Less is More: Computational Regularization by Subsampling

Lorenzo Rosasco
University of Genova - Istituto Italiano di Tecnologia
Massachusetts Institute of Technology
lcsl.mit.edu

joint work with Alessandro Rudi, Raffaello Camoriano

Paris

Laboratory for Computational and Statistical Learning

A Starting Point

Classically:
Statistics and optimization **distinct steps** in algorithm design

Empirical process theory + Optimization

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Large Scale:

Consider **interplay** between statistics and optimization!

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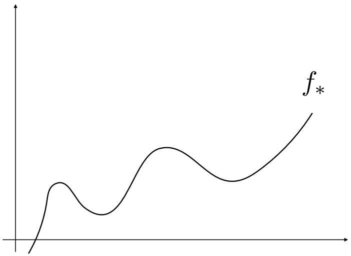
Computational Regularization:
Computation "tricks"=regularization

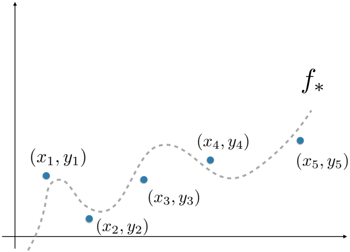
Supervised Learning

Problem: Estimate f^*



Supervised Learning

Problem: Estimate f^* given $S_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$



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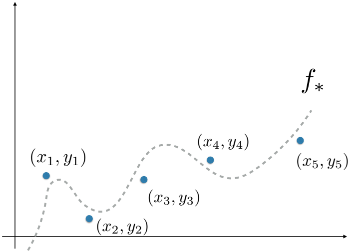

The Setting

$$y_i = f^*(x_i) + \varepsilon_i \qquad i \in \{1, \ldots, n\}$$

- $\varepsilon_i \in \mathbb{R}, x_i \in \mathbb{R}^d$ **random** (bounded but with unknown distribution)
- f^* **unknown**

Outline

Non-linear/non-parametric learning

$$\widehat{f}(x) \;=\; \sum_{i=1}^{M} c_i\, q(x, w_i)$$

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Question: How to choose w_i, c_i and M given S_n ?

Learning with Positive Definite Kernels

There is an *elegant* answer if:

- q is **symmetric**
- *all* the matrices $\widehat{Q}_{ij} = q(x_i, x_j)$ are **positive semi-definite**[1]

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Representer Theorem (Kimeldorf, Wahba '70; Schölkopf et al. '01)

- $M = n$,
- $w_i = x_i$,
- c_i by **convex** optimization!

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Kernel Ridge Regression (KRR)

a.k.a. Tikhonov Regularization

$$\widehat{f}_\lambda = \operatorname*{argmin}_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \|f\|^2$$

where[2]

$$\mathcal{H} = \{ f \mid f(x) = \sum_{i=1}^{M} c_i q(x, w_i),\ c_i \in \mathbb{R}, \underbrace{w_i \in \mathbb{R}^d}_{\text{any center!}},\ \underbrace{\color{red}{M \in \mathbb{N}}}_{\text{any length!}} \}$$

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Solution

$$\widehat{f}_\lambda = \sum_{i=1}^{n} c_i\, q(x, x_i) \quad \text{with} \quad c = (\widehat{Q} + \lambda n I)^{-1} \widehat{y}$$

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1. **Optimal nonparametric bound**
2. More refined results for smooth kernels

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3. **Adaptive tuning**, e.g. via cross validation
4. **Proofs**: inverse problems results + random matrices
   (Smale and Zhou + Caponnetto, De Vito, R.)

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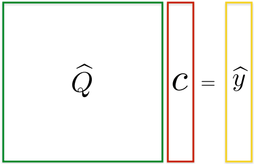
Linear System



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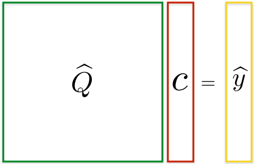

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BIG DATA?

Running out of time and space ...

Can this be fixed?

