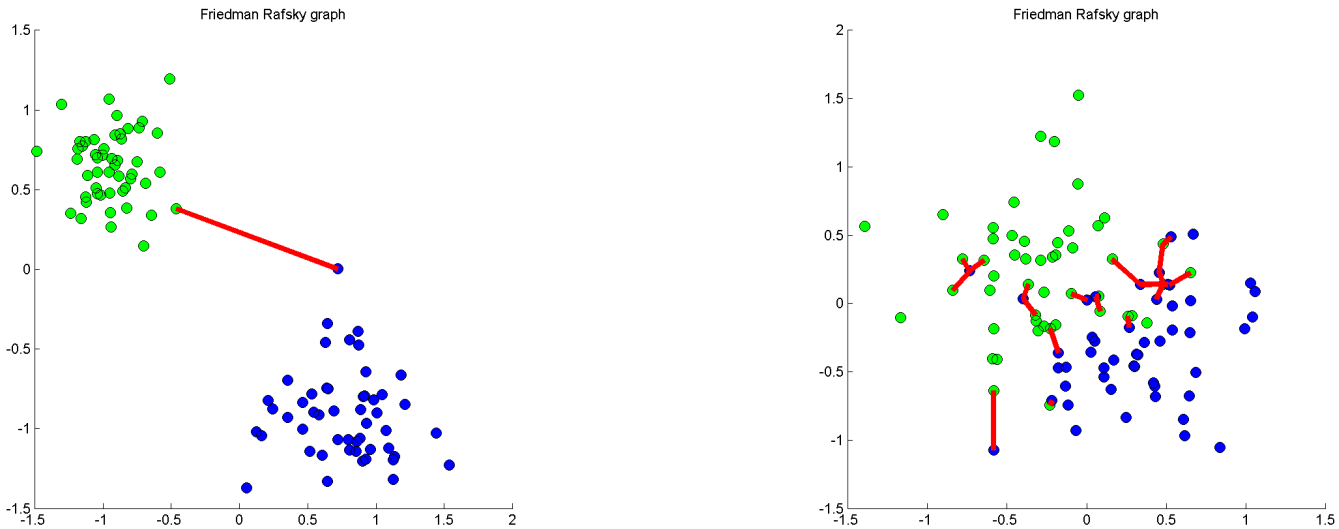

Figure: Friedman-Rafsky statistic converge to bounds on Bayes classification error.

- Q: Can we empirically estimate tight upper and lower bounds on Bayes misclassification error?

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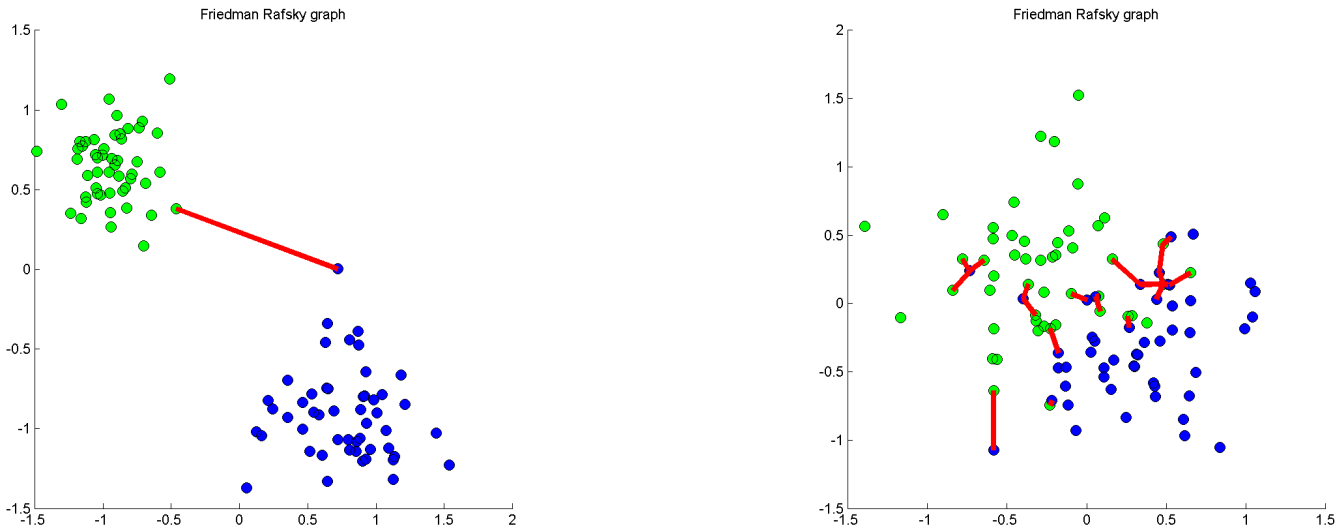

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- Q: Can we empirically estimate tight upper and lower bounds on Bayes misclassification error?
- A: Boosted ensembles of modified FR information divergence estimators[1] are rate-optimal estimates of a divergence measure[2] for smooth distributions[3]

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Bayes optimal classifier

Consider classification problem

- $Y \in \{1, \ldots, K\}$ an unknown label with priors $\{p_k\}$, $\sum_{k=1}^{K} p_k = 1$.

$$P(Y = k) = \begin{cases} p_1, & k = 1 \\ \vdots, & \vdots \\ p_K, & k = K \end{cases}$$

- X an observed random variable with conditional distribution

$$f(x|Y = k) = \begin{cases} f_1(x), & k = 1 \\ \vdots, & \vdots \\ f_K(x), & k = K \end{cases}$$

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Let $C(x)$ be (Bayes) optimal classifier that minimizes avg 0-1 loss (probability of error)

$$C(x) = \text{argmax}_{1 \leq k \leq K} P(Y = k|X = x)$$

Bayes error rate: best achievable misclassification error probability

Bayes error rate is avg missclassification error probability of Bayes classifier

$$\epsilon_{p_1,\ldots,p_K}(f_1, f_2, \ldots, f_K) = P(C(X) \neq Y)$$

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Integral representation

$$\epsilon_{p_1,\ldots,p_K}(f_1, f_2, \ldots, f_K) = 1 - \int \max_{1 \leq k \leq K} \{f_k(x) p_k\} dx$$

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Benchmark learning objective: empirically estimate the Bayes error rate

- directly from n training samples $\{(X_i, Y_i)\}_{i=1}^n$
- assuming (X_i, Y_i) i.i.d., where
- given Y_i: $X_i \sim f(x|Y_i = k) = f_k(x)$, $k = 1, \ldots, K$
- $P(Y_i = k) = p_k$

Bayes error rate for binary case ($Y \in \{0, 1\}$)

For special case of binary classification ($K = 2$)

$$\epsilon_{p,q}(f_1, f_2) = \frac{1}{2} - \frac{1}{2} \int |pf_1(x) - qf_2(x)| dx,$$

where $q = 1 - p$

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Alternative representation:

$$\epsilon_{p_1,p_2}(f_1, f_2) = \frac{1 + |p - q|}{2} - \frac{1}{2} \int g(f_1(x)/f_2(x)) f_2(x) dx,$$

where $g(u)$ is the convex function

$$g(u) = |pu - q| - |p - q|$$

The f-divergence between a pair of distributions

The f-divergence (Csiszár)[1], (Ali-Silvey)[2]:

$$D_g(f_1 \| f_2) = \int g\left(\frac{f_1(x)}{f_2(x)}\right) f_2(x) dx$$

where $g(u)$ is a convex function on $\mathbb{R}^+$ and $g(1) = 0$.

[1] I. Csiszár (1963), Eine informationstheoretische Ungleichung und ihre Anwendung auf den Beweis der Ergodizitat von Markoffschen Ketten. Magyar. Tud. Akad. Mat. Kutato Int. Kozl. 8:85108.

[2] S. M. Ali and S. D. Silvey (1966), A general class of coefficients of divergence of one distribution from another, J. Royal Stat. Soc., Ser.B , 28:131-142.

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Properties: if g is strictly convex then $D_g(f_1 \| f_2)$ is

- reflexive non-negative: $D_g(f_1 \| f_2) \geq 0$ with equality iff $f_1 = f_2$
- monotone: $D_g(f_1 \| f_2)$ non-increasing under transformations $x \to T(x)$
- jointly convex: $D_g(f_1 \| f_2)$ is convex in (f_1, f_2)

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Instances of f-divergences

The following are common instances of f-divergence[1]

- Total variation distance $g(u) = \frac{1}{2}|u-1|$

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- Kullback-Liebler divergence: $g(u) = u\log u$:

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- Hellinger-Bhattacharyya divergence $g(u) = (\sqrt{u}-1)^2$

$$D^{H}(f_1\|f_2) = \int \left(\sqrt{f_1(x)} - \sqrt{f_2(x)}\right)^2 dx$$

[1] Csiszár, I., and Shields, P. C. (2004). Information theory and statistics: A tutorial. Foundations and Trends in Communications and Information Theory, 1(4), 417-528.

Other instances of f-divergences

- Generalized total variation distance[1]: $g(u) = |pu - q|/2 - |p - q|/2$

$$D_p^{GTV} = \frac{1}{2} \int |pf_1(x) - qf_2(x)| dx + |p - q|/2$$

- Henze-Penrose divergence[2]: $g(u) = \frac{1}{4pq} \left[\frac{(pt-q)^2}{pt+q} - (p-q)^2 \right]$

$$D_p^{HP} = \frac{1}{4pq} \left[\int \frac{(pf_1(x) - qf_2(x))^2}{pf_1(x) + qf_2(x)} dx - (p-q)^2 \right].$$

[1] T. Kailath (1967), The divergence and Bhattacharyya distance measures in signal selection, IEEE T. Communication Technology, 15:1:5260

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f-divergences and Bayes error rate

These divergences can each be related to minimum probability of error

- Exact f-divergence representation

$$\epsilon_{p,q}(f_1, f_2) = \frac{1 + |p - q|}{2} - D_p^{GTV}(f_1(x) \| f_2(x))$$

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- Bhattacharyya bound[1]

$$\frac{1}{2} - \frac{1}{2}\sqrt{1 - BC_p^2} \leq \epsilon_{p,q} \leq \frac{1}{2} BC_p,$$

where $BC_p = \frac{\sqrt{pq}}{2}(1 - D_p^H)$ is the Bhattacharyya coefficient

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- *Learning to benchmark* can be reduced to f-divergence estimation.
- f-divergences are widely used in signal processing[2] and machine learning[3].
- Density plug in estimation strategies are often applied.

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Henze-Penrose divergence bound on Bayes error rate

Bound based on the Henze-Penrose divergence[1]

$$\frac{1}{2} - \frac{1}{2}\sqrt{\widetilde{D}_p^{HP}(f_1, f_2)} \leq \epsilon_p \leq \frac{1}{2} - \frac{1}{2}\widetilde{D}_p^{HP}(f_1, f_2), \tag{1}$$

where $\widetilde{D}_p^{HP} = 4pqD_p^{HP} + (p-q)^2$.

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where $\widetilde{D}_p^{HP} = 4pqD_p^{HP} + (p-q)^2$.

- For $p = 1/2$ this is a tighter bound than the Bhattacharyya bound.

