The quest for provably efficient ML algorithms

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Joint with:
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Data

⟺

Computations

Outline

Learning theory: statistics and computations

A case study: scalable kernel methods

Empirical results

Supervised learning

From data

$$(x_i, y_i)_{i=1}^n$$

to predictions

$$f(x_{\text{new}}) \approx y_{\text{new}}$$

Statistical supervised learning

Given $(x_i, y_i)_{i=1}^n \sim P(x, y)^n$ find $\widehat{f}$ with small

$$L(\widehat{f}) = \mathbb{E}[\ell(y, \widehat{f}(x))]$$

Empirical risk minimization

Minimize

$$\widehat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i))$$

over some space $\mathcal{H}$, e.g.

- $f(x) = \theta^\top x$
- $f(x) = \theta^\top \Phi(x)$ (kernels)
- $f(x) = w^\top \sigma(Wx)$, $\theta = (w, W)$, (neural nets)

+weights constraint:

Error analysis

How good is the ERM solution $\widehat{f}_R$?

$$\mathbb{E}[L(\widehat{f}_R)] - \min L$$

Bias and variance

Idealized ERM: f_R minimize L (**with** weights constraint).

$$
\begin{aligned}
&\mathbb{E}[L(\widehat{f}_R)] - \min L \\
&= \mathbb{E}[L(\widehat{f}_R)] - L(f_R) + L(f_R) - \min L
\end{aligned}
$$

A typical bound

$$
\begin{aligned}
&\mathbb{E}[L(\widehat{f}_R)] - \min L \\
&= \mathbb{E}[L(\widehat{f}_R)] - L(f_R) + L(f_R) - \min L \\
&\lesssim \frac{R}{n} + \frac{1}{R}
\end{aligned}
$$

$$
R = \sqrt{n} \quad \Longrightarrow \quad \mathbb{E}[L(\widehat{f}_R)] - \min L \lesssim \frac{1}{\sqrt{n}}
$$

A grain of salt

It's just an example of bound!

$$\mathbb{E}[L(\widehat{f}_R)] - \min L \lesssim \frac{R}{n} + \frac{1}{R}$$

$$R = \sqrt{n} \quad \Longrightarrow \quad \mathbb{E}[L(\widehat{f}_R)] - \min L \lesssim \frac{1}{\sqrt{n}}$$

- bounds depend on P! Much better/worse bounds possible.
- bounds depend on setting! e.g. classification, $n \ll d$ (interpolation)...

What about computations?

Optimization

ERM

$$\min_{\theta} \widehat{L}(f_{\theta})$$

by gradient descent

$$\widehat{\theta}_{t+1} = \widehat{\theta}_t + \gamma_t \nabla \widehat{L}(f_{\widehat{\theta}_t})$$

Another error decomposition

$$\mathbb{E}[L(f_{\widehat{\theta}_t})] - \min L$$
$$= \mathbb{E}[L(f_{\widehat{\theta}_t})] - \mathbb{E}[L(\widehat{f}_R)] + \mathbb{E}[L(\widehat{f}_R)] - \min L$$
$$= \mathbb{E}[L(f_{\widehat{\theta}_t})] - \mathbb{E}[L(\widehat{f}_R)] + \mathbb{E}[L(\widehat{f}_R)] - L(f_R) + L(f_R) - \min L$$

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ERM with square loss

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_\theta(x_i)))^2 + \lambda \|\theta\|^2$$

- $f_\theta(x) = \theta^\top x$
- $f_\theta(x) = \theta^\top \Phi(x), \quad \Phi(x)^\top \Phi(x') = k(x, x')$

Optimization: solving a linear system!

A typical bound and its cost

$$\mathbb{E}[L(\widehat{f}_\lambda)] - \min L \lesssim \frac{1}{\lambda n} + \lambda$$

$$\lambda = 1/\sqrt{n} \quad \Longrightarrow \quad \mathbb{E}[L(\widehat{f}_\lambda)] - \min L \lesssim \frac{1}{\sqrt{n}}$$

For large feature space/kernels the computational cost is

- time $O(n^3)$
- memory $O(n^2)$.

Can we do better? Statistically no but computationally...

An efficient approach: FALKON

- Conjugate gradient+
- subsampling/sketching (Nyström)+
- sketched preconditioning.

