Performance-complexity Trade-off in Large Dimensional Spectral Clustering

Statistics Seminar, RSFAS, Australian National University

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- **Example**: unsupervised (kernel) spectral clustering

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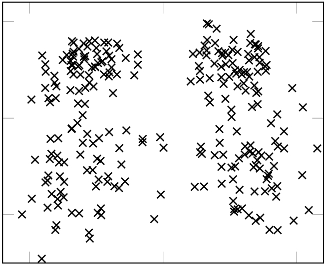

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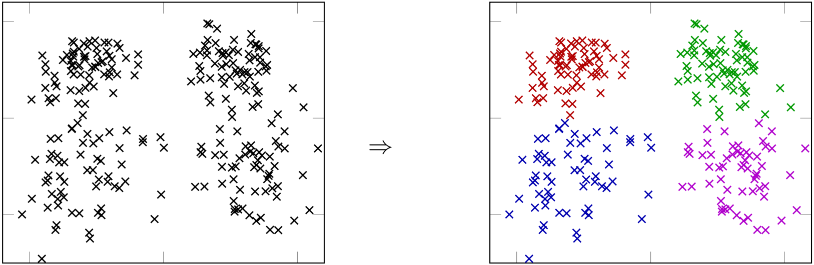

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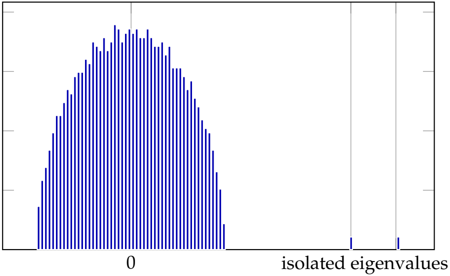

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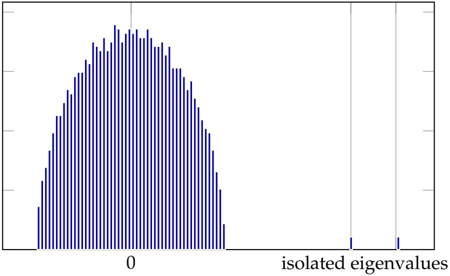
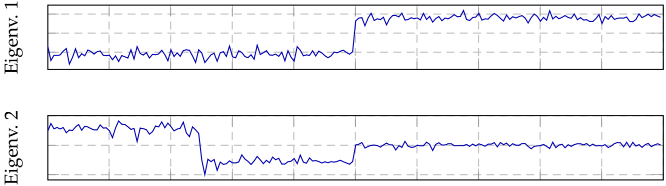


$\Downarrow$ **Top eigenvectors** $\Downarrow$



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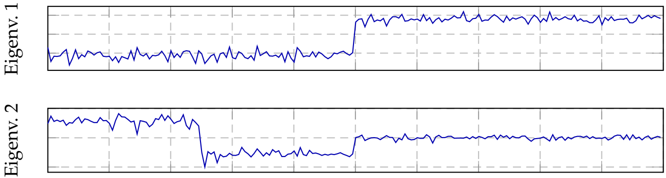

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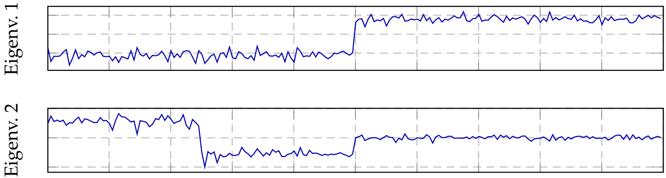

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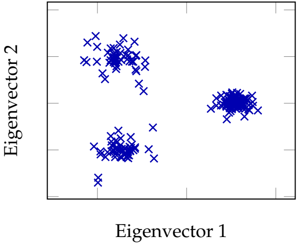

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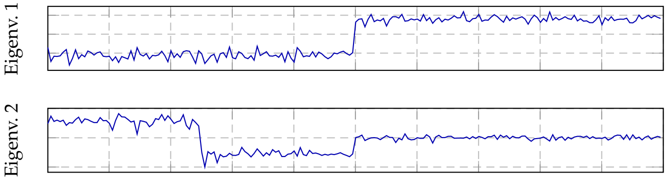

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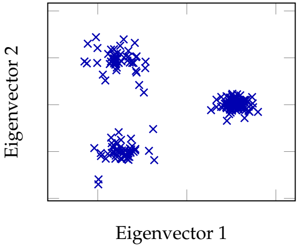

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EM or k-means clustering.

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- **Key object**: eigenspectrum of the "compressed" kernel matrix, in particular, statistics of top eigenvectors!

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2. Main Results
   - Model and problem setting
   - Uniform sparsification
   - Non-uniform sparsification, quantization, and binarization

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Data: two-class signal-plus-noise mixture

Let $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^p$ be independently drawn (non-necessarily uniformly) from:

$$\mathcal{C}_1 : \mathbf{x}_i \sim \mathcal{N}(-\boldsymbol{\mu}, \mathbf{I}_p), \quad \mathcal{C}_2 : \mathbf{x}_i \sim \mathcal{N}(+\boldsymbol{\mu}, \mathbf{I}_p). \tag{1}$$

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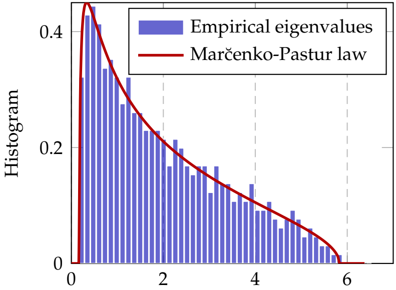