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Numerical comparisons[1]

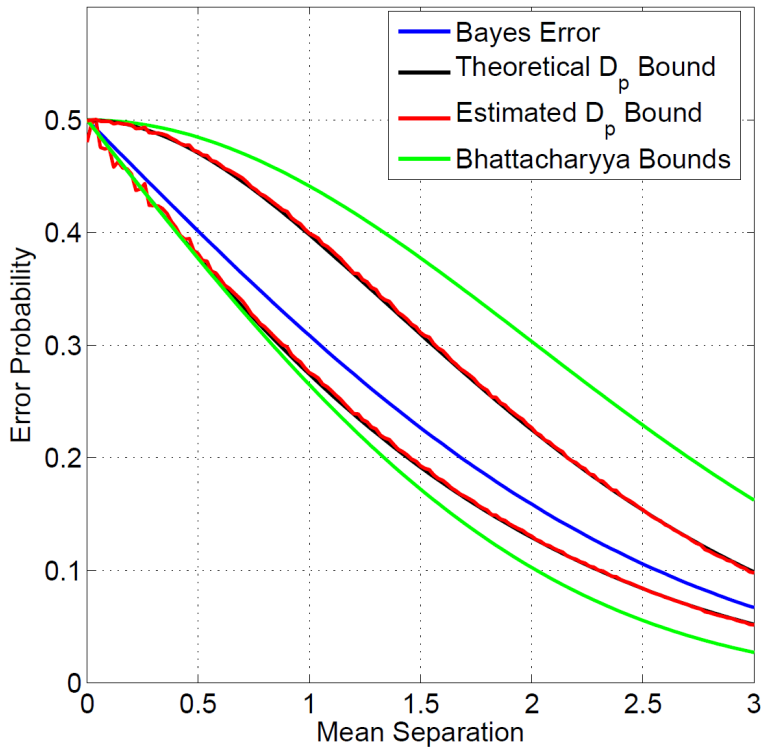

Figure: The HP bound using D_p is tighter than the Bhattacharrya bound using BC for bivariate normal distribution.

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Information divergence estimation

Set up:

- Given: samples $\{(X_i, Y_i)\}_{i=1}^{n}$ from $f_k(x)P(Y = k)$

$\Rightarrow$ $f_k(x) = f(x|Y = k)$

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Two main approaches to estimation of D

- Density-plug-in: construct density estimators $\hat{f}_1$, $\hat{f}_2$ and form $\hat{D} = D(\hat{f}_1, \hat{f}_2)$
- Direct methods: find a simpler statistic $\hat{D}$ that converges to $D(f_1 \| f_2)$

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Estimation strategies compared along two dimensions

- Sample complexity: rate γ at which estimator RMSE decreases in n

$$RMSE = \sqrt{\mathbb{E}[(\hat{D} - D)^2]} = O(1/n^\gamma)$$

- Computational complexity: measured by memory and runtime requirements

Sample complexity for divergence estimators

Assume that $X \in \mathbb{R}^d$, $0 < c_l \leq f_X \leq c_u < \infty$, and f_X in a smooth class $\mathcal{H}_{s,K}$

Convergence results for divergence estimation:

- Minimax estimators of density functionals [1],[2]
- Minimax estimators of divergence functionals [3]
- Common behavior of minimax RMSE

$$\inf_{\widehat{D}} \sup_{f_X \in \mathcal{H}_{s,K}} E\left[\left|D(X) - \widehat{D}(X_{1:n})\right|^2\right]^{1/2} = \begin{cases} cn^{-\phi(s,d)} & s < d/m \\ cn^{-1/2} & s \geq d/2 \end{cases}$$

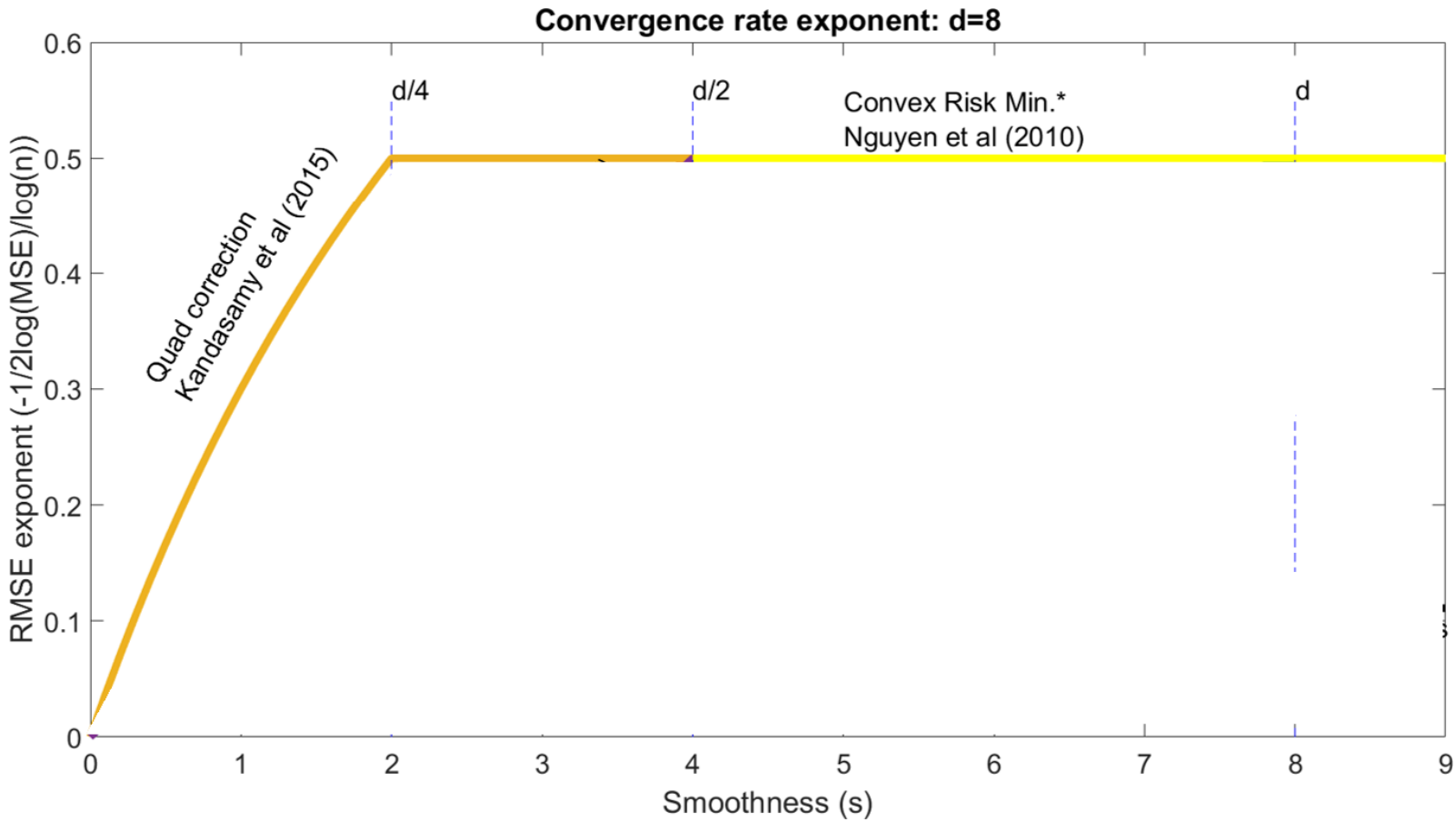
where $\phi(s,d)$ increases in s and decreases in d, and m is integer

[1] Birgé, L., and Massart, P. (1995). Estimation of integral functionals of a density. The Annals of Statistics, 11-29.

[2] Bickel, P. J., and Ritov, Y. A. (2003). Nonparametric estimators which can be "plugged-in". Annals of Statistics, 1033-1053.

[3] Nguyen, X., Wainwright, M., and Jordan, M. (2010). Estimating divergence functionals and the likelihood ratio by convex risk minimization. IEEE T. on Inform Theory, 56(11), 5847-5861.

RMSE convergence rate comparisons[1][2]



$\Rightarrow$ Kandasami's quadratic estimator achieves $O\left(\min\{n^{-3s/(2s+d)}, n^{-1/2}\}\right)$

[1] A. Krishnamurthy, K. Kandasamy, B. Póczos. Nonparametric estimation of Rényi divergence and friends, NIPS 2014.

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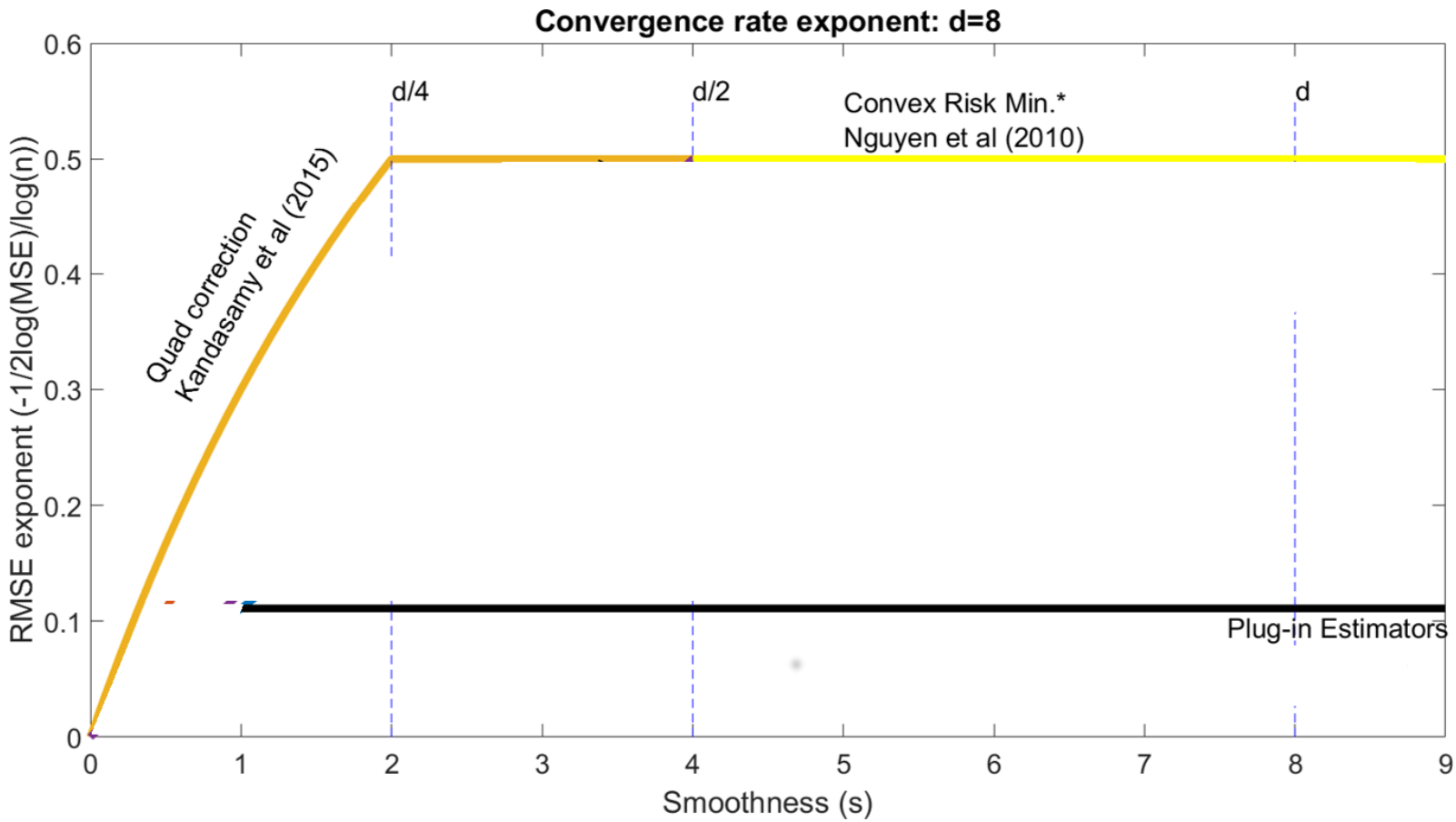

$\Rightarrow$ Density plug-in is a weak learner: RMSE rate is $O(n^{-1/d})$

[1] K Moon, K Sricharan, K Greenewald, A. Hero. Ensemble Estimation of Information Divergence," Entropy, vol. 20, no. 8, p. 560, July 2018.

