Learning to benchmark

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- Morteza Noshad - Stanford
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- Dennis Wei - IBM AI

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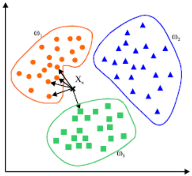
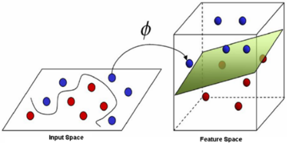
- DARPA Predicting Health and Disease, Biochronicity and Prometheus Programs
- NSF: Theoretical Foundations Program
- NIH: Biomedical Imaging Institute
- DOE: NNSA Consortia for Verfication Technology (CVT) and Exploitation of Technolological Innovations (ETI)

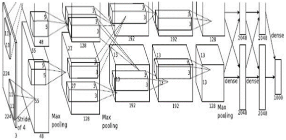
Benchmarks in Machine Learning



kNN classifier

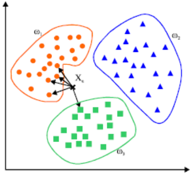


SVM classifier



CNN classifier

Benchmarks in Machine Learning



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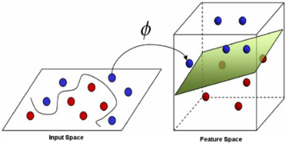

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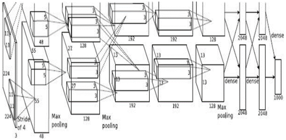

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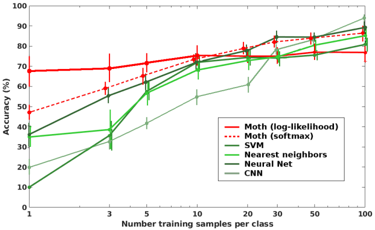
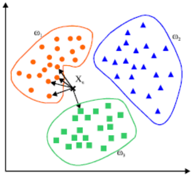


Accuracy for MNIST (Delahunt *et al* 2019)

Benchmarks in Machine Learning



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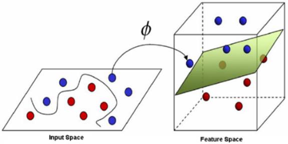

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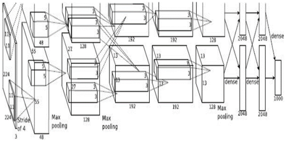

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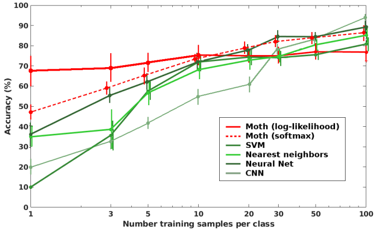

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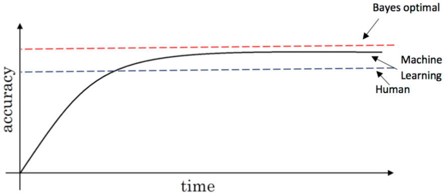

Bayes-optimal benchmark
(Andrew Ng's Blog, Dec. 22, 2018)

Learning to benchmark classification accuracy without learning a classifier

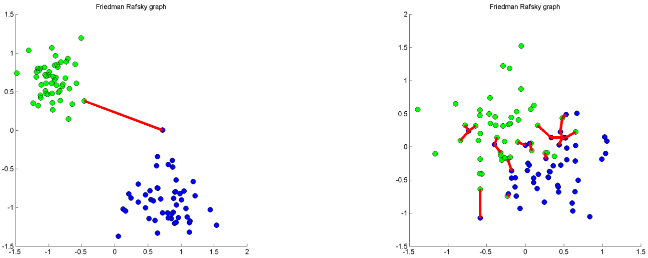

Figure: Friedman-Rafsky statistic converges to bound on Bayes classification error.

- Q: Can we find data-driven empirical upper and lower bounds on Bayes error?

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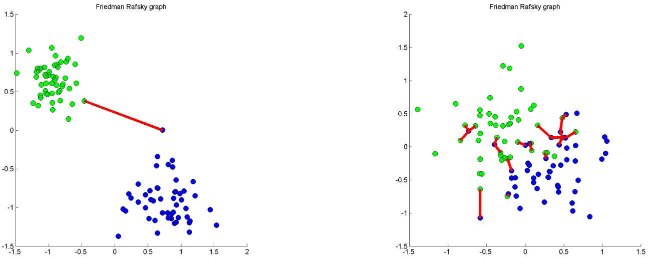

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- Q: Can we find data-driven empirical upper and lower bounds on Bayes error?
- A: The FR statistic[1] directly estimates a bound[2] on Bayes error[3]

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Benchmarking performance of Bayes classifier

Consider classification problem

- $Y \in \{0, 1\}$ an unknown label with priors $\{q, p\}$, $p + q = 1$.