Statistical and computational error

$$\mathbb{E}[L(f_{\hat{\theta}_t})] - \min L$$
$$= \mathbb{E}[L(f_{\hat{\theta}_t})] - \mathbb{E}[L(\widehat{f}_\lambda)] + \mathbb{E}[L(\widehat{f}_\lambda)] - \min L$$
$$\lesssim e^{-t/\lambda} + \frac{1}{M^2} + \frac{1}{\lambda n} + \lambda$$

$$\lambda = 1/\sqrt{n}, \quad t = \log n, \quad M = \sqrt{n} \quad \Longrightarrow \quad \mathbb{E}[L(f_{\hat{\theta}_t})] - \min L \lesssim \frac{1}{\sqrt{n}}$$

Just theory?

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Falkon 1.0: some experiments

	MillionSongs ($n \sim 10^6$)			YELP ($n \sim 10^6$)		TIMIT ($n \sim 10^6$)	
	MSE	Relative error	Time(s)	RMSE	Time(m)	c-err	Time(h)
FALKON	**80.30**	$\mathbf{4.51 \times 10^{-3}}$	**55**	**0.833**	**20**	32.3%	**1.5**
Prec. KRR	-	4.58×10^{-3}	$289^{\dagger}$	-	-	-	-
Hierarchical	-	4.56×10^{-3}	$293^{\star}$	-	-	-	-
D&C	80.35	-	737^{*}	-	-	-	-
Rand. Feat.	80.93	-	772^{*}	-	-	-	-
Nyström	80.38	-	876^{*}	-	-	-	-
ADMM R. F.	-	5.01×10^{-3}	$958^{\dagger}$	-	-	-	-
BCD R. F.	-	-	-	0.949	$42^{\ddagger}$	34.0%	$1.7^{\ddagger}$
BCD Nyström	-	-	-	0.861	$60^{\ddagger}$	33.7%	$1.7^{\ddagger}$
KRR	-	4.55×10^{-3}	-	0.854	$500^{\ddagger}$	33.5%	$8.3^{\ddagger}$
EigenPro	-	-	-	-	-	32.6%	$3.9^{\wr}$
Deep NN	-	-	-	-	-	32.4%	-
Sparse Kernels	-	-	-	-	-	**30.9%**	-
Ensemble	-	-	-	-	-	33.5%	-

Table: MillionSongs, YELP and TIMIT Datasets. Times obtained on: $\ddagger$ = cluster of 128 EC2 r3.2xlarge machines, $\dagger$ = cluster of 8 EC2 r3.8xlarge machines, $\wr$ = single machine with two Intel Xeon E5-2620, one Nvidia GTX Titan X GPU and 128GB of RAM, $\star$ = cluster with 512 GB of RAM and IBM POWER8 12-core processor, $*$ = unknown platform.

Falkon 1.0: some more experiments

	SUSY ($n \sim 10^6$)			HIGGS ($n \sim 10^7$)		IMAGENET ($n \sim 10^6$)	
	c-err	AUC	Time(m)	AUC	Time(h)	c-err	Time(h)
FALKON	**19.6%**	0.877	**4**	0.833	**3**	20.7%	**4**
EigenPro	19.8%	-	$6^{\wr}$	-	-	-	-
Hierarchical	20.1%	-	$40^{\dagger}$	-	-	-	-
Boosted Decision Tree	-	0.863	-	0.810	-	-	-
Neural Network	-	0.875	-	0.816	-	-	-
Deep Neural Network	-	**0.879**	$4680^{\ddagger}$	**0.885**	$78^{\ddagger}$	-	-
Inception-V4	-	-	-	-	-	**20.0%**	-

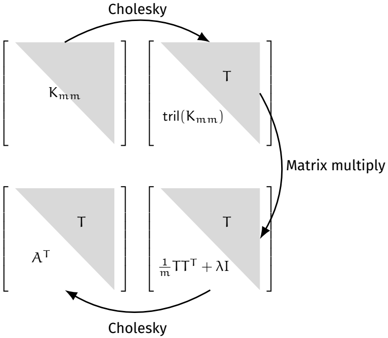
Table: Architectures: $\dagger$ = cluster with IBM POWER8 12-core cpu, 512 GB RAM, $\wr$ = single machine with two Intel Xeon E5-2620, one Nvidia GTX Titan X GPU, 128GB RAM, $\ddagger$ = single machine.