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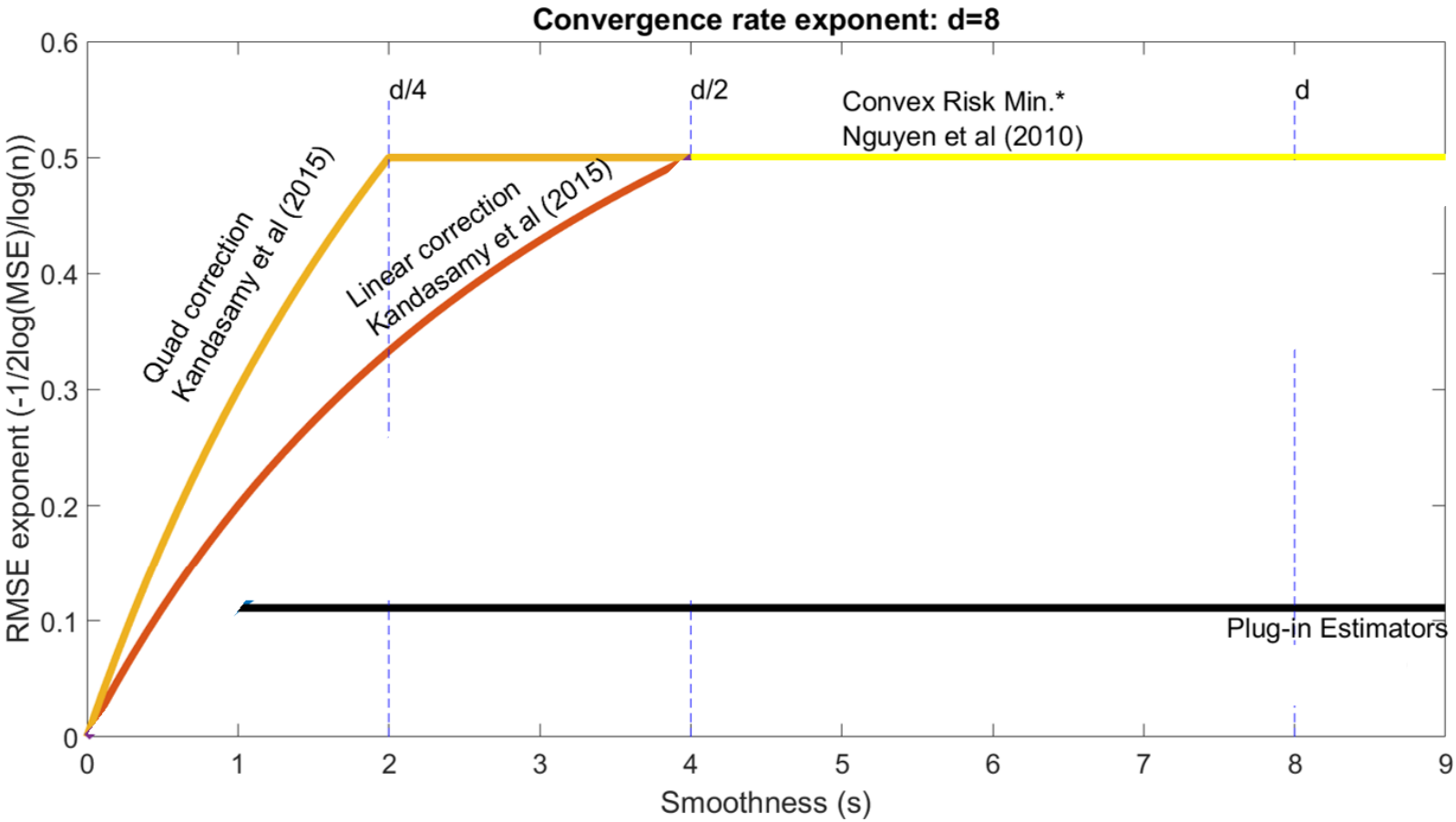

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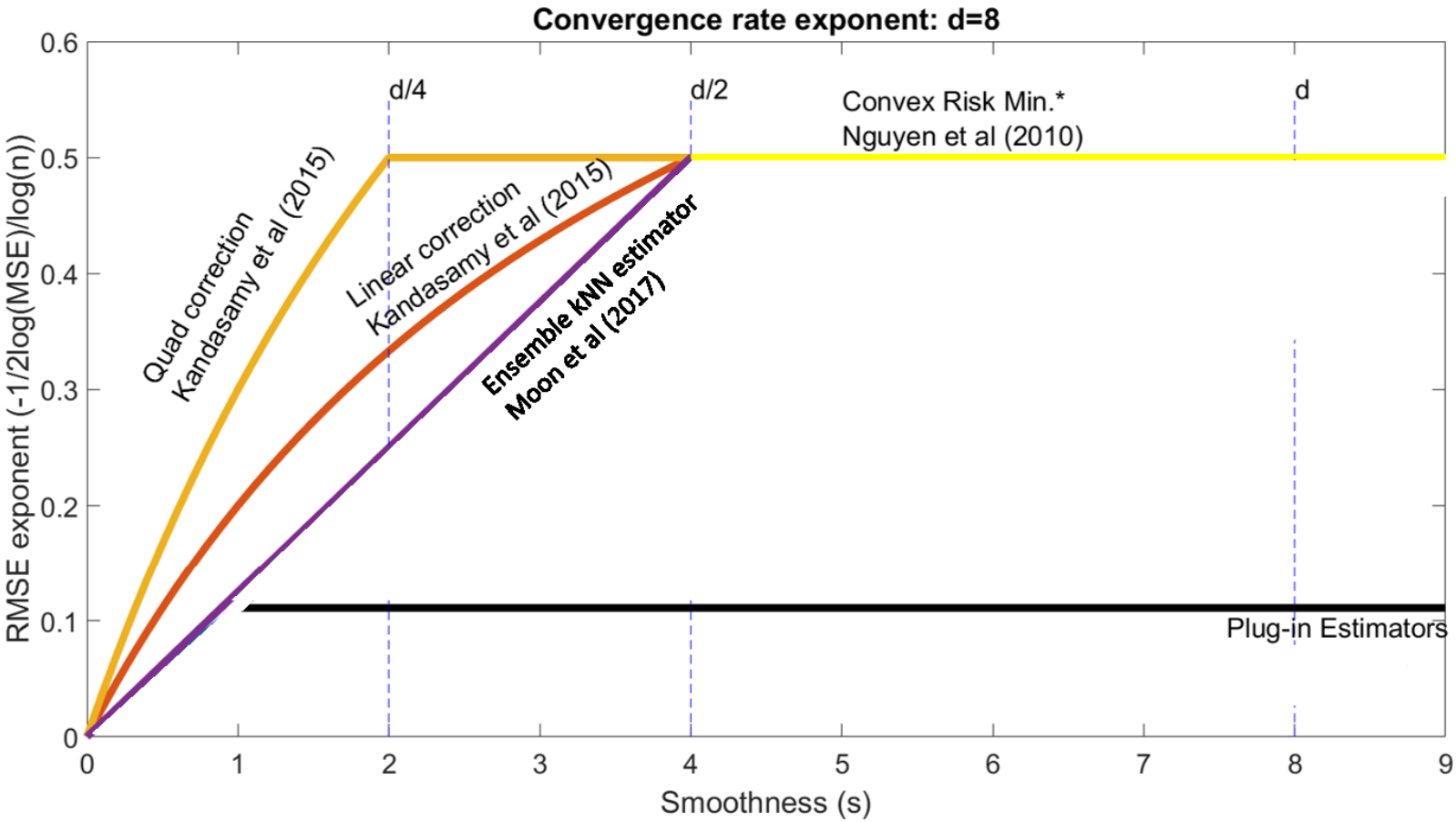

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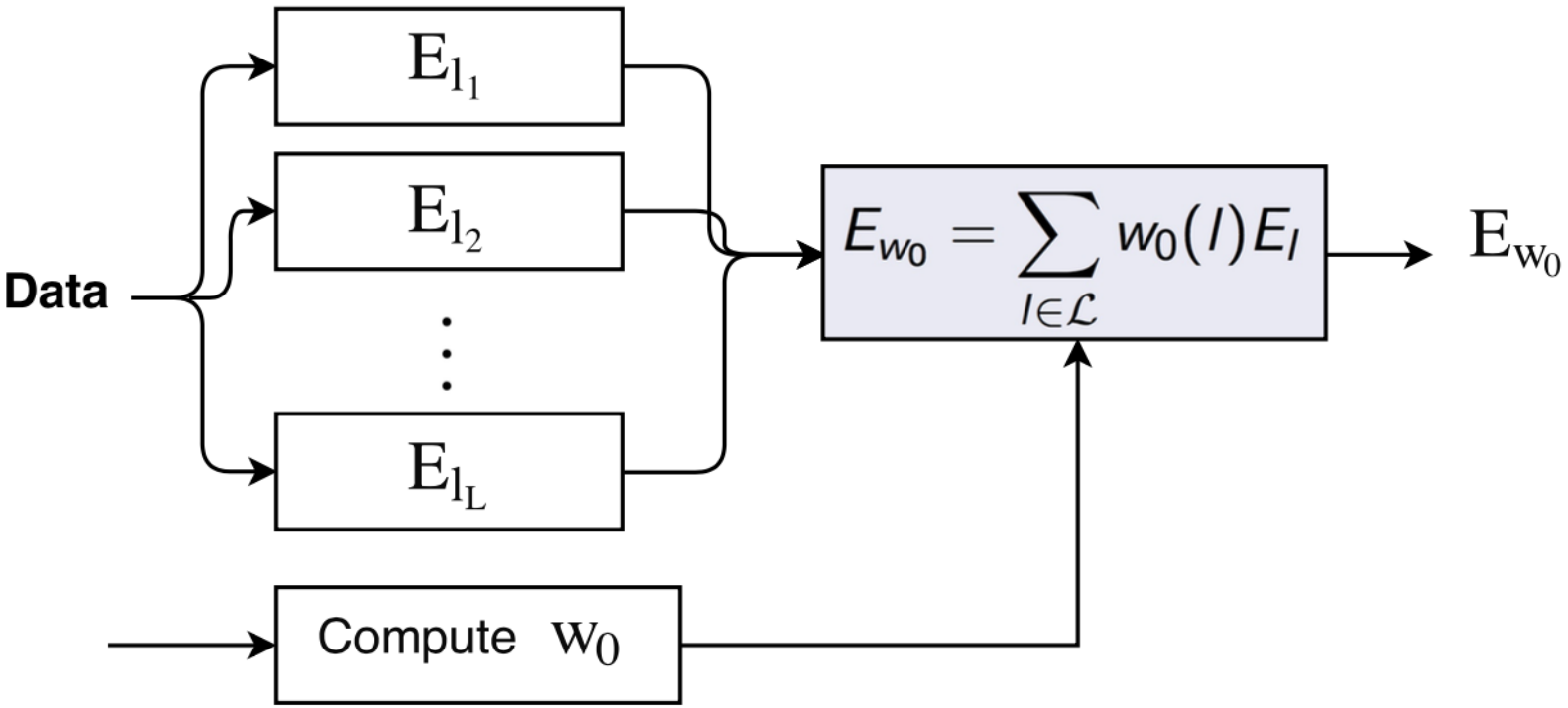
Boosting ensembles concept



- $\{E_{l_i}\}_{i=1}^{L}$ ensemble of base estimators (weak learners)
- $\mathbf{w} = (w_0(l))_{l=1}^{L}$ a vector of boosting weights
- E_{w_0}: combined base estimators (boosted learner)

Choice of boosting weights

Approaches to weight selection

- Boosting classifiers with Adaboost[1] and other objective functions.
- Consensus clustering: unsupervised classification[2]
- Matching pursuit for dictionary learning[3]

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[2] L. Tao, C. Ding and M. I. Jordan. "Solving consensus and semi-supervised clustering problems using nonnegative matrix factorization." Intl Conf on Data Mining, 2007, pp. 577-582.