$$P(Y = k) = p^k q^{1-k}, \quad k = 0, 1$$

- X an observed random variable with conditional distribution

$$f(x|Y = k) = [f_1(x)]^k [f_0(x)]^{1-k}, \quad k = 0, 1$$

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

$$C(x) = \mathrm{argmax}_{k\in\{0,1\}}\{P(Y=k|X=x)\}$$

Bayes error rate: best achievable misclassification error probability

Bayes error rate is avg missclassification error probability of Bayes classifier

$$\epsilon_p(f_0, f_1) = P(C(X) \neq Y)$$

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Integral representation

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Alternative representation as an f-divergence btwn distributions

$$\epsilon_p(f_0, f_1) = \frac{1 + |p - q|}{2} - \frac{1}{2} \int g(f_1(x)/f_0(x)) f_0(x) dx,$$

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]:

$$D_g(f_1 \| f_0) = \int g\left(\frac{f_1(x)}{f_0(x)}\right) f_0(x) dx$$

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

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Properties: if g is strictly convex then $D_g(f_1\|f_0)$ is

- reflexive non-negative: $D_g(f_1\|f_0) \geq 0$ with equality iff $f_1 = f_0$
- monotone: $D_g(f_1\|f_0)$ non-increasing under transformations $x \to T(x)$
- jointly convex: $D_g(f_1\|f_0)$ is convex in (f_0, f_1)

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Examples: $g(u) = u\log(u)$ (KL); $g(u) = (1 - u^\alpha)\frac{1}{1-\alpha}$ (Rényi-α), etc.

[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.

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Instances of f-divergences

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

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

$$D^{TV}(f_1\|f_2) = \frac{1}{2}\int |f_1(x) - f_2(x)|dx$$

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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].

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HP bound tighter than Bhattacharya for $p = 1/2$. [1]

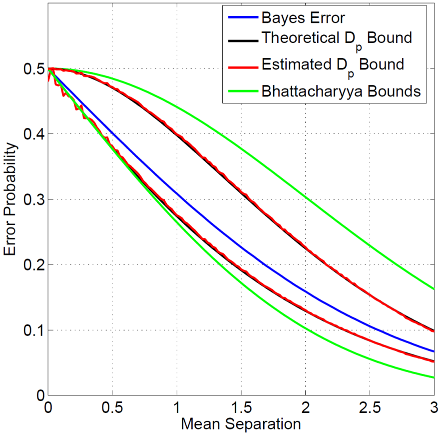

Figure: The HP bound using D_p is tighter than the Bhattacharrya bound using BC for bivariate normal distribution.

[1] V. Berisha, A. Wisler, A.O. Hero, and A. Spanias (2016), Empirically Estimable Classification Bounds Based on a Nonparametric Divergence Measure IEEE T. Signal Processing, 64:3:580-591.

Empirical Estimation of f-Divergence

- **Goal**: Accurate and computationally fast estimation of f-divergence
- **Density plug-in estimator of f-divergence:**

$$\widehat{D_g}(f_1 \| f_0) = \int g\left(\frac{\widehat{f_1}(x)}{\widehat{f_0}(x)}\right)\widehat{f_0}(x)dx$$

where

  - $\widehat{f_0}, \widehat{f_1}$ are density estimates, e.g., with kernel bandwidth parameter ϵ
  - Gabor kernel, histogram, k-NN kernel[1] (Devroye 2012)

- **Root mean squared error (RMSE)** decreases slowly in n=#samples

$$\mathrm{RMSE} = \sqrt{\mathrm{Bias}^2 + \mathrm{Variance}} = cn^{-1/2d}$$

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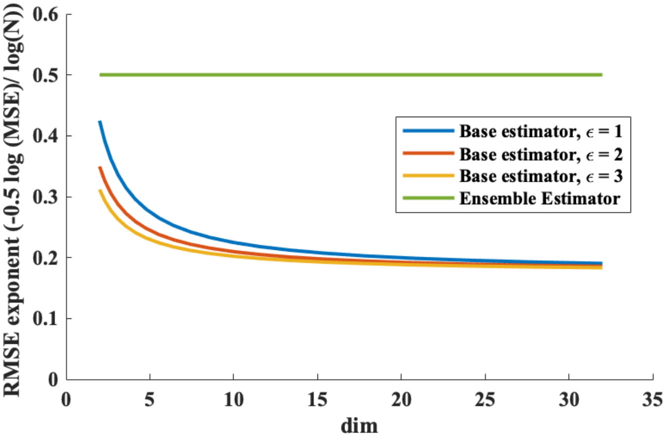
$\Rightarrow$ Compare to optimal *parametric* RMSE rate:

$$\mathrm{RMSE} = \sqrt{\mathrm{MSE}} = cn^{-1/2}$$

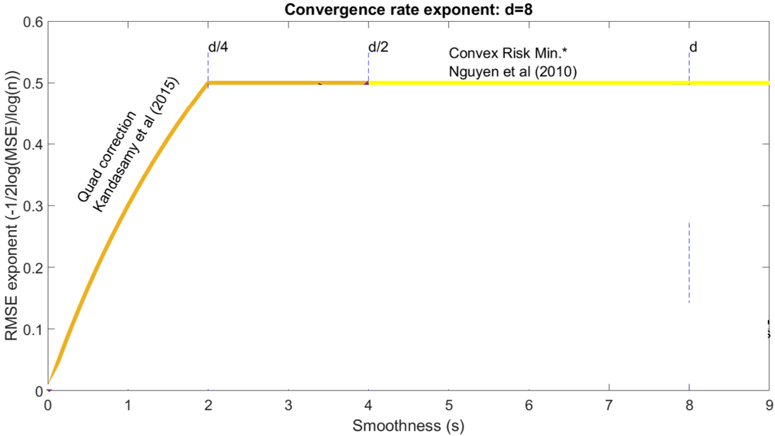
[1] L. Devroye, G. Lugosi, "Combinatorial methods in density estimation," Springer 2012.

Optimal $\sqrt{n}$ RMSE rates are achievable with ensemble estimation[1]



[1] K.R. Moon, K. Sricharan, K. Greenewald, and A.O. Hero (2018), "Ensemble Estimation of Information Divergence," Entropy

RMSE convergence rate comparisons[1,2]

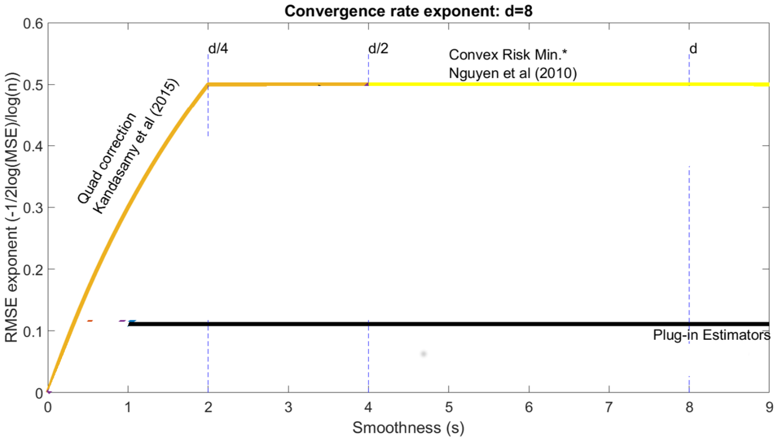


$\Rightarrow$ Kandasami's quadratic estimator achieves $O\left(\min\{n^{-3s/(2s+d)}, n^{-1/2}\}\right)$

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

[2] X. Nguyen, M. Wainwright, M. Jordan "Estimating divergence functionals and the likelihood ratio by convex risk minimization." IEEE Trans on Information Theory, 2010.

RMSE convergence rate comparisons[1]



⇒ 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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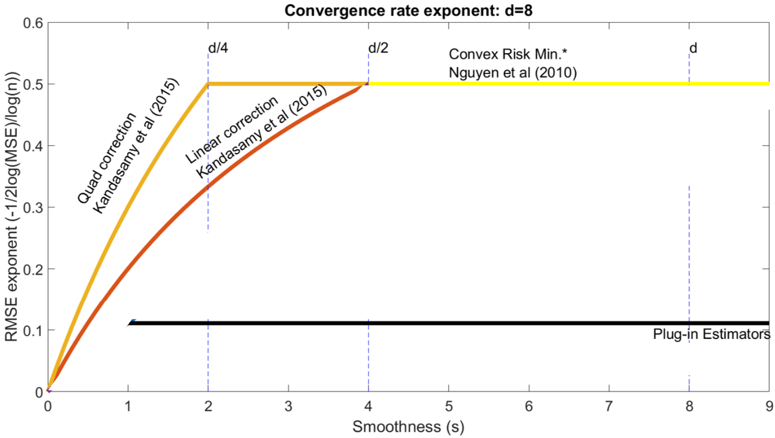