Implementing Falkon 2.0

[Meanti, Carratino, R., Rudi '20]

Function Falkon($X \in \mathbb{R}^{n \times d}$, $y \in \mathbb{R}^n$, λ, m, t):

- $X_m \leftarrow$ RamdomSubsample(X, m);
- $T, A \leftarrow$ Preconditioner(X_m, λ);
- **Function** LinOp(β):
  - $v \leftarrow A^{-1}\beta$;
  - $c \leftarrow k(X_m, X)k(X, X_m)T^{-1}v$;
  - **return** $A^{-\top}T^{-\top}c + \lambda n v$;
- $\text{rhs} \leftarrow A^{-\top}T^{-\top}k(X, X_m)y$;
- $\beta \leftarrow$ ConjugateGradient(LinOp, rhs, t);
- **return** $T^{-1}A^{-1}\beta$;



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Falkon2.0

- Least squares and logisitic loss [Marteau Ferey, Bach, Rudi '18,'19]
- Multi-GPU
- Mixed precision
- Optimized matrix-vector product
- Optimized kernel computation
- Out of core modules

Falkon2.0

Table: Relative performance improvement wrt Falkon 1.0

Experiment	Preconditioner		Iterations	
	Time	Improvement	Time	Improvement
Falkon1.0	2337 s	—	4565 s	—
Float32 precision	1306 s	1.8×	1496 s	3×
GPU preconditioner	179 s	7.3×	1344 s	1.1×
2 GPUs	118 s	1.5×	693 s	1.9×
KeOps	119 s	1×	232 s	3×
Overall improvement		19.7×		18.8×

Falkon2.0: thousands of points in seconds

	MNIST $n = 6 \cdot 10^4, d = 780$	CIFAR10 $n = 6 \cdot 10^4, d = 1024$	SVHN $n = 7 \cdot 10^4, d = 1024$
Falkon	10.9 s	13.7 s	17.2 s
ThunderSVM	19.6 s	82.9 s	166.4 s

Table: Comparing running times of FALKON and ThunderSVM. Parameters were tuned to have approximately the same accuracy.

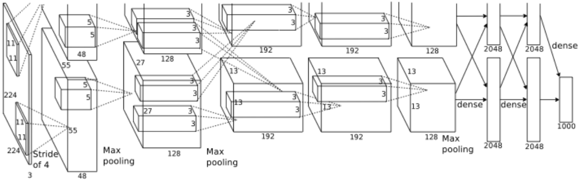
Falkon2.0: millions/billions (!) of points in minutes

	TAXI $n \approx 10^9$		HIGGS $n \approx 10^7$		YELP $n \approx 10^6$, $d \approx 10^7$		TIMIT $n \approx 10^6$	
	RMSE	time(h)	AUC	time(m)	RMSE	time(m)	c-err	time(m)
FALKON	**311.7**	**1**	0.8196	**7.4**	**0.810**	**16.8**	32.27%	**4.8**
LogFALKON	–	–	**0.8213**	37.8	–	–	–	–
EigenPro2	FAIL		FAIL		FAIL		**31.91%**	29
GPyTorch	322.5	10.8	0.8005	52.9	FAIL		–	–
GPflow	313.2	8.5	0.8042	24.3	FAIL		33.78%	44.5

	AIRLINE-CLS $n \approx 10^6$		AIRLINE $n \approx 10^6$		MSD $n \approx 10^5$		SUSY $n \approx 10^6$	
	c-err	time(m)	MSE	time(m)	relative error	time(m)	c-err	time(m)
FALKON	31.5%	**3.1**	**0.758**	**4.1**	4.4834×10^{-3}	**1**	19.67%	**0.4**
LogFALKON	**31.3%**	21.5	–	–	–	–	**19.58%**	1.4
EigenPro2	32.5%	27.2	0.785	24.5	4.4778×10^{-3}	6.3	20.08%	1.5
GPyTorch	33.0%	24.2	0.803	31	4.5344×10^{-3}	15.5	19.71%	16.5
GPflow	32.6%	10.5	0.790	28.7	4.4986×10^{-3}	8.8	19.65%	9.3

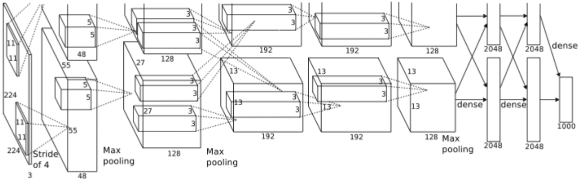
Deep neural networks (DNN)

$$f(x) = \langle w, \Phi(x) \rangle \,, \qquad \underbrace{x \mapsto \Phi_L \circ \cdots \circ \Phi_1(x)}_{\text{compositional representation}}$$