[3] S. Mallat and Z. Zhang (1993). Matching pursuit with time frequency dictionaries. IEEE T. on Signal Processing 41:3397-3415

[4] Bickel, P. J., Ritov, Y. A., and Zakai, A. (2006). Some theory for generalized boosting algorithms. J. of Machine Learning Research, 705-732.

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$\Rightarrow$ Our proposed ensemble divergence estimator has rate-optimal weights that are not data dependent

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Back to information divergence estimation problem

Information divergence function

$$D_g(f_1 \| f_2) = \int g\left(\frac{f_1(x)}{f_2(x)}\right) f_2(x) dx$$

where $g(u)$ is a convex function on $\mathbb{R}^+$ and $g(1) = 0$.

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Proposed base estimator: Locality Sensitive Hashing (LSH) plug-in estimator[1]

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Proposed base estimator: Locality Sensitive Hashing (LSH) plug-in estimator[1]

Assumptions[2] (similar to kernel density plug-in entropy estimator [3])

- f_1 and f_2 have common bounded support set $\Omega \subset \mathbb{R}^d$.
- $0 < C_L \leq f_1, f_2 \leq C_U < \infty$ on Ω.
- Densities f_1 and f_2 are both differentiable of order d.
- g is Lipschitz continuous.

---

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Locality sensitive hashing plug-in estimator

Define numbers of samples N and M in class 1 and class 2, respectively,

$$N = \sum_{i=1}^{n} Y_i, \qquad M = \sum_{i=1}^{n} (1 - Y_i) = n - N$$

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LSH-based divergence estimator

- Step 1: Apply LSH quantizer $\{Q_i(x)\}_{i=1}^{F}$ to bin X_i into F buckets

$$N_i = \sum_{j=1}^{n} Y_j Q_i(X_j), \qquad M_i = \sum_{j=1}^{n} (1 - Y_j) Q_i(X_j),$$

- Step 2: Compute divergence plug-in estimator using histograms $\{(N_i, M_i)\}$

$$\widehat{D}_g(f_1 \| f_2) := \sum_{i: M_i > 0} g\left(\frac{N_i/N}{M_i/M}\right) M_i/M$$

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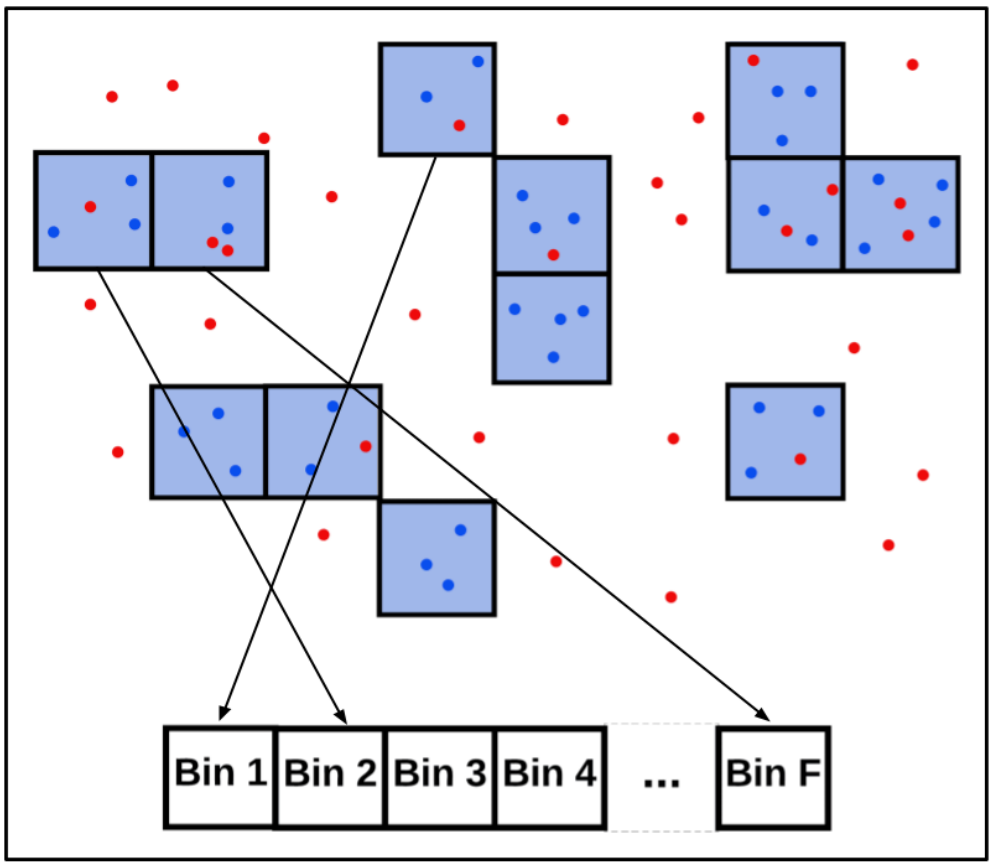

Figure: LSH quantizes **X** data with random displacement b and cell resolution ϵ

Locality sensitive hashing plug-in estimator: bias and variance

Theorem (Bias Expansion)

If f_1 and f_2 are d-times differentiable, the mean of $\widehat{D}_g$ is

$$\mathbb{E}[\widehat{D}_g] = D(f_1 \| f_2) + \mathbb{B}(\widehat{D}_g)$$

$$\mathbb{B}(\widehat{D}_g) = \sum_{i=1}^{d} C_i \epsilon^i + O\left(\frac{1}{n\epsilon^d}\right).$$

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The variance of the hash-based estimator can be bounded as

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$\Rightarrow$ This makes the slowest term in the bias decay as $\mathbb{B}(\widehat{D}_g) = O(n^{-1/2d})$

Ensemble bias reduction

- Let $\{\widehat{D}_g^{\epsilon(t)}\}_{t\in\mathcal{L}}$ be a set of $L = |\mathcal{L}|$ base learners.
- $\mathcal{L} := \{t_1, ..., t_L\}$ is a set of index values.
- $\epsilon(t) = tn^{-1/2d}$ is a set of histogram bandwidth parameters.

Define: Ensemble divergence estimator $\widehat{D}_w := \sum_{t\in\mathcal{L}} w(t)\widehat{D}_{\epsilon(t)}$

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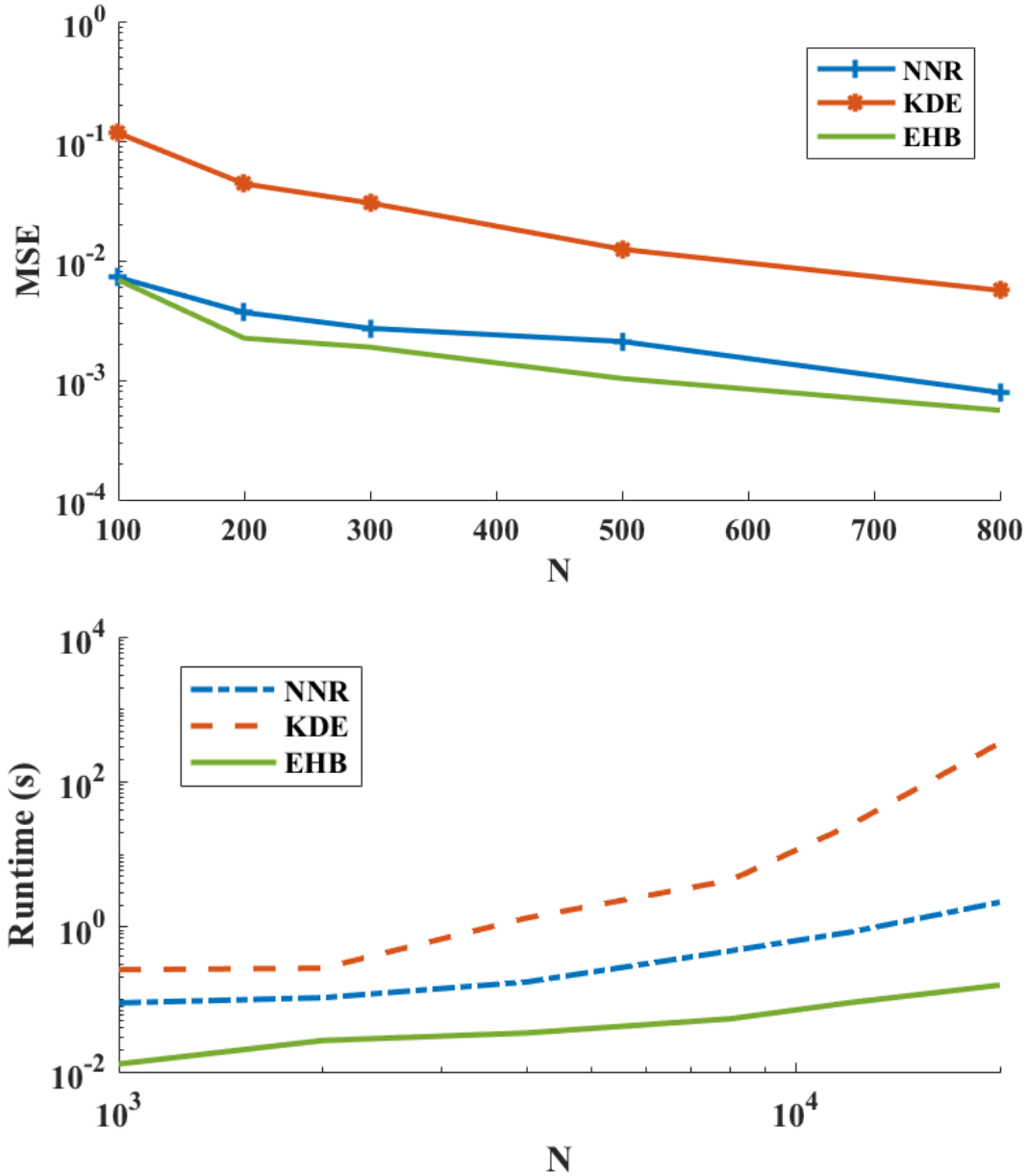
$$\mathbb{B}\left[\widehat{D}_w\right] = \sum_{i=1}^{d} C_i n^{-i/2d} \sum_{t=1}^{d} w(t)t^i + O\left(\frac{1}{\sqrt{n}}\right)$$

$\Rightarrow$ Bias becomes $O(1/\sqrt{n})$ if $w(t)$ is selected (offline) according to

$$\begin{aligned} \min_{w} \quad & \|w\|_2 \\ \textit{subject to} \quad & \sum_{t\in\mathcal{L}} w(t) = 1, \\ & \sum_{t\in\mathcal{L}} w(t)t^i = 0, i \in \mathbb{N}, i \leq d \end{aligned}$$

Simulation validation: Hellinger divergence for 2D shifted normals.