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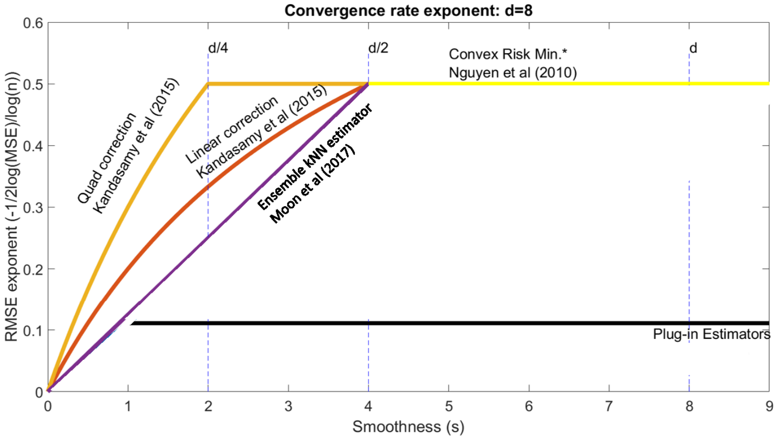

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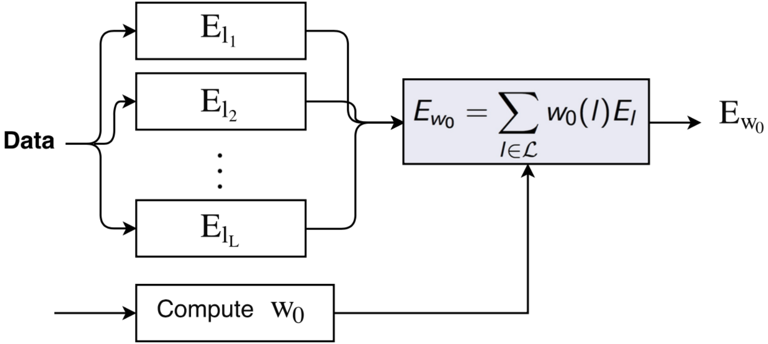
Boosting ensembles concept



- $\{E_{l_i}\}_{i=1}^{L}$ ensemble of base estimators (weak learners)
- $\mathbf{w}_0 = (w_0(l))_{l=1}^{L}$ a vector of boosting weights
- $E_{\mathbf{w}_0}$: combined base estimators (boosted learner)

Choice of boosting weights

Most boosting approaches use *data-dependent* weights:

- Boosting classifiers with Adaboost[1] and other objective functions.

[1] Y. Freund and R. E. Schapire (1996). Experiments with a new boosting algorithm. Intl Conf on Machine Learning. pp. 148-156.

[2] 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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Choice of boosting weights

Most boosting approaches use *data-dependent* weights:

- Boosting classifiers with Adaboost[1] and other objective functions.

Under some conditions such methods achieve Bayes optimal performance[2]

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This can be applied to different base estimation methods:

- Kernel density estimates (KDE)
- k-NN density estimates
- NN ratio estimates
- Locality sensitive hashing (LSH) density estimates

---

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Locality sensitive hashing (LSH) plug-in estimator

$$\widehat{D}_g(f_1 \| f_0) := \sum_{i: M_i > 0} g\left(\frac{N_i/N}{M_i/M}\right) M_i/M$$

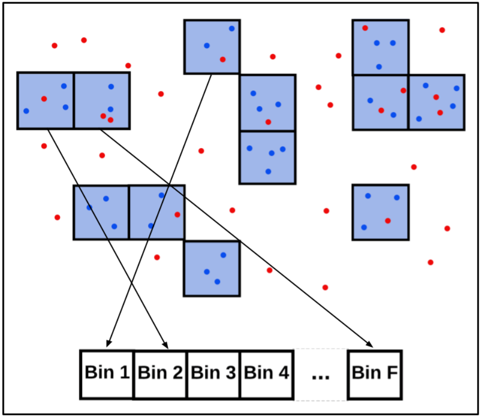

Figure: LSH quantizes **X** data with cell resolution ϵ and random displacement b

Locality sensitive hashing plug-in estimator: bias and variance

Theorem (Bias Expansion)

If f_0 and f_1 are d-times differentiable, the mean of $\widehat{D}_g$ has representation

$$\mathbb{E}[\widehat{D}_g] = D(f_1 \| f_0) + \mathbb{B}(\widehat{D}_g)$$

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

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

Ensemble bias reduction: an inverse problem

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

Define: Ensemble divergence estimator $\widehat{D}_{\mathbf{w}} := \sum_{j=1}^{L} w_j \widehat{D}_{\epsilon(t_j)} = \mathbf{w}^T \hat{\mathbf{D}}_\epsilon$

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$\Rightarrow$ For large d, Chebychev methods used to stabilize solution (Noshad '19)

Ensemble estimator variance needs also to be controled

Variance of ensemble divergence estimator is quadratic in **w**

$$\mathbb{V}(\widehat{D}_{\mathbf{w}}) = \mathbb{V}(\mathbf{w}^T \hat{\mathbf{D}}_{\epsilon}) = \mathbf{w}^T \mathrm{cov}(\hat{\mathbf{D}}_{\epsilon}) \mathbf{w} \leq \|\mathbf{w}\|^2 \lambda_{max}.$$