Convolutional and fully connected DNN

$$f(x) = \langle w, \Phi(x) \rangle \,, \qquad x \mapsto \underbrace{\Phi_L \circ \ldots \Phi_K}_{\text{Fully connected}} \circ \underbrace{\Phi_{K-1} \cdots \circ \Phi_1(x)}_{\text{Convolutional}}$$



- Convolutional layers, thousands parameters.
- Fully connected layers, million parameters.

$\rightarrow$ End to end learning.

(LeCun et al. ’98)

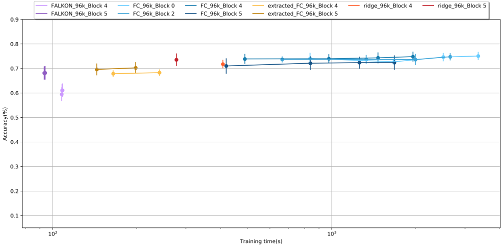
Trading DNN for kernel methods

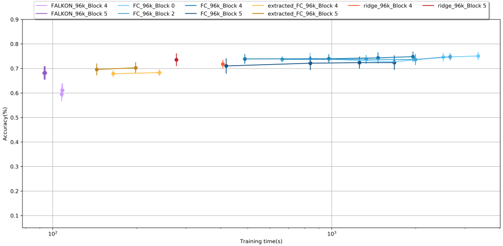
$$f(x) = \langle w, \Phi(x) \rangle , \quad x \mapsto \underbrace{\Phi_L}_{\text{Kernel representation}} \circ \underbrace{\Phi_{L-1} \cdots \circ \Phi_1(x)}_{\text{Convolutional}}$$

- not about data representation…
- …but scaling kernel methods to millions of points.

Don’t fine tune, use kernel methods

[Alfano, Pastore, R., Odone ’20]





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Wrapping up

- Efficiency: don't separate optimization and statistics.
- Beyond supervised learning: PCA, K-means...
- Beyond statistica learning: online learning and bandits.

TBD

- Develop theory for special settings: classification/Interpolation/
- Combine Nyström and multiscale approaches [Chen, Avron, Sindawhani '16].

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PhD/Postdoc positions available!

Relevant papers

Papers

Less is More: Nyström Computational Regularization
A. Rudi, R. Camoriano and L. Rosasco · NIPS15

FALKON: An Optimal Large Scale Kernel Method
A. Rudi, L. Carratino and L. Rosasco · NIPS17

Gaussian Process Optimization with Adaptive Sketching: Scalable and No Regret
D. Calandriello, L. Carratino, A. Lazaric, M. Valko and L. Rosasco · COLT19

Statistical and computational trade-offs in kernel k-means
D. Calandriello, L. Rosasco · NeurIPS18

Gain with no Pain: Efficient Kernel-PCA by Nyström Sampling
N. Sterge, B. Sriperumbur, L. Rosasco, A. Rudi · AISTATS20

Code

FALKON
G. Meanti,L. Carratino, L. Rosasco and A. Rudi · `http://lcsl.mit.edu`

BKB
D. Calandriello, L. Carratino, A. Lazaric, M. Valko and L. Rosasco · `http://lcsl.mit.edu`

More relevant papers

Papers

Learning with SGD and Random Features
L. Carratino, A. Rudi and L. Rosasco · NeurIPS18

On Fast Leverage Score Sampling and Optimal Learning
A. Rudi, D. Calandriello, L. Carratino and L. Rosasco · NeurIPS18

Exact sampling of determinantal point processes with sublinear time preprocessing
M. Dereziński , D. Calandriello, M. Valko · NeurIPS19

Near-linear Time GP Optimization with Adaptive Batching and Resparsification
D. Calandriello, L. Carratino, A. Lazaric, M. Valko and L. Rosasco · Preprint 2020

Code

BLESS: leverage score sampling
A. Rudi, D. Calandriello, L. Carratino and L. Rosasco · `http://lcsl.mit.edu`

DPP sampling

M. Dereziński , D. Calandriello, M. Valko · `http://lcsl.mit.edu`