Benchmark learner vs HP bound learner

Simulation: classification of 2 mean shifted 10 dim Gaussian densities

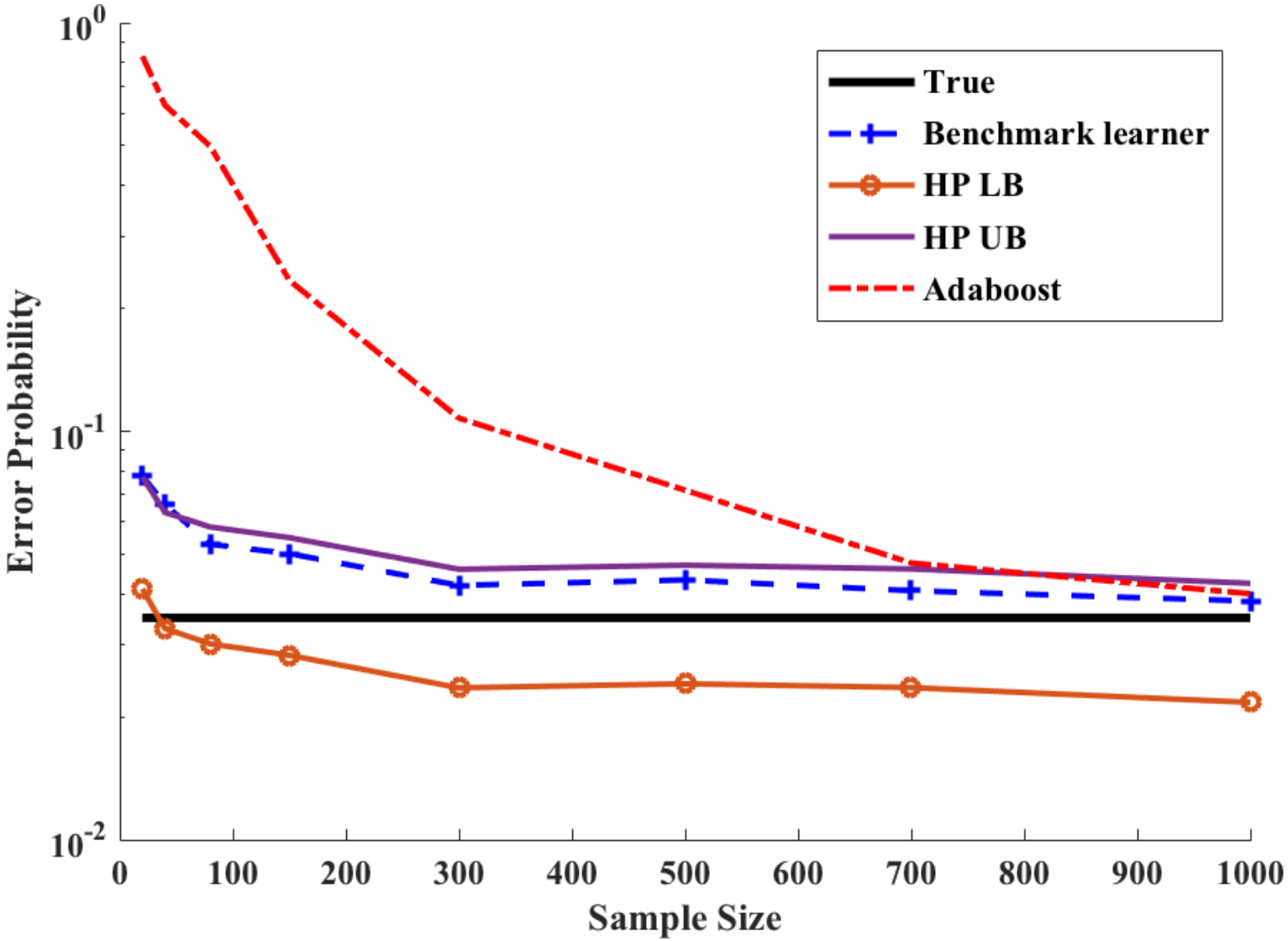


Figure: Note: ensemble benchmark learner is within envelope of HP bound learner.

Benchmark learner for multiclass classification

Gaussian $\mathcal{N}_2(\mu, \mathbf{I}_2)$, $K = 4$ classes $\mu_1, \ldots, \mu_4$

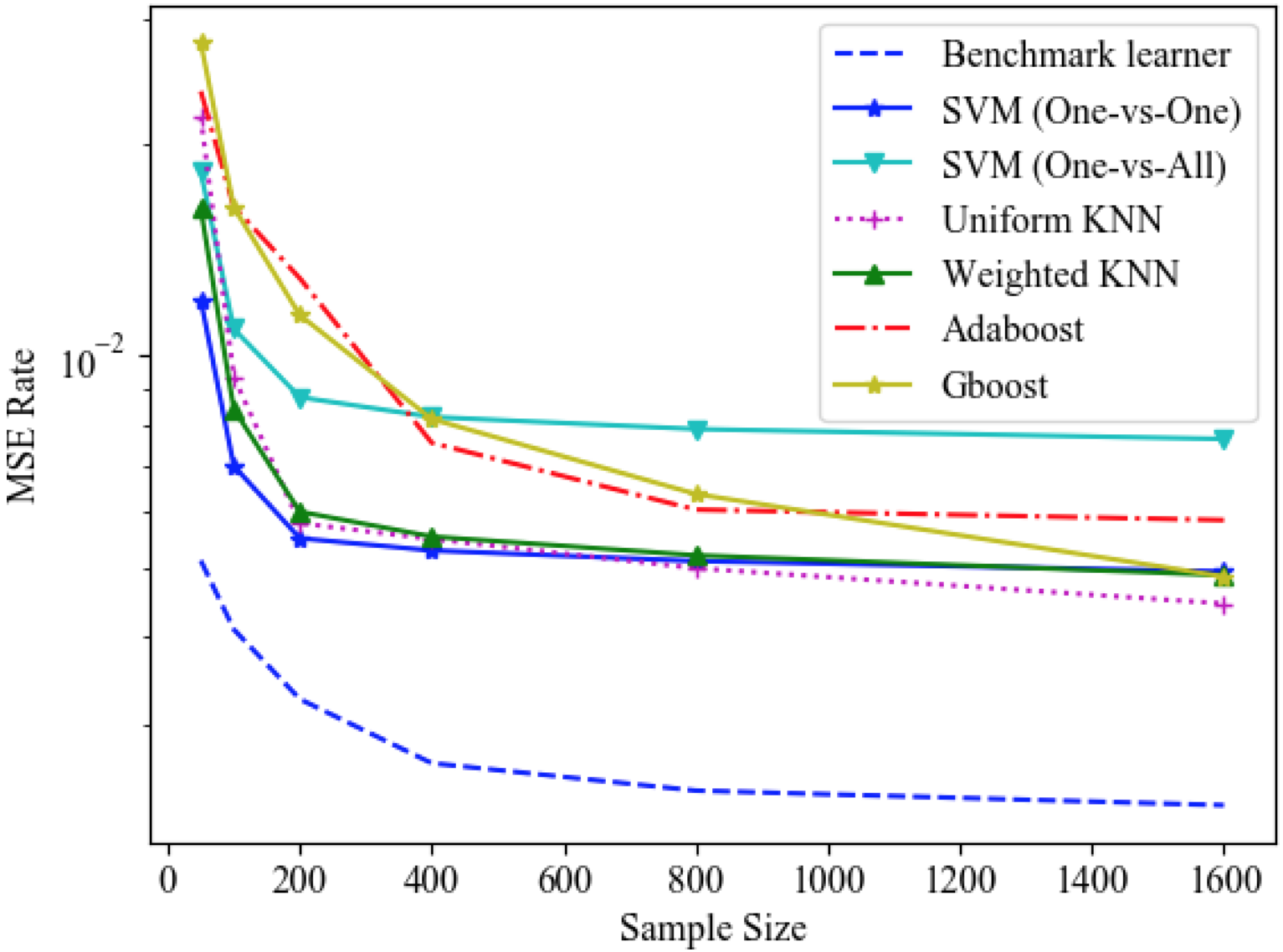
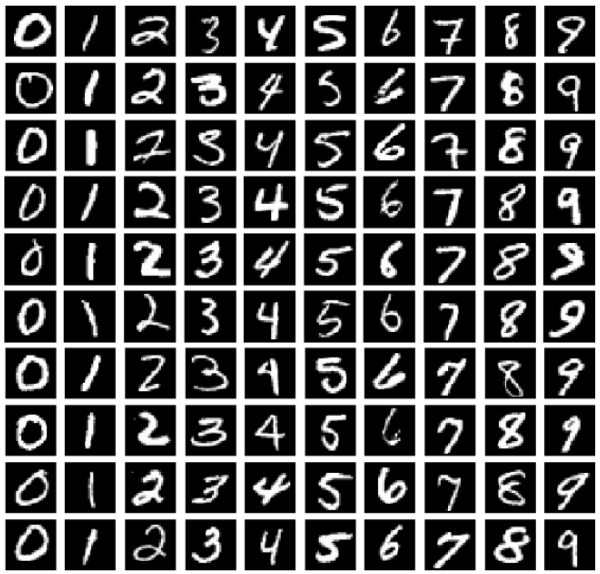
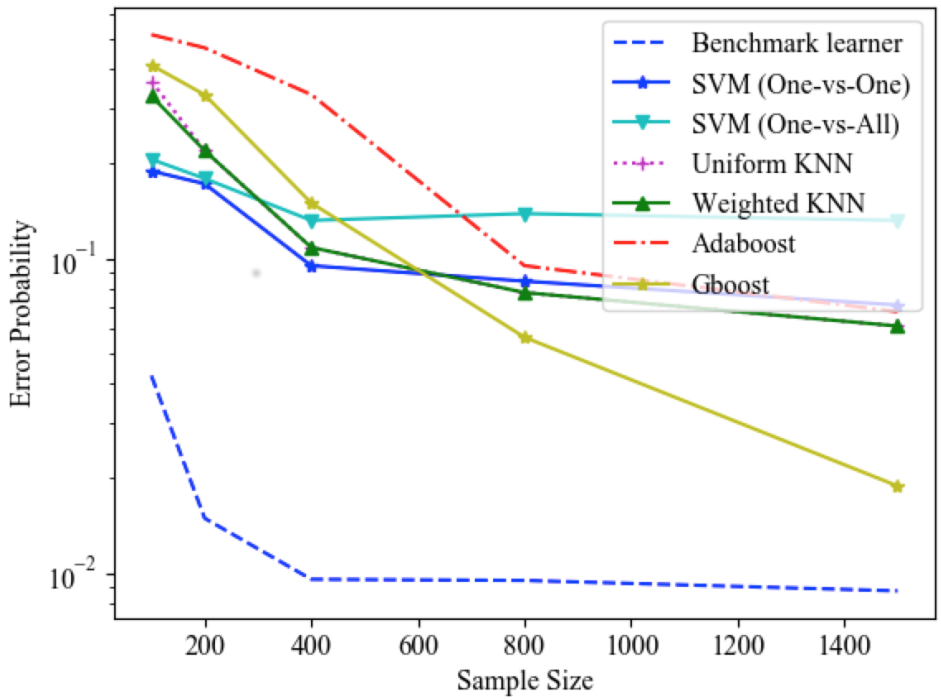