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$\Rightarrow$ Select **w** as solution to linearly constrained quadratic program

$$\begin{aligned} \min_{\mathbf{w}} \quad & \|\mathbf{w}\|_2 \\ \textit{subject to} \quad & \sum_{j=1}^{L} w_j = 1, \\ & \sum_{j=1}^{L} w_j t_j^i = 0, i \in [d] \end{aligned}$$

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Variance of ensemble divergence estimator is quadratic in $\mathbf{w}$

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$\Rightarrow$ Select $\mathbf{w}$ as solution to linearly constrained quadratic program

$$\begin{aligned} \min_{\mathbf{w}} \quad & \|\mathbf{w}\|_2 \\ \textit{subject to} \quad & \sum_{j=1}^{L} w_j = 1, \\ & \sum_{j=1}^{L} w_j t_j^i = 0, \, i \in [d] \end{aligned}$$

- If $L > d$, the solution $\mathbf{w}^*$ ensures MSE of $O(1/n)$.
- Weights are computed offline, not dependent on data or data's distribution

Benchmark learner for multiclass classification

Simulation: $K = 4$ classes in concentric sphere regions over $d = 20$ dimensions

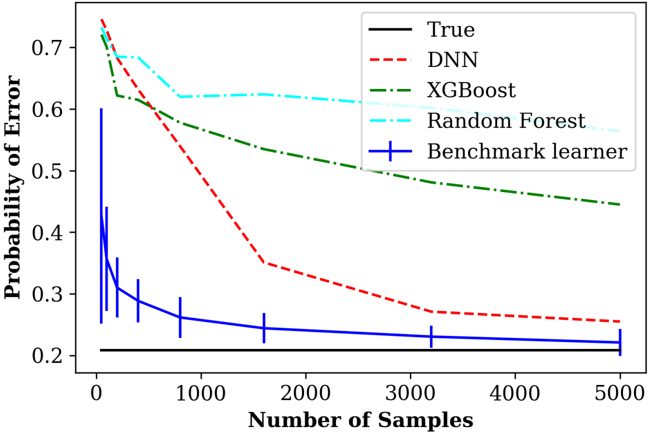
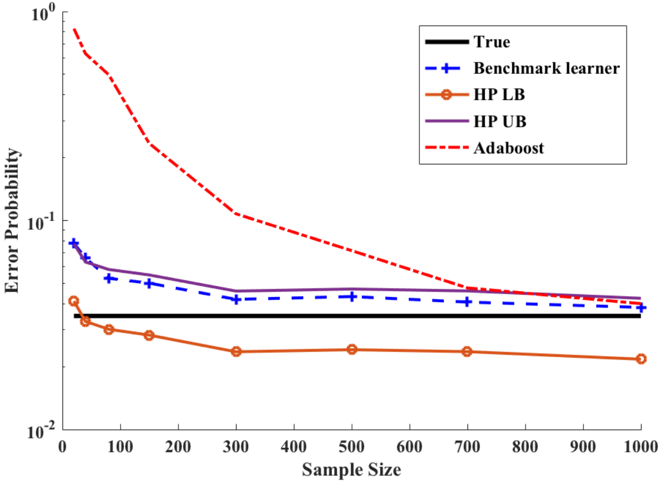


Figure: Benchmark learner indicates small margin for improvement. DNN: 5 hidden layers with [20,64,65,10,40 RELU neurons trained with ADAM and 10% dropout.

Benchmark learner as a minibatch stopping rule

Simulation: classification of 2 mean shifted 10 dim Gaussian densities

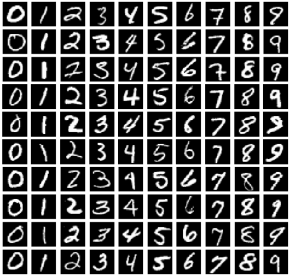


Ref: Noshad and Hero, AISTAT 2018

Benchmarking MNIST digit classification

MNIST handwritten digit corpus:

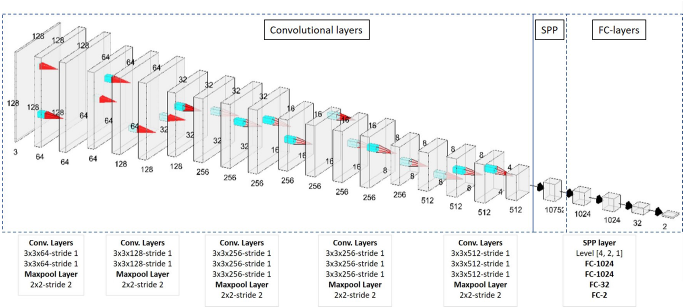
- $K = 10$ classes
- $d = 784$ dimensions
- $n = 60,000$ samples



