

Random Moments for Sketched Statistical Learning

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PLAN

- 1 The sketched learning approach
- 2 A framework for sketched learning
- 3 Two examples
 - Sketched PCA
 - Sketched clustering
- 4 How to construct a sketching operator

OUTLINE

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- ▶ Training collection $\mathbf{X} = (x_1, \dots, x_n)$ seen as a (d, n) matrix

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 - ▶ Want to find a predictor (“hypothesis”) $h \in \mathcal{H}$ suited to data
 - ▶ Performance on data point x measured by loss function $\ell(x, h)$
 - ▶ Goal is to minimize averaged loss and approximate the minimizer

$$h^* = \underset{h \in \mathcal{H}}{\text{Arg Min}} \mathcal{R}(h) = \underset{h \in \mathcal{H}}{\text{Arg Min}} \mathbb{E}[\ell(X, h)]$$

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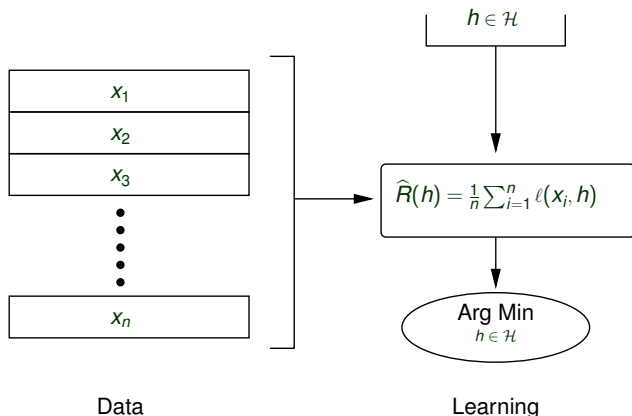
$$h^* = \underset{h \in \mathcal{H}}{\text{Arg Min}} \mathcal{R}(h) = \underset{h \in \mathcal{H}}{\text{Arg Min}} \mathbb{E}[\ell(X, h)]$$

- ▶ Assuming (x_1, \dots, x_n) are drawn i.i.d., natural proxy is empirical risk minimizer

$$\hat{h}_{ERM} = \min_{h \in \mathcal{H}} \hat{\mathcal{R}}(h) = \min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(x_i, h)$$

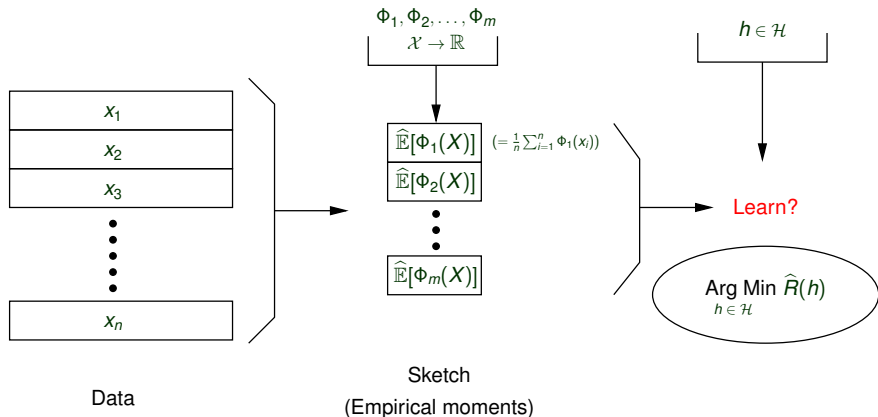
(can possibly be combined with regularization)

CLASSICAL FRAMEWORK



- ▶ Storage cost: $O(nd)$
- ▶ Computation cost: $O((nd)^k)$
- ▶ Stochastic gradient can improve computation bottlenecks but usually requires several data passes

SKETCHED LEARNING APPROACH



- ▶ Storage cost after sketching: $O(m)$
- ▶ Computation cost: hopefully polynomial in m
- ▶ Sketch can be updated very easily
- ▶ Which moments Φ_i ? How large should m be?