Figure: Note: Benchmark learner attains much lower MSE in estimating Bayes error

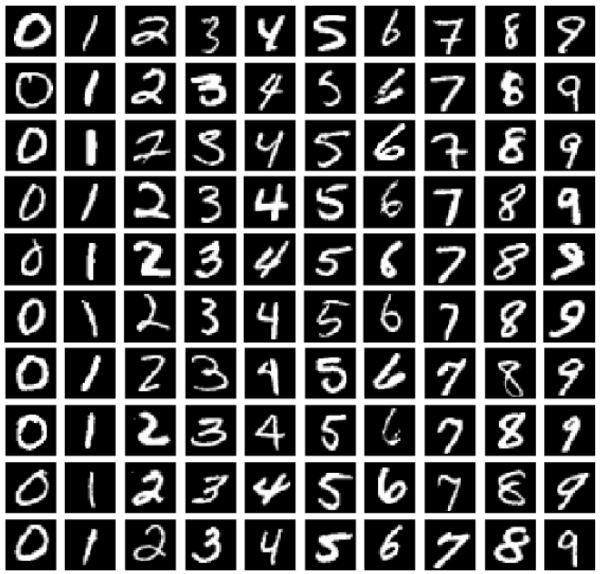
Benchmarking MNIST digit classification

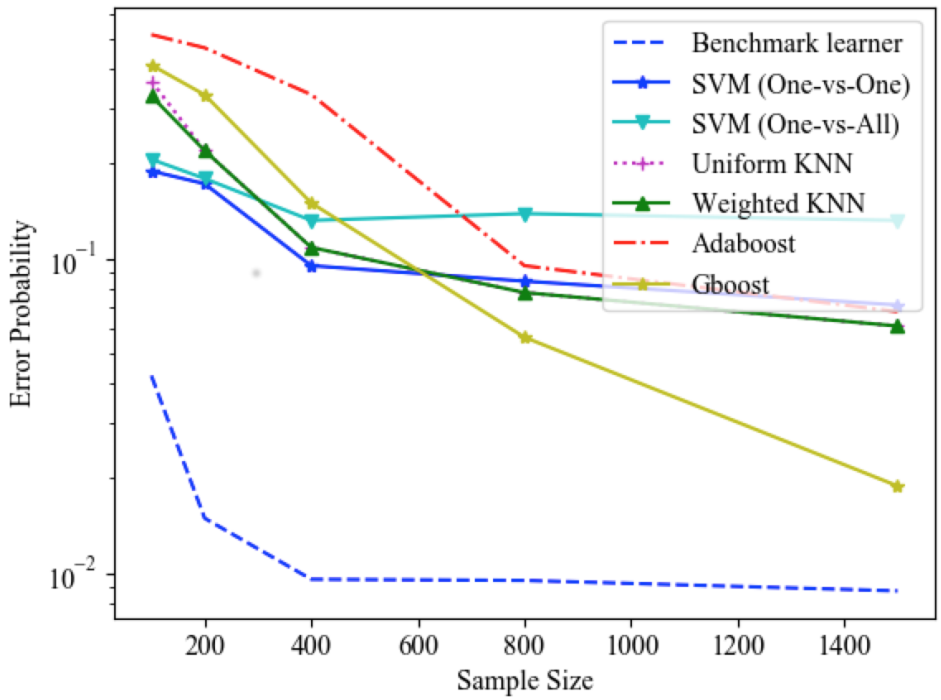




- MNIST handwritten digits with $K = 10$ classes
- Digit image data has $d = 64$ dimensions
- $n = 1795$ samples

Benchmarking MNIST digit classification





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Note: Gboost comes closest to benchmark but there is large margin for improvement.

Action classification for navigating SCITOS G5 robot

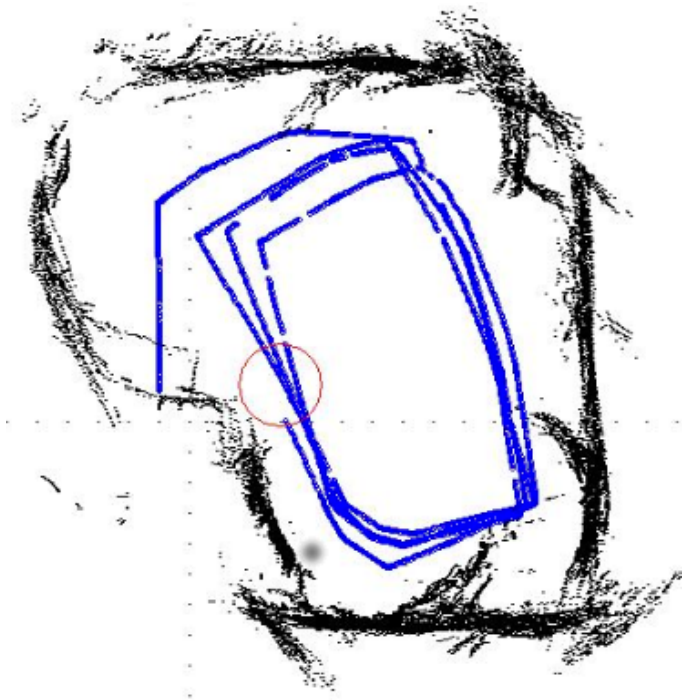

Figure: SCITOS G5 w/ 24 sensors

Robot's navigation path

- SCITOS robot navigation data from UCI database
- 4 robot control actions: Sharp R, Slight R, Forward, Slight L
- 24 equispaced ultrasound sensors on robot skirt
- $n = 5456$ action instances collected in experiment

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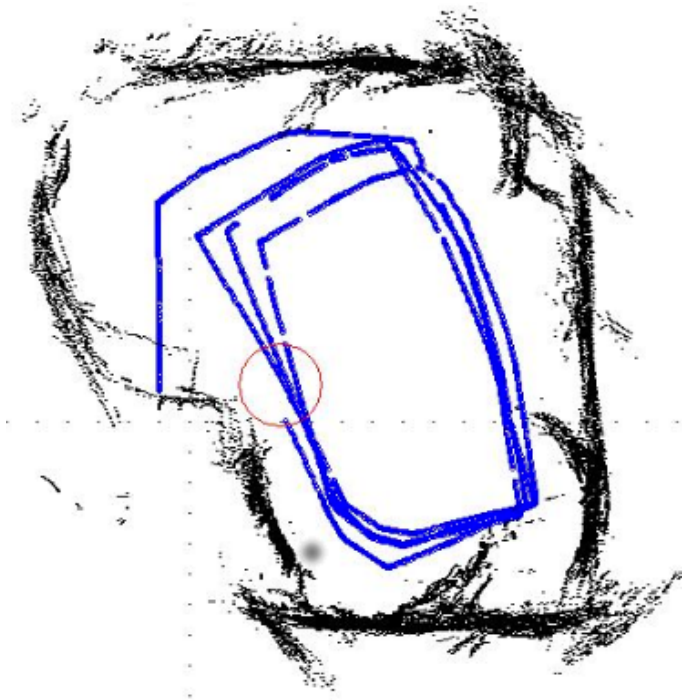

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Q. Without knowing control law, how well can we learn to predict the actions from the sensor readings?

Action classification: DoE w/ navigating SCITOS G5 robot

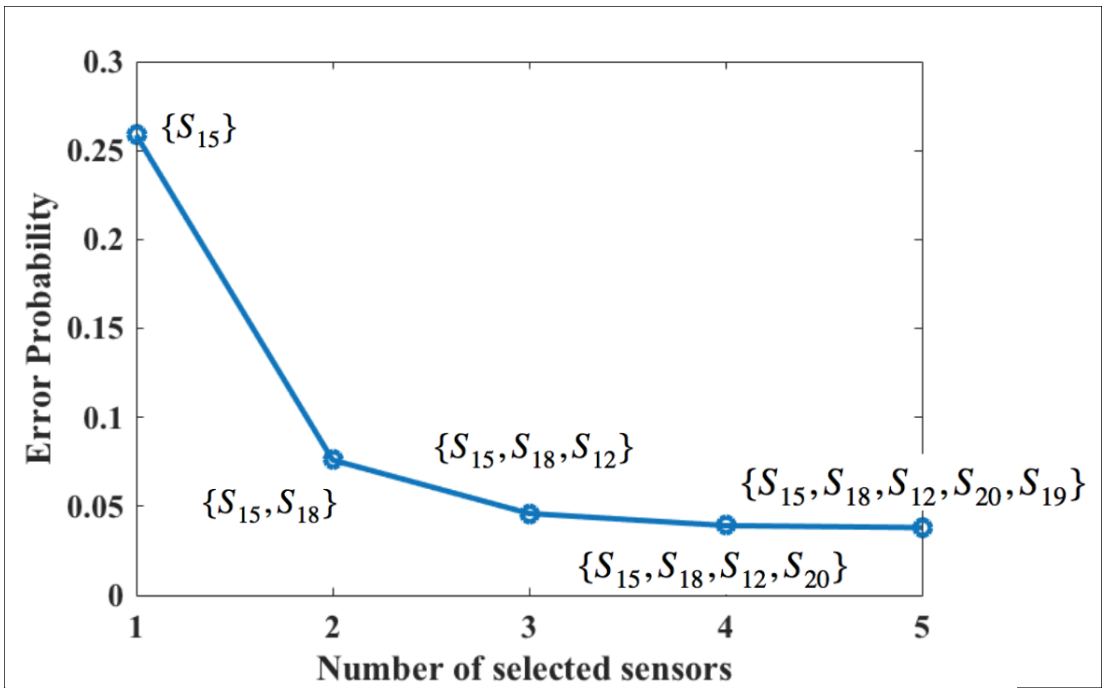
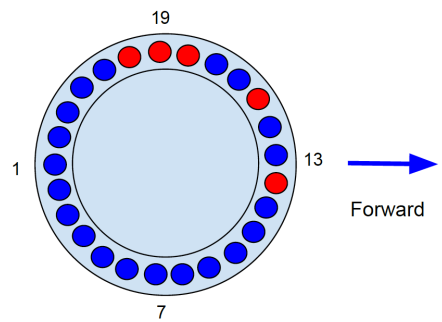