Papers	Method	Error rate
(Cireşan et al., 2010)	Single 6-layer DNN	0.35%
(Ciresan et al., 2011)	Ensemble of 7 CNNs and training data expansion	0.27%
(Cireşan et al., 2012)	Ensemble of 35 CNNs	0.23%
(Wan et al., 2013)	Ensemble of 5 CNNs and DropConnect regularization	0.21%
Benchmark learner	Ensemble ϵ-ball estimator	0.14%

Table 1: Comparison of error probabilities of several the state of the art deep models with the benchmark learner, for the MNIST handwriting image classification dataset

Mutual information estimation: application to DNN information bottleneck



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

- DNNs have remarkable empirical performance,

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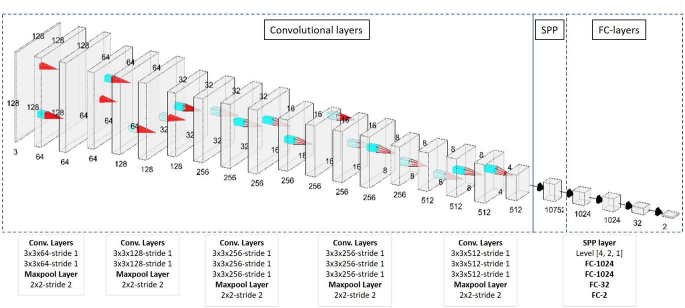

Convolutional neural network (CNN) for image classification[1]

- DNNs have remarkable empirical performance, but there is limited understanding of why DNN perform so well

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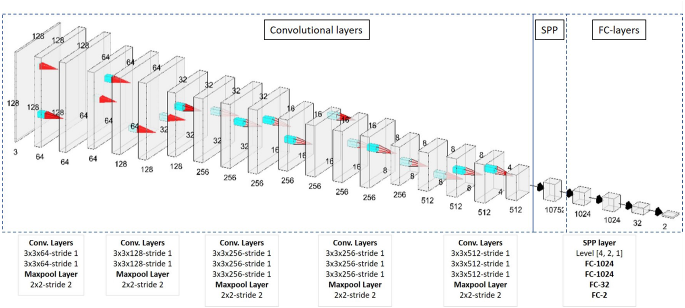


Convolutional neural network (CNN) for image classification[1]

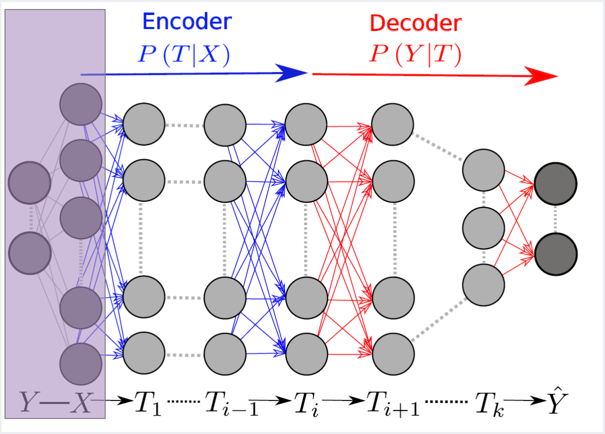
- DNNs have remarkable empirical performance, but there is limited understanding of why DNN perform so well

The compositional learning hypothesis:
DNN's learn in two phases:

- Phase 1: learn the easy cases (**memorize**)
- Phase 2: generalize to the hard cases (**compress**)

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

Tishby's framework: encoder/decoder information bottleneck

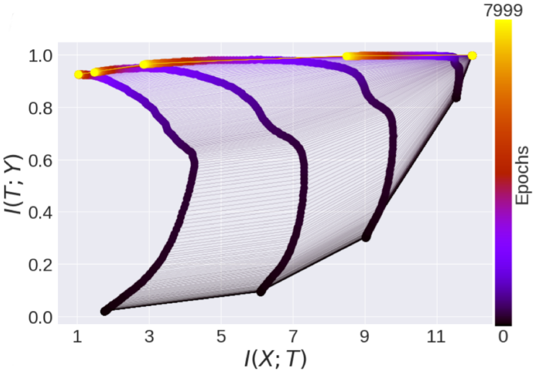


- Encoder I/O: input X, ouptut T (features)
- Decoder I/O: input T, output Y (labels)

[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

Information plane: a layer-by-layer plot of discrimination vs. compression



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

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

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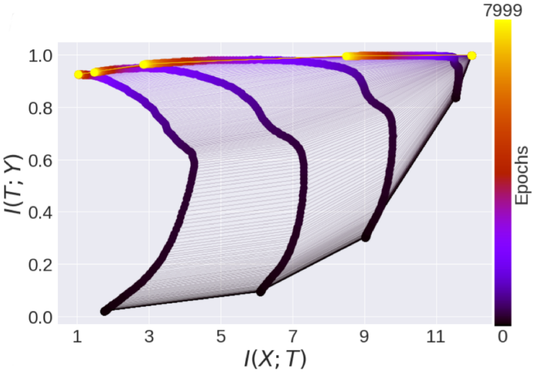

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- Schwartz-Ziv&Tishby[1] observed **memorization→compression** for *tanh* activation (MLP 10-8-6-4-2 and classification of 10D Gaussian)

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

Does memorization→compression depend on activation function?