FIRST CONSIDERATIONS

- ▶ In the classical approach, learning theory guarantees are of the form

$$\sup_{h \in \mathcal{H}} \left| \mathcal{R}(h) - \widehat{\mathcal{R}}(h) \right| \leq \varepsilon(n),$$

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- ▶ This implies that the ERM estimator satisfies the risk bound

$$\mathcal{R}(\widehat{h}_{ERM}) \leq \mathcal{R}(h^*) + \varepsilon(n).$$

- ▶ To preserve this property up to constant factor for an estimator $\widetilde{h}_{Sketched}$ it is sufficient to ensure that

$$\left| \mathcal{R}(\widehat{h}_{ERM}) - \mathcal{R}(\widetilde{h}_{Sketched}) \right| \lesssim \sup_{h \in \mathcal{H}} \left| \mathcal{R}(h) - \widehat{\mathcal{R}}(h) \right|.$$

A NAIVE APPROACH

- ▶ A first thought is to discretize the hypothesis space into h_1, \dots, h_m and take $\Phi_i(x) = \ell(x, h_i), i = 1, \dots, m$.
- ▶ Then we simply have

$$\mathbb{E}[\Phi_i(X)] = \frac{1}{n} \sum_{j=1}^n \ell(x_j, h_i) = \widehat{R}(h_i), \quad i = 1, \dots, m.$$

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- ▶ With the moment information, we can replace ERM by “discretized ERM” over h_1, \dots, h_m .
- ▶ To ensure $\left| \mathcal{R}(\widehat{h}_{ERM}) - \mathcal{R}(\widetilde{h}_{disc.ERM}) \right| \leq \varepsilon(n)$, require (h_1, \dots, h_m) to be an $\varepsilon(n)$ -covering of the space \mathcal{H} (say for supremum norm).
- ▶ If \mathcal{H} is of metric dimension γ a covering typically requires $m = O(\varepsilon^{-\gamma}) = O(n^{\gamma/2})$, seems hopeless!

SOME HOPE (1)

- ▶ Consider “trivial” example $\ell(x, h) = \|x - h\|^2$, goal is to learn mean $h^* = \mathbb{E}[X]$; obviously only need to store only the empirical mean $\hat{\mathbb{E}}[h(X)] = \frac{1}{n} \sum_{i=1}^n x_i$ i.e. $m = 1!$

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- ▶ Can this phenomenon be generalized?

SOME HOPE (2)

- ▶ **Example 2: PCA.** Since we only need the estimated (covariance) matrix to find PCA directions, we only need to keep moments of order 2 ($m = O(d^2)$).
- ▶ We can even hope do to better by using low-rank approximations of the covariance. Using random projections on Gaussian vectors is a well-known mean to this goal.

TOWARDS SKETCHED CLUSTERING

- ▶ **Example 3:** We will be interested in learning goals where the target cannot be easily represented in terms of moments, i.e. *k*-means/*k*-medians.

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AN ABSTRACT FRAMEWORK

- ▶ Let \mathfrak{M} denote the set of probability measures on $\mathcal{X} = \mathbb{R}^d$.
- ▶ Define the **Risk Operator**

$$\mathcal{R}(\pi, h) = \mathbb{E}_{X \sim \pi}[\ell(X, h)].$$

Note that the empirical risk is

$$\widehat{\mathcal{R}}(h) = \mathcal{R}(\widehat{\pi}_n, h), \quad \text{with } \widehat{\pi}_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i} \text{ (empirical measure).}$$

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- ▶ Observe that $\mathcal{R}(\pi, h)$ is linear in π .
- ▶ Given $\Phi(x) = (\Phi_1(x), \dots, \Phi_m(x))$ define the **sketching operator**

$$\mathcal{A}_\Phi(\pi) = \mathbb{E}_{X \sim \pi}[\Phi(X)].$$

The data sketch is $s = \widehat{\mathbb{E}}[\Phi(X)] = \mathcal{A}_\Phi(\widehat{\pi}_n)$.

- ▶ Note that \mathcal{A}_Φ is a linear operator on probability measures.