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Spectral filtering (Engl '96- inverse problems, Rosasco et al. 05- ML)

$$g_\lambda(\hat{Q}) \sim \hat{Q}^\dagger$$

The filter function g_λ defines the form of the approximation

Spectral filtering

Examples

- Tikhonov- ridge regression
- Truncated SVD– principal component regression
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$$c_t = g_t(\hat{Q}) = \gamma \sum_{r=0}^{t-1} (I - \gamma \hat{Q})^r \widehat{y}$$

...it's GD for ERM!!

$$r = 1 \dots t \quad c_r = c_{r-1} - \gamma(\hat{Q} c_{r-1} - \hat{y}), \quad c_0 = 0$$

Statistics and computations with spectral filtering

The different filters achieve *essentially* **the same** optimal statistical error!

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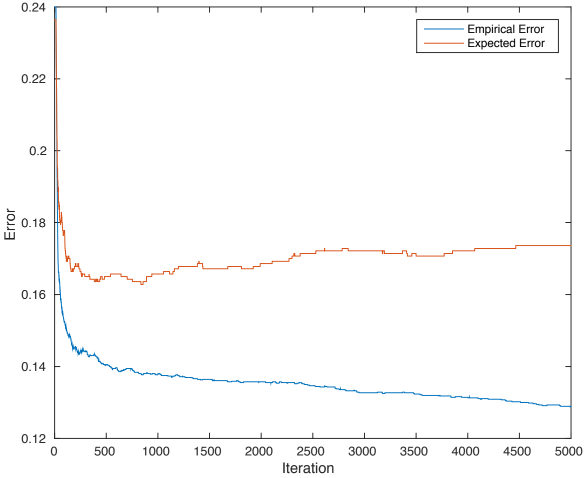
Difference is in computations

Filter	*Time*	*Space*
Tikhonov	n^3	n^2
GD	$n^2\lambda_*^{-1}$	n^2
Accelerated GD	$n^2\lambda_*^{-1/2}$	n^2
Truncated SVD	$n^2\lambda_*^{-\gamma}$	n^2

Notet: $\lambda_*^{-1} = t$, for iterative methods

Semiconvergence



- Iterations control statistics **and** time complexity

Computational Regularization

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Is there a principle to control statistics, time **and space** complexity?

Outline

Nonparametric Learning

Data Dependent Subsampling

Data Independent Subsampling

Subsampling

1. pick w_i at random...

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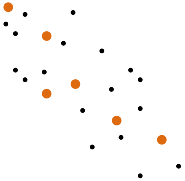
   (Smola, Schölkopf '00)

$$\tilde{w}_1, \ldots, \tilde{w}_M \subset x_1, \ldots x_n \qquad M \ll n$$



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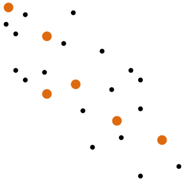

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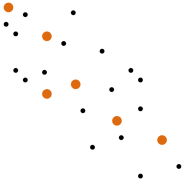

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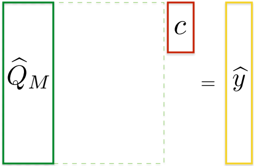

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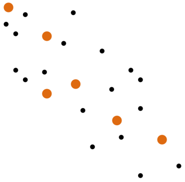

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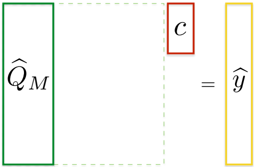

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What about statistics? What's the price for efficient computations?

Putting our Result in Context

- *Many* **different subsampling** schemes
  (Smola, Scholkopf '00; Williams, Seeger '01; ... 20+)

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- **Theoretical guarantees** mainly on **matrix approximation**
  (Mahoney and Drineas '09; Cortes et al '10, Kumar et al.'12 ... 10+)

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- Statistical guarantees **suboptimal** or in **restricted setting**
  (Cortes et al. '10; Jin et al. '11, Bach '13, Alaoui, Mahoney '14)

Main Result

(Rudi, Camoriano, Rosasco, '15)

Theorem

If $f^* \in \mathcal{H}$, then

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Note: An interesting insight is obtained rewriting the result...

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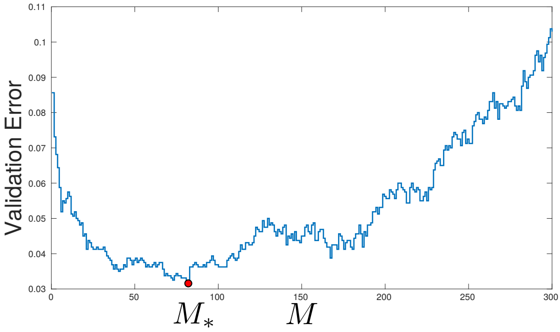
3. *Pick another center ...*

Nÿstrom CoRe Illustrated

n, λ are fixed



Computation controls stability!