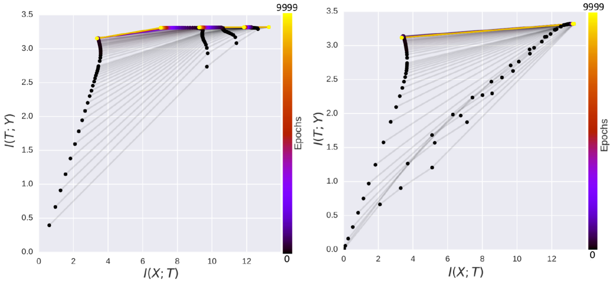

Figure: Figure 1.C (*tanh*) and 1.D (*ReLU*) from Saxe *et al*[1]

- 784-1024-20-20-20-10 MLP trained on MNIST dataset
- Output layer: *sigmoid*. Hidden layers: *tanh* at left and *ReLu* at right.
- Trained using SGD on cross–entropy loss with minibatch size 128
- Learning rate= 0.001 and, at convergence, achieved error rate 0.98

[1] Saxe, Bansal, Dapello, Advani, Kolchinsky, Tracey, and Cox, "On the information bottleneck theory of deep learning," ICLR, 2018.

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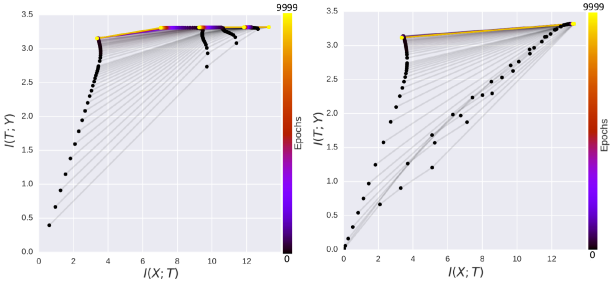

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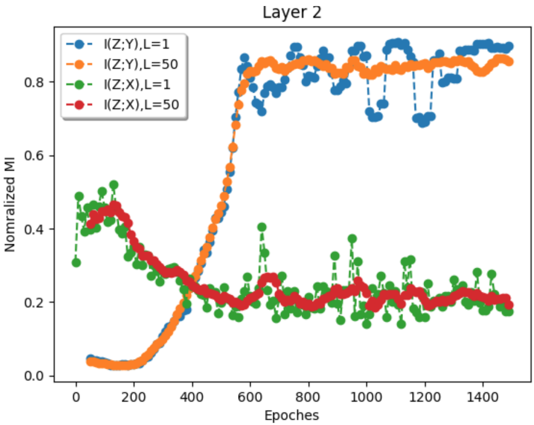
- Saxe *et al* claim that *ReLU* inner layers **exhibit no compression**

[1] Saxe, Bansal, Dapello, Advani, Kolchinsky, Tracey, and Cox, "On the information bottleneck theory of deep learning," ICLR, 2018.

Information plane for MLP/*ReLU* using ensemble MI estimation



- 10-8-6-4-2 MLP/*ReLU* trained on 10,000 samples of 10D Gaussian
- MI with $L = 1$ (green&blue) is the Schwartz-Ziv&Tishby MI estimate
- Proposed ensemble MI implementation[1] (red&orange) is more stable

[1] Noshad, Yu, Hero, "Scalable MI estimation using dependence graphs," ICASSP 2019.

Ensemble estimation provides confirmatory evidence

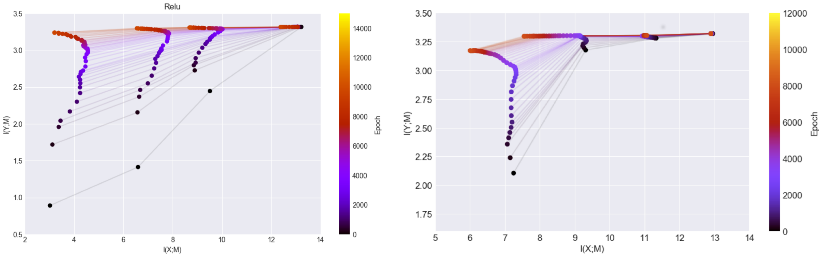


Figure: Left: **MLP/ReLU** 784-1024-20-20-20-10. Right: **CNN/ReLU** 784-4-8-16-10

- MLP and CNN trained on MNIST dataset[1]

⇒ Memorization→Compression phenonomon occurs in both MLP and CNN

[1] Noshad, Yu, Hero, "Scalable MI estimation using dependence graphs," ICASSP 2019.