APPROACH (FORMAL VERSION)

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- ▶ Approximate learning step:

$$\tilde{h} = \underset{h \in \mathcal{H}}{\text{Arg Min}} \mathcal{R}(\tilde{\pi}, h).$$

GOAL FOR THEORY

- ▶ Remember from initial considerations we aim (ideally) at

$$\left| \mathcal{R}(\hat{h}_{ERM}, \pi) - \mathcal{R}(\tilde{h}_{Sketched}, \pi) \right| \lesssim \sup_{h \in \mathcal{H}} |\mathcal{R}(h, \pi) - \mathcal{R}(h, \hat{\pi}_n)|.$$

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- ▶ Since \hat{h}_{ERM} and $\tilde{h}_{Sketched}$ are two ERMs based on the true empirical $\hat{\pi}_n$ and its reconstruction $\tilde{\pi}$, a sufficient condition for the above is

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Using notation $\|\rho\|_{\mathcal{L}(\mathcal{H})} := \sup_{h \in \mathcal{H}} |\mathcal{R}(h, \rho)|$, rewrite as

$$\|\pi - \Delta(\mathcal{A}_\Phi(\pi'))\|_{\mathcal{L}(\mathcal{H})} \lesssim \|\pi - \pi'\|_{\mathcal{L}(\mathcal{H})}.$$

- Since the reconstruction is obtained from the sketch information only, it is reasonable to aim at

$$\|\pi - \Delta(\mathcal{A}_\Phi(\pi'))\|_{\mathcal{L}(\mathcal{H})} \lesssim \|\mathcal{A}_\Phi(\pi - \pi')\|_2.$$

ABSTRACT COMPRESSION/DECODING RESULTS

- ▶ Assume we have a “model” $\mathfrak{G} \subset \mathfrak{M}$ so that the sketching operator satisfies the following **lower restricted isometry property**:

$$\forall \pi, \pi' \in \mathfrak{G} \quad \|\pi - \pi'\|_{\mathcal{L}(\mathcal{H})} \leq C_{\mathcal{A}} \|\mathcal{A}(\pi - \pi')\|_2. \quad (\text{LRIP})$$

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- ▶ Then the “ideal decoder”

$$\Delta(\mathbf{s}) = \underset{\pi \in \mathfrak{G}}{\text{Arg Min}} \|\mathbf{s} - \mathcal{A}(\pi)\|_2$$

satisfies the following instance optimality property for any π, π' :

$$\|\pi - \Delta(\mathcal{A}(\pi'))\|_{\mathcal{L}(\mathcal{H})} \lesssim d(\pi, \mathfrak{G}) + \|\mathcal{A}(\pi - \pi')\|_2,$$

with

$$d(\pi, \mathfrak{G}) = \inf_{\sigma \in \mathfrak{G}} \left(\|\pi - \sigma\|_{\mathcal{L}(\mathcal{H})} + 2C_{\mathcal{A}} \|\mathcal{A}(\pi - \sigma)\|_2 \right).$$

- ▶ (Conversely, the above property implies a LRIP inequality).

(Bourrier et al, 2014)

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- ▶ Find suitable sketching dimension m and features Φ so that the corresponding sketching operator \mathcal{A}_Φ satisfies a LRIP inequality, restricted to model \mathcal{G} .
- ▶ Define the ideal decoder from sketch s

$$\Delta(s) = \underset{\pi \in \mathcal{G}}{\text{Arg Min}} \|\mathbf{s} - \mathcal{A}_\Phi(\pi)\|_2.$$

- ▶ **For theory:** interpret the resulting instance optimality bound in terms of the learning risk.
- ▶ **For practice:** find suitable approximation of the ideal decoder if it is computationally too demanding.

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WARM UP: SKETCHED PCA

- ▶ The risk is the PCA reconstruction error

$$\mathcal{R}_{PCA}(\pi, h) = \mathbb{E}_{X \sim \pi} \left[\|X - P_h X\|_2^2 \right],$$

where hypothesis space \mathcal{H} = linear subspaces of dimension k and P_h = orthogonal projector onto h .