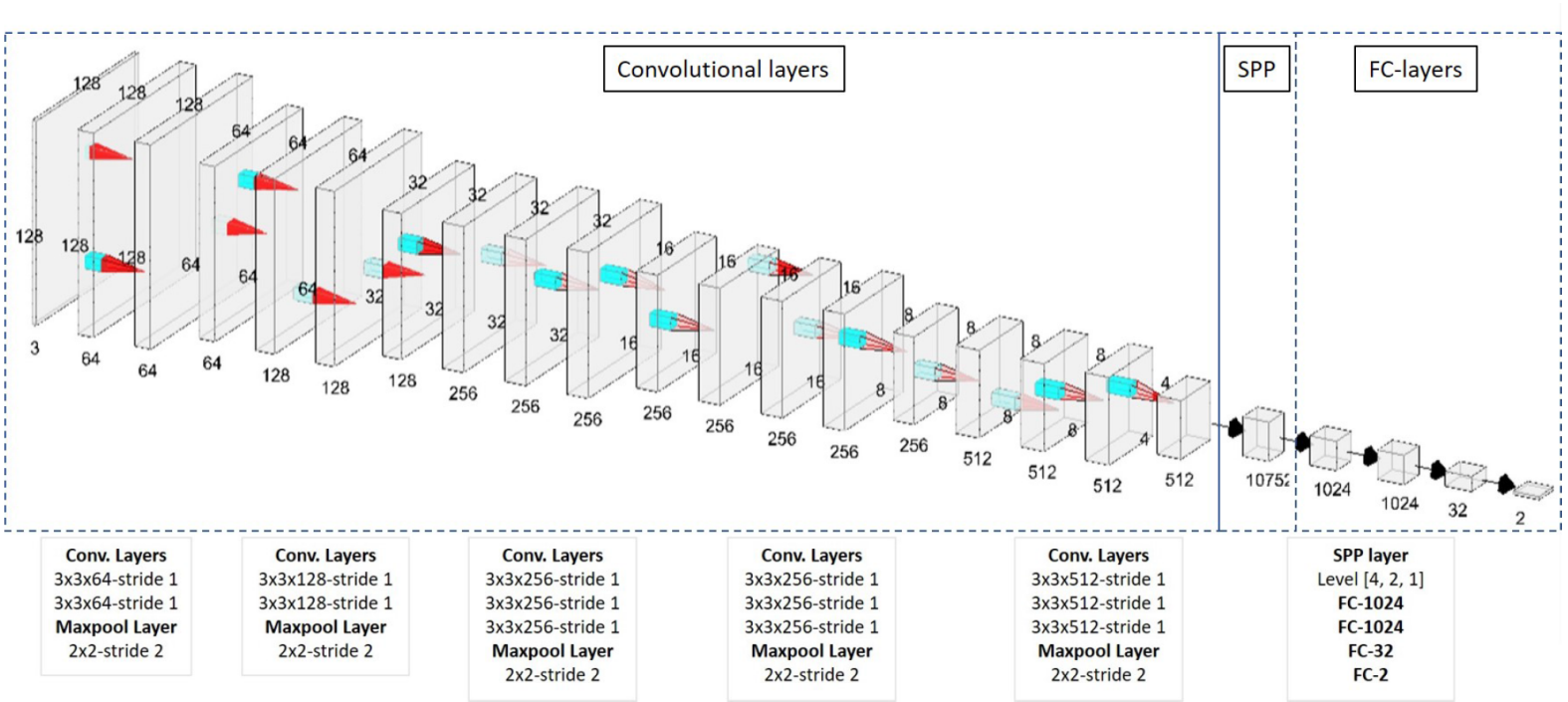
Figure: Sensor-selection curve



The top ranked 5 sensors selected

- 4 HP divergences estimated for each of 4 one-vs-all-classifiers
- These estimates mapped to average Bayes error using upper HP bound
- Greedy step-up and step down sensor selection procedures implemented
- 3 sensors suffice to force estimated misclassification error below 0.05.

Mutual information estimation: application to DNN information bottleneck



Convolutional neural network (CNN) for image classification[1]

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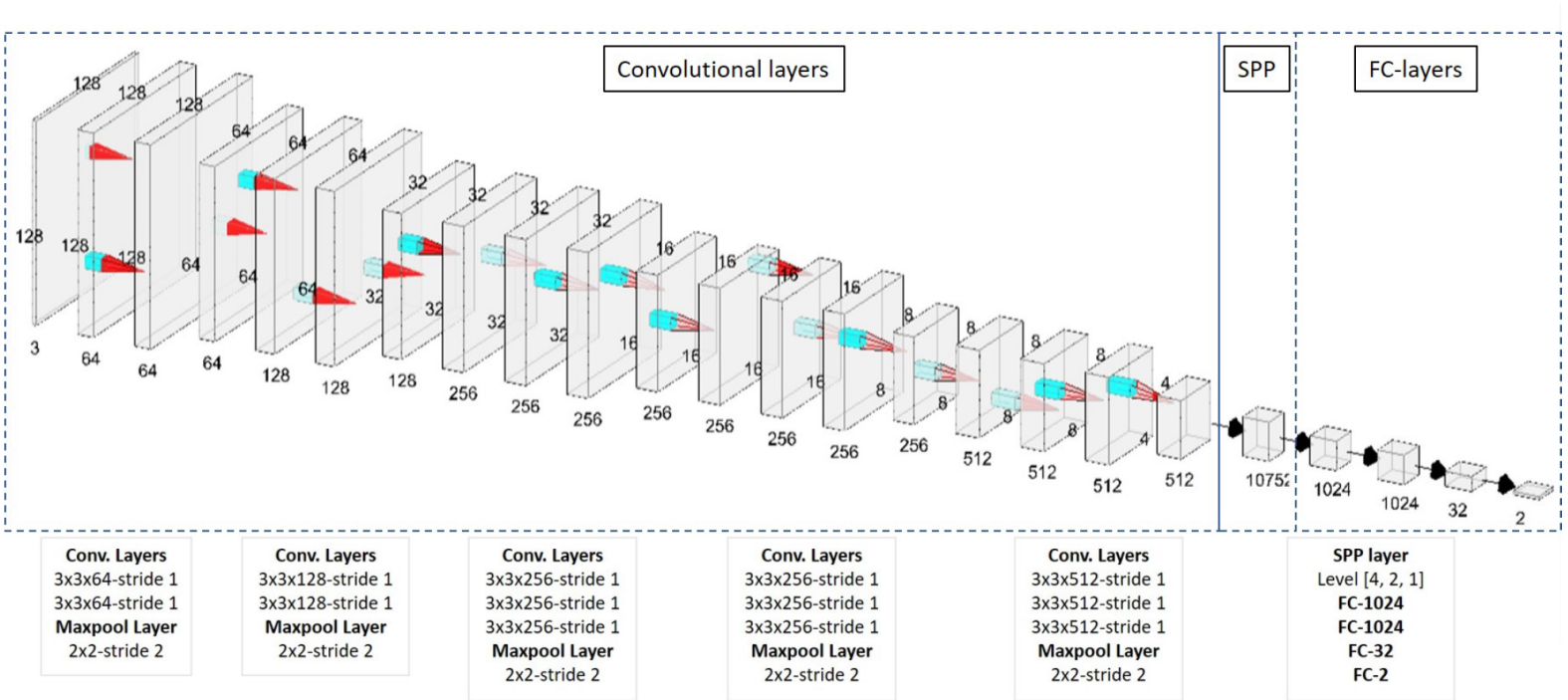


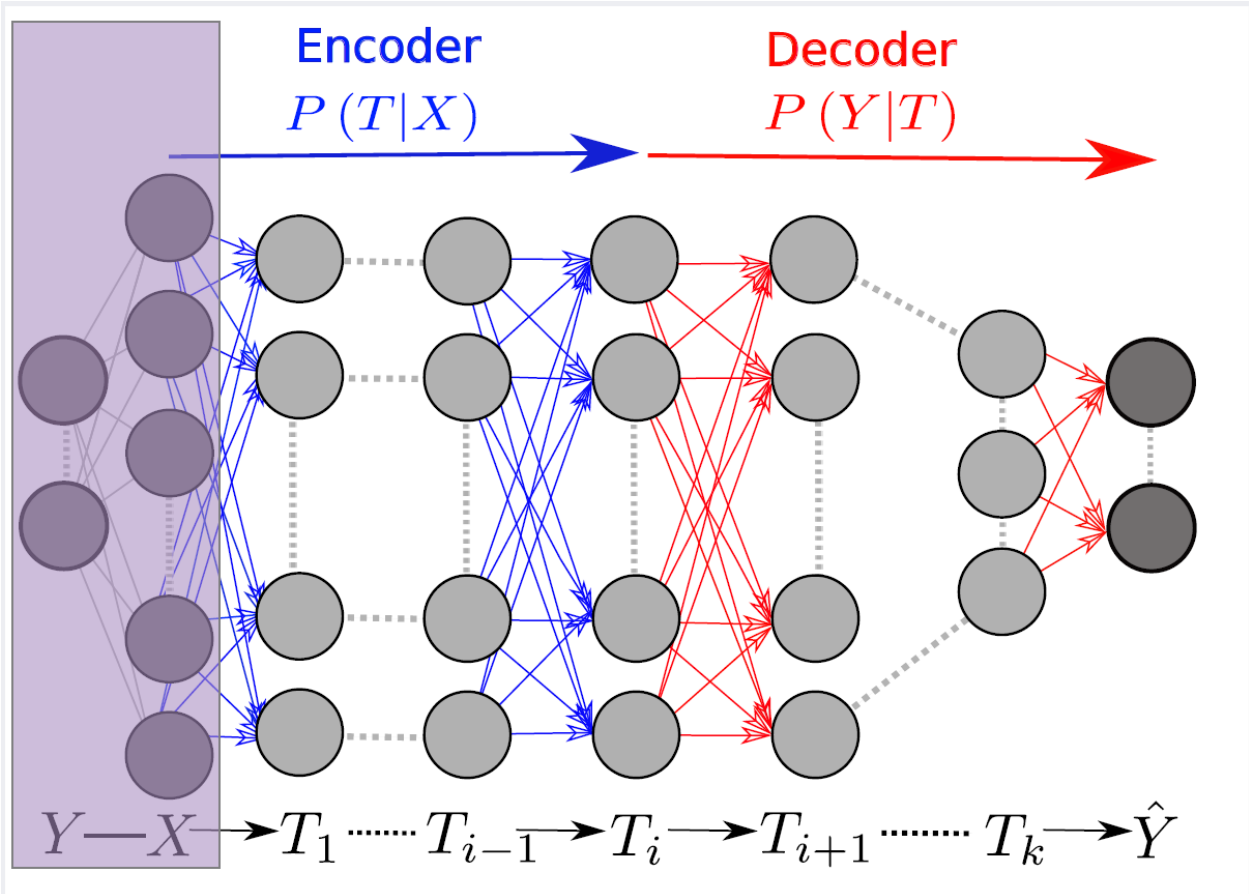
Convolutional neural network (CNN) for image classification[1]

DNN design questions:

- How many input (convolution) layers?
- How many output (discrimination) layers?
- How much pooling and what kind of activation functions?
- How to set learning rate parameters?