Summary

Main takeaways

- Learning to benchmark involves 2 types of meta-learning
  - Meta-learning v0: Learning ensembles of weak base-learners (Freund&Schapire 1996)
  - Meta-learning v1: Learning the Bayes error rate (BER)[1][2][3]

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- LSH ensemble method achieves rate optimal performance in both computational complexity and sample complexity
- Benchmark learning applications demonstrated:
  - Performance monitoring: learning sufficient sample size
  - Feature learning: performing data-driven feature selection
  - Interpretable learning: exploring DNN compositional learning hypothesis

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Supplement: Chebyshev stabilization of ensemble wieghts ($L = 10$)

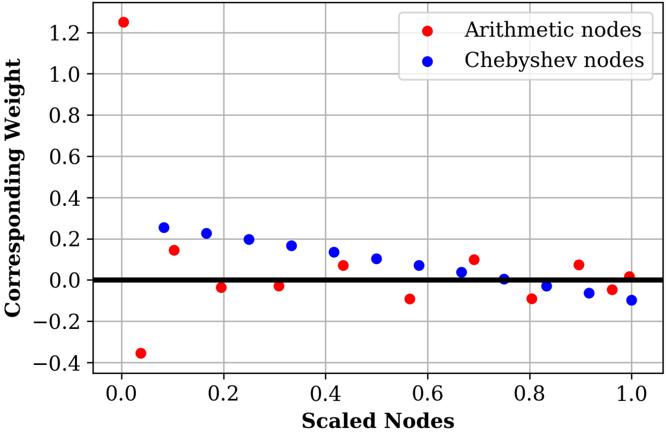

Figure: For $L = 10$ the arithmetic nodes (bandwidth scaled by $k, k+1, \ldots$) give weights with higher dynamic range than the proposed Chebyshev node approach.

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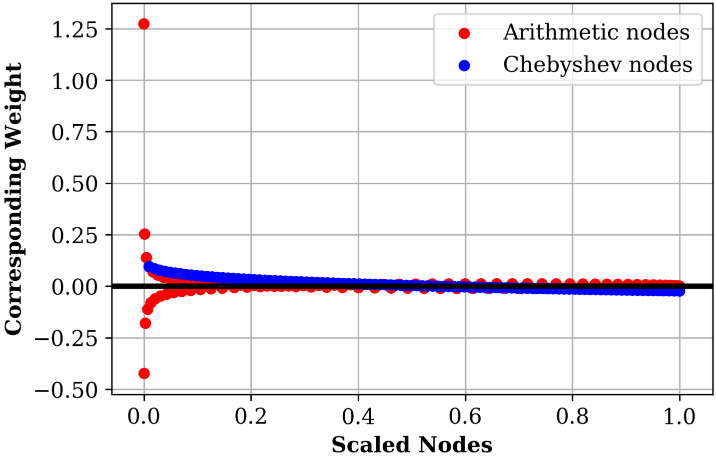

Figure: For $L = 100$ the arithmetic nodes (bandwidth scaled by $k, k+1, \ldots$) give weights with much higher dynamic range than the proposed Chebyshev node approach.

Supplement: Chebyshev wieghts improve MSE of benchmark learner

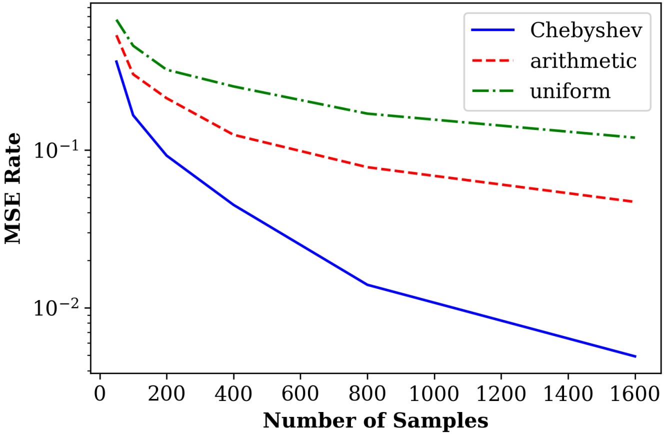

Figure: For a binary classification problem (mean of Gaussian isotropic dsn in dim $d = 100$) the proposed Chebyshev node approach provides significant improvement of MSE in Bayes estimation error rate.

Thanks

Questions?