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- ▶ To construct \mathcal{A}_Φ , use a linear operator \mathcal{M} to \mathbb{R}^m satisfying the RIP

$$1 - \delta \leq \frac{\|\mathcal{M}(M)\|_2^2}{\|M\|_{Frob}^2} \leq 1 + \delta$$

for all matrices M of rank less than k .

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- ▶ **Sketch:** $\mathcal{A}_\Phi(\hat{\pi}_n) = \mathcal{M}(\hat{\Sigma}_n)$ (apply \mathcal{M} to empirical covar. matrix $\hat{\Sigma}_n$.)
- ▶ **Reconstruct from a sketch s :** find

$$\tilde{\Sigma} = \underset{\text{rank}(M) \leq k}{\text{Arg Min}} \|s - \mathcal{M}(M)\|_2.$$

- ▶ **Output:** \tilde{h} = space spanned by k first eigenvectors of $\tilde{\Sigma}$.

THEORETICAL GUARANTEE

For any distribution π on $B(0, R)$, we have the bound (w.h.p. over data sampling)

$$\mathcal{R}_{PCA}(\pi, \tilde{h}) - \mathcal{R}_{PCA}(\pi, h^*) \leq C \left(\sqrt{k} \mathcal{R}_{PCA}(\pi, h^*) + R^2 \sqrt{\frac{k}{n}} \right).$$

- ▶ independent of total data dimension
- ▶ the first factor \sqrt{k} may be spared using more precise results from low rank matrix sensing (also convex relaxation of reconstruction program for better computational efficiency)

SKETCHED CLUSTERING: SETTING

- ▶ Consider k -means or k -medians. Assume data is bounded by R .
- ▶ **Hypothesis space:** $\mathcal{H} = \mathcal{H}_{k,2\varepsilon,R}$, set of cluster centroids $h = (c_1, \dots, c_k)$ that are R -bounded and pairwise 2ε -separated.
- ▶ Loss function

$$\ell(x, h) = \min_{1 \leq i \leq k} \|x - c_i\|_2^p,$$

with $p = 1$ for k -medians, $p = 2$ for k -means.

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- ▶ **Restricted model:** $\mathcal{G} = \mathcal{G}_{k,2\varepsilon,R}$ set of k -point distributions whose support is in $\mathcal{H}_{k,2\varepsilon,R}$.

SKETCHED CLUSTERING: SKETCHING

- ▶ **Fourier features:** consider scaled Fourier features

$$\Phi_{\omega}(x) = \frac{C_{\omega}}{\sqrt{m}} e^{j\omega^t x},$$

where $C_{\omega} \simeq d / ((1 + \varepsilon \|\omega\|) \log k)$.

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- ▶ **Random frequency vectors:** draw $\omega_1, \dots, \omega_m$ i.i.d. in \mathbb{R}^d from the distribution with density

$$\Lambda(\omega) \propto (1 + \varepsilon^2 \|\omega\|^2) \exp(-\varepsilon^2 \|\omega\|^2 / (2 \log k)).$$

- ▶ The sketching operator \mathcal{A}_{Φ} corresponds to the random Fourier features (Φ_{ω_i}) , $i = 1, \dots, m$.

SKETCHED CLUSTERING: RECONSTRUCTION

- ▶ **Reconstruct from a sketch \mathbf{s} :** find

$$\tilde{\pi} = \underset{\pi \in \mathfrak{S}_{k, 2\varepsilon, R}}{\text{Arg Min}} \|\mathbf{s} - \mathcal{A}_{\Phi}(\pi)\|_2.$$

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- ▶ **Theoretical guarantee on reconstruction:** if

$$m \geq k^2 d^3 \text{polylog}(k, d) \log\left(\frac{R}{\varepsilon}\right),$$

then for any distribution π on $\mathcal{B}(0, R)$, with high probability on the draw of frequencies and of the data, it holds

$$\mathcal{R}(\pi, \tilde{h}) - \mathcal{R}(\pi, h^*) \lesssim \frac{R^p \sqrt{k \log k}}{\varepsilon} \mathcal{R}(\pi, h^*)^{\frac{1}{p}} + \frac{R^p d \sqrt{k \log k}}{\sqrt{n}}.$$