[1] B. DuFumier. A new deep learning approach to solar flare prediction. ENSTA internship report, Sept. 2018

Tishby's framework: encoder/decoder information bottleneck

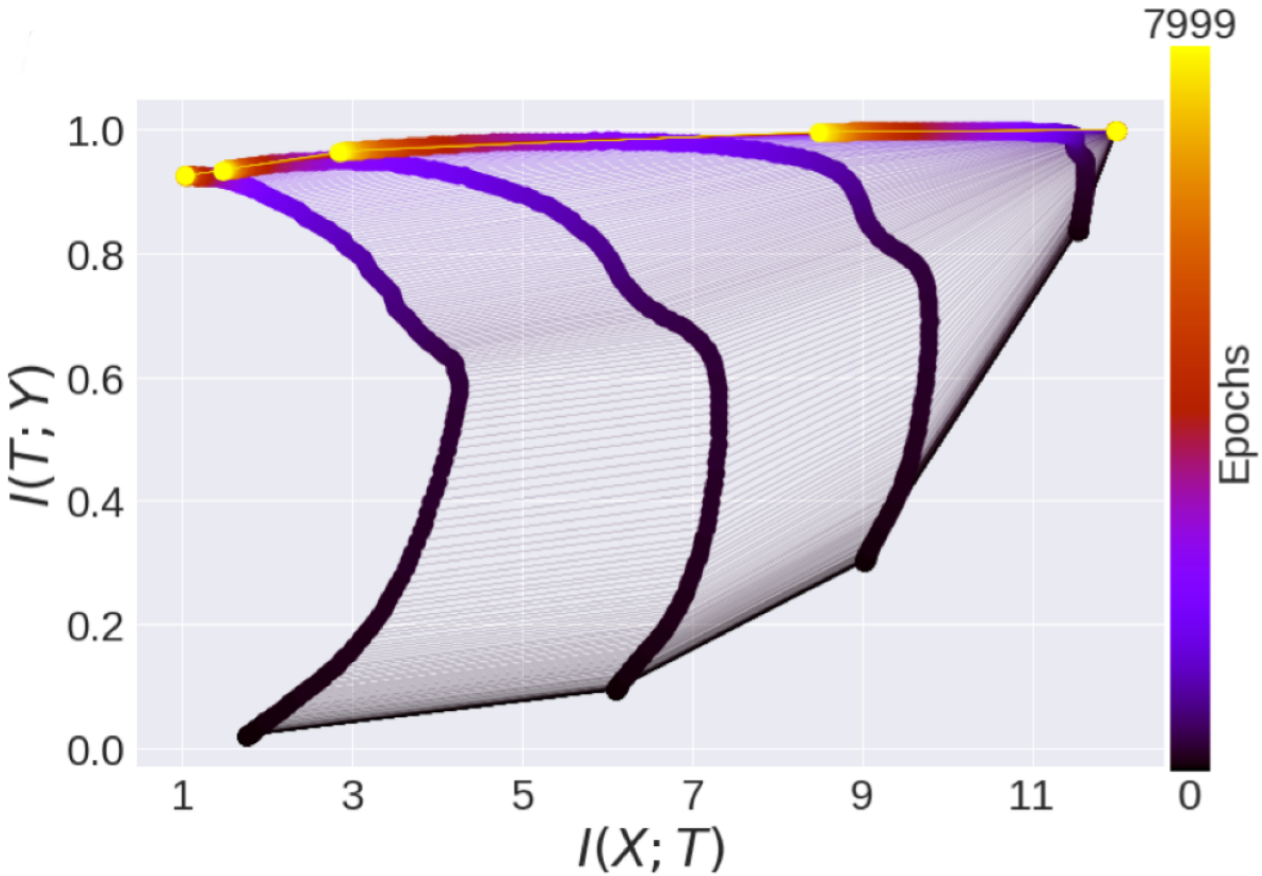


- Encoder I/O: input X, ouptut T (features)
- Decoder I/O: input T, output Y (labels)

[1] R Schwartz-Ziv and N Tishby. Opening the black box of deep neural networks via information. arXiv 2017

[2] AM Saxe, Y. Bansal, J. Dapello, M. Advani, A. Kolchinsky, BD Tracey, DD. Cox, "On the information bottleneck theory of deep learning," ICLR 2018

The information plane



- Plot of training-trajectories of $[I(X;T_i), I(T_i;Y)]$ for different layers T_i

$$I(X;T) = \int f_{XT} \log\left(\frac{f_{XT}}{f_X f_T}\right), \quad I(T;Y) = \int f_{TY}\left(\frac{f_{TY}}{f_T f_Y}\right)$$

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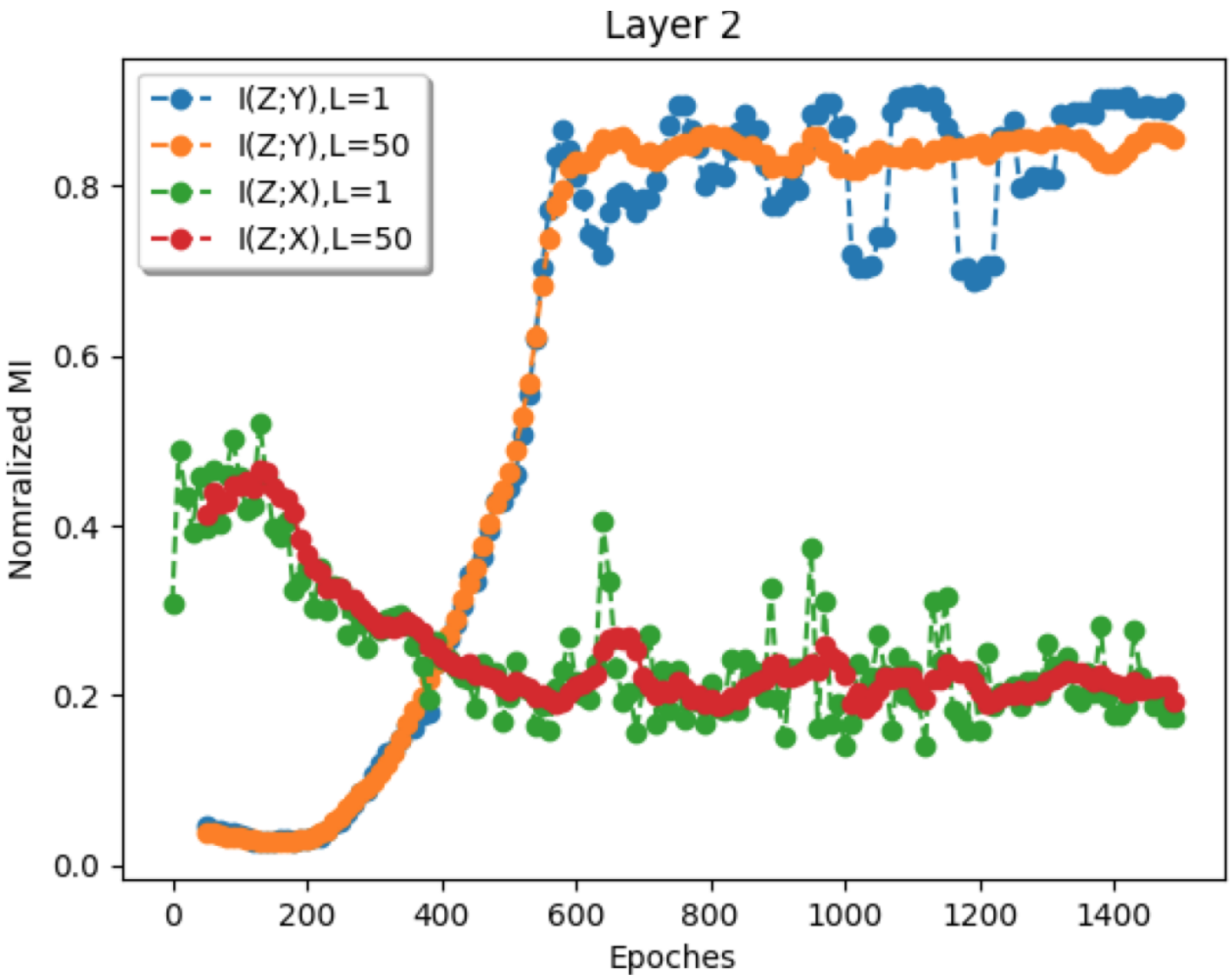
Information plane improvements via ensemble MI estimation



- 10-8-6-4-2 ReLu MLP trained on 10,000 samples of 10D Gaussian
- MI with $L = 1$ (green&blue) is identical to Tishby's implementation
- Proposed ensemble MI implementation (red&orange) is more stable

Summary and open problems

Main takeaways

- Meta-learning v0: Constructing weak base learners of Bayes error rate (BER) for multiclass
- Meta-learning v1: Ensemble learning of BER with optimized data-independent weights
- LSH ensemble method achieves rate optimal performance in both computational complexity and sample complexity
- Illustrated for MNIST digit classification, feature selection, and DNN information bottleneck

Summary and open problems

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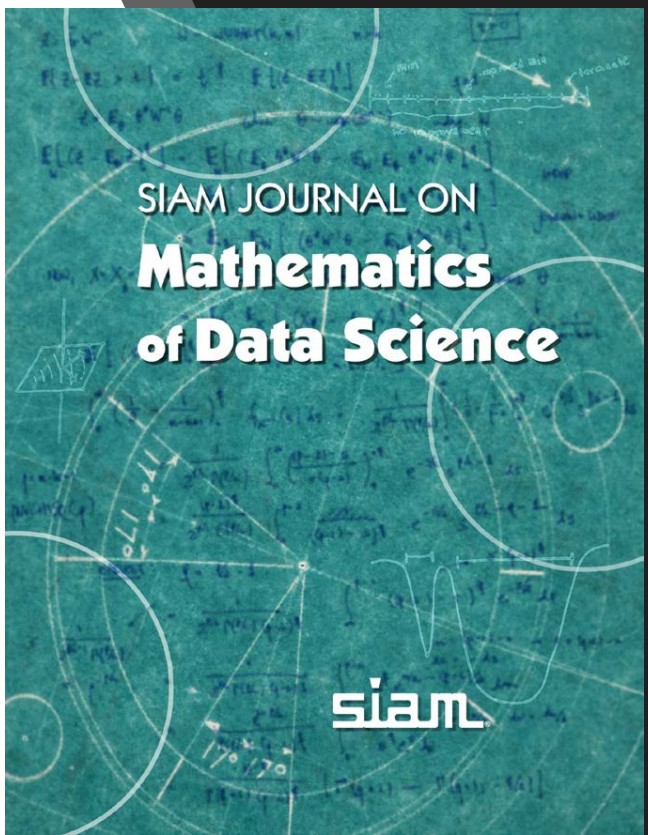
Open problems

- Weakening of d-times differentiability and strict boundedness on density
- High-dimensional learning regimes: $n, d \to \infty$
- Partially labeled data: Learning to benchmark semisupervised classification

New journal



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- http://www.siam.org/journals/simods.php

Thanks

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Hoanan Zhu (EECS)
Oskar Singer (EECS)
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Yun Wei (AIM)
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Byoung Jang (Statistics)

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Geoff Ginsburg (Duke)
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Ed Zelnio (AFRL)
Sutunay Choudhouri (PNNL)
Earl Lawrence (LANL)

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