Time/space requirement tailored to **generalization**

Experiments

comparable/better w.r.t. the state of the art

Dataset	n_{tr}	d	*Incremental CoRe*	*Standard KRLS*	*Standard Nyström*	*Random Features*	*Fastfood RF*
Ins. Co.	5822	85	$0.23180 \pm 4 \times 10^{-5}$	**0.231**	0.232	0.266	0.264
CPU	6554	21	$\mathbf{2.8466 \pm 0.0497}$	7.271	6.758	7.103	7.366
CT slices	42800	384	$\mathbf{7.1106 \pm 0.0772}$	NA	60.683	49.491	43.858
Year Pred.	463715	90	$\mathbf{0.10470 \pm 5 \times 10^{-5}}$	NA	0.113	0.123	0.115
Forest	522910	54	0.9638 ± 0.0186	NA	**0.837**	0.840	0.840

- Random Features (Rahimi, Recht '07)
- Fastfood (Le et al. '13)

Summary so far

- **Optimal** learning with data dependent subsampling
- Computational regularization: subsampling **regularizes**!

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- **Optimal** learning with data dependent subsampling
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- Can one do better than **uniform** sampling?

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- **Optimal** learning with data dependent subsampling
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Few more questions:

- Can one do better than **uniform** sampling?
  Yes: leverage score sampling...
- What about **data independent** sampling?

Outline

Nonparametric Learning

Data Dependent Subsampling

Data Independent Subsampling

Random Features

$$\widehat{f}(x) \;=\; \sum_{i=1}^{M} c_i \, q(x, w_i)$$

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- perform KRR on

$$\mathcal{H}_M = \{f \mid f(x) = \sum_{i=1}^{M} c_i q(x, \tilde{w}_i),\; c_i \in \mathbb{R}\}.$$

Random Fourier Features

(Rahimi, Recht '07)

Consider

$$q(x, w) = e^{iw^T x},$$

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By sampling $\tilde{w}_1, \dots, \tilde{w}_M$ we are considering the **approximating kernel**

$$\frac{1}{M} \sum_{i=1}^{M} \left[q(x, \tilde{w}_i) \overline{q(x', \tilde{w}_i)} \right] = \widetilde{K}_M(x, x')$$

More Random Features

- **translation invariant** kernels $K(x, x') = H(x - x')$,

$$q(x, w) = e^{iw^T x}, \qquad w \sim \mu = \mathcal{F}(H)$$

- infinite **neural nets** kernels

$$q(x, w) = |w^T x + b|_+, \qquad (w, b) \sim \mu = U[\mathbb{S}^d]$$

- infinite **dot product** kernels
- homogeneous **additive** kernels
- **group invariant** kernels
- ...

Note: Connections with **hashing** and **sketching** techniques.

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Optimization

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Statistics

As before: **do we pay a price for efficient computations?**

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- Statistical guarantees **suboptimal or in restricted setting**
  (Rahimi, Recht '09, Yang et al. '13 ...,Bach '15)

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- Random features achieve **optimal** bound!
- Efficient worst case subsampling $M_* \sim \sqrt{n}$– but cannot exploit smoothness.

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Nÿstrom vs Random features

- Both achieve optimal rates
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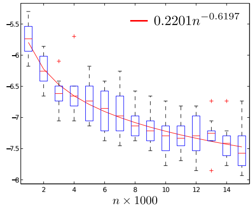
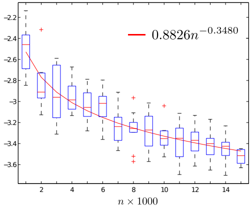
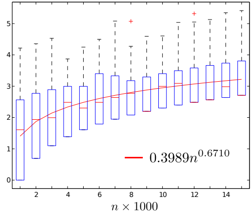
$\log \lambda$



Test Error



$\log M$



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- **Optimal bounds** for data dependent/independent subsampling
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- **Regularization by projection**: inverse problems and preconditioning
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- Beyond randomization: **non convex neural nets optimization**?

Some perspectives:

- **Computational regularization**: subsampling regularizes
- **Algorithm design**: control **stability** for good statistics/computations