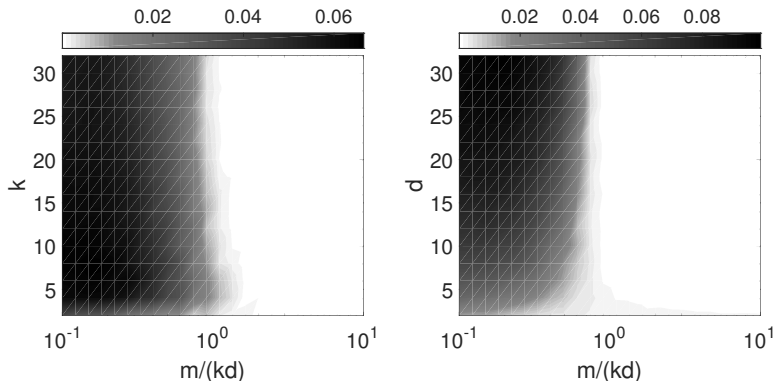
SKETCHED CLUSTERING: EXPERIMENTS

Simplifications (or cut corners...) for experiments:

- ▶ Use regular Gaussian density for frequency drawing (no weighting)
- ▶ Use heuristic greedy search for the reconstruction operator
- ▶ Ignore the 2ε -separation constraint for reconstruction

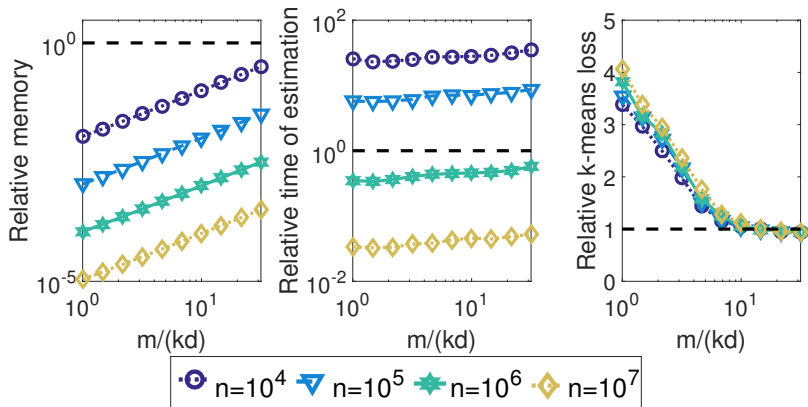
SKETCHED CLUSTERING: EXPERIMENTS

Data: mixture of 10 Gaussians with uniform weights and centers drawn from a Gaussian



Normalized k -means risk, on $n = 10^4 k$ points uniformly drawn in $[0, 1]^d$, $d = 10$ (left), $k = 10$ (right).

SKETCHED CLUSTERING: EXPERIMENTS



Relative time, memory and k -means risk of CKM with respect to k -means (10^0 represents the k -means result). ($d = 10$)

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CONSTRUCTING A SUITABLE SKETCHING OPERATOR

- ▶ **Core of approach:** finding a sketching operator \mathcal{A}_Φ satisfying LRIP.

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- ▶ Use as **intermediary** a kernel Hilbert norm $\|\cdot\|_\kappa$ satisfying LRIP:

$$\forall \pi, \pi' \in \mathfrak{G} \quad \|\pi - \pi'\|_{\mathcal{L}(\mathcal{H})} \lesssim \|\pi - \pi'\|_\kappa,$$

where κ is a reproducing kernel and $\|\pi\|_\kappa^2 = \mathbb{E}_{\mathbf{X}, \mathbf{X}' \sim \pi \otimes 2}[\kappa(\mathbf{X}, \mathbf{X}')]$.

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- ▶ Assume on the other hand the following representation holds:

$$\kappa(\mathcal{X}, \mathcal{X}') = \mathbb{E}_{\omega \sim \Lambda} \left[\phi_\omega(\mathcal{X}) \overline{\phi_\omega(\mathcal{X}')} \right],$$

where (ϕ_ω) is a family of complex-valued feature functions.

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where (ϕ_ω) is a family of complex-valued feature functions.

- ▶ **Strategy:** sample random features $\omega_j \sim \Lambda$, ensuring (w.h.p.) the corresponding sketching operator delivers good enough approximation to $\|\cdot\|_\kappa$ i.e.

$$\forall \pi, \pi' \in \mathfrak{G} \quad \|\pi - \pi'\|_\kappa \lesssim \|\mathcal{A}_\Phi(\pi - \pi')\|_2 .$$

DIMENSION OF SKETCH REQUIRED

- ▶ Uniform approximation of the kernel norm by the sketching norm obtained via Bernstein's inequality + covering argument on the normalized **secant set**

$$\mathcal{S}_{\|\cdot\|_{\kappa}}(\mathfrak{G}) = \left\{ \frac{\pi - \pi'}{\|\pi - \pi'\|_{\kappa}} \mid \pi, \pi' \in \mathfrak{G} \right\}.$$

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- ▶ More precisely we find the sufficient condition

$$m \gtrsim \log \mathcal{N}(\mathcal{S}_{\|\cdot\|_{\kappa}}(\mathfrak{G}), d_{\mathcal{F}}, 1/2),$$

$$\text{where } d_{\mathcal{F}}(\pi, \pi') = \sup_{\omega} \left| |\mathbb{E}_{X \sim \pi}[\Phi_{\omega}(X)]|^2 - |\mathbb{E}_{X \sim \pi'}[\Phi_{\omega}(X)]|^2 \right|.$$

DIMENSION OF SKETCH REQUIRED

- ▶ Uniform approximation of the kernel norm by the sketching norm obtained via Bernstein's inequality + covering argument on the normalized **secant set**

$$\mathcal{S}_{\|\cdot\|_{\kappa}}(\mathfrak{G}) = \left\{ \frac{\pi - \pi'}{\|\pi - \pi'\|_{\kappa}} \mid \pi, \pi' \in \mathfrak{G} \right\}.$$

- ▶ More precisely we find the sufficient condition

$$m \gtrsim \log \mathcal{N}(\mathcal{S}_{\|\cdot\|_{\kappa}}(\mathfrak{G}), d_{\mathcal{F}}, 1/2),$$

where $d_{\mathcal{F}}(\pi, \pi') = \sup_{\omega} \left| |\mathbb{E}_{X \sim \pi}[\Phi_{\omega}(X)]|^2 - |\mathbb{E}_{X \sim \pi'}[\Phi_{\omega}(X)]|^2 \right|$.

- ▶ Finally, the vectorial form of Bernstein's inequality can be used again (this time on the data) to control the estimation noise $\|\mathcal{A}_{\Phi}(\pi - \hat{\pi}_n)\|_2$.

APPLICATION TO MIXTURES AND CLUSTERING

Overview of remaining steps to obtain bound on risk and sketch dimension:

- ▶ **Establish** the LRIP between the risk norm $\|\cdot\|_{\mathcal{L}(\mathcal{H})}$ and the kernel norm $\|\cdot\|_{\kappa}$ on the model \mathfrak{G} .
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- ▶ Once the instance optimality inequality is obtained, relate back the terms of the bound to the learning task (learning risk).

CONCLUSION

- ▶ The sketched learning framework holds promise to reduce computation and memory burden
- ▶ General theoretical framework based on:
 - ▶ LRIP/compressed sensing recovery principles
 - ▶ Kernel embeddings and random features
- ▶ Theoretical recovery guarantees and bounds on the sketch dimension needed
- ▶ Applications:
 - ▶ sketched PCA
 - ▶ sketched clustering
 - ▶ sketched mixture of Gaussians estimation
 - ▶ ... more to come?

SketchML matlab toolbox available:
(large-scale mixture learning using sketches)

<http://sketchml.gforge.inria.fr/>

ArXiv Preprint:

Compressive Statistical Learning with Random Feature Moments

R. Gribonval, G. Blanchard, N. Keriven, Y. Traonmilin

<https://arxiv.org/abs/1706.07180>