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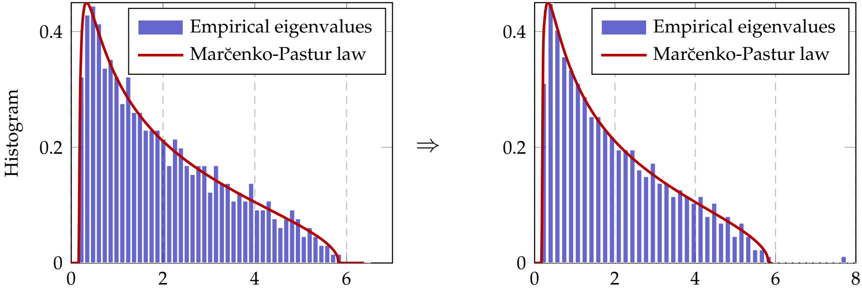

Figure: Eigenvalues of $\mathbf{X}^\mathsf{T}\mathbf{X}/p$ versus the Marčenko-Pastur law, $p = 512$, $n = 1\,024$, with $\rho = 0$ **(left)** and $\rho = 2$ **(right)**.

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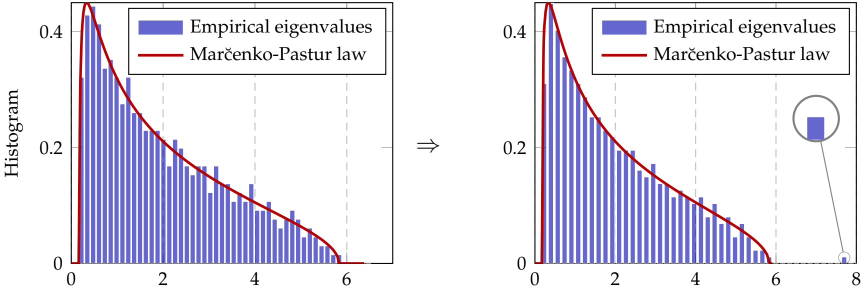

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Objective: "compress" linear Gram matrix $\mathbf{X}^\mathsf{T}\mathbf{X} \in \mathbb{R}^{n\times n}$.

Uniform sparsification

Setting uniformly a proportion $1-\varepsilon$ entries to zero with a symmetric Bernoulli mask $\mathbf{B} \in \{0,1\}^{n\times n}$

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- for $(\hat\lambda, \hat{\mathbf{v}})$ an eigenpair of $\mathbf{K}$ and label vector $\mathbf{v} \in \mathbb{R}^n$, by Cauchy's integral formula, the "angle": $|\hat{\mathbf{v}}^\mathsf{T}\mathbf{v}|^2 = -\frac{1}{2\pi\imath}\oint_{\Gamma(\hat\lambda)} \mathbf{v}^\mathsf{T}\mathbf{Q}(z)\mathbf{v}\,dz$, for $\Gamma(\hat\lambda)$ positively circling $\hat\lambda$

Uniform sparsification: performance analysis

Theorem (Limiting spectral measure)

As $n, p \to \infty$ with $p/n \to c \in (0, \infty)$, the empirical spectral measure $\omega_{\mathbf{K}} = \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(\mathbf{K})}$ of $\mathbf{K}$ converges to a deterministic limit ω, uniquely defined through its Stieltjes transform $m(z) = \int (t-z)^{-1} \omega(dt)$ solution to

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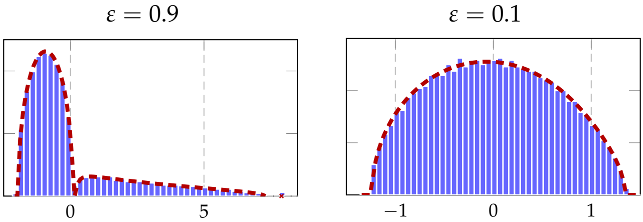
Theorem (Isolated eigenpair and a phase transition)

Define $F(x) = x^4 + 2x^3 + \left(1 - \frac{c}{\varepsilon}\right) x^2 - 2cx - c$, $G(x) = \frac{\varepsilon}{c}(1+x) + \frac{1}{1+x} + \frac{\varepsilon}{x(1+x)}$ and let γ be the largest real solution to $F(\gamma) = 0$. Then, the largest eigenpair $(\hat{\lambda}, \hat{\mathbf{v}})$ of $\mathbf{K}$ satisfies

$$\hat{\lambda} \to \lambda = \begin{cases} G(\rho), & \rho > \gamma \\ G(\gamma), & \rho \le \gamma \end{cases}, \quad \frac{1}{n}|\hat{\mathbf{v}}^\mathsf{T}\mathbf{v}|^2 \to \alpha = \begin{cases} \frac{F(\rho)}{\rho(1+\rho)^3}, & \rho > \gamma \\ 0, & \rho \le \gamma \end{cases} \tag{4}$$

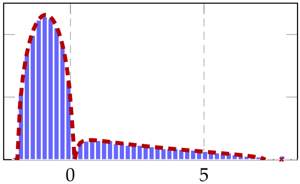
as $n,p \to \infty$ with $p/n \to c \in (0,\infty)$, for SNR $\rho = \lim \|\boldsymbol{\mu}\|^2$.

Uniform sparsification: implications

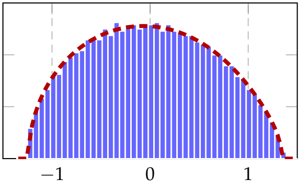


Uniform sparsification: implications

$\varepsilon = 0.9$



$\varepsilon = 0.1$



Remark: becomes the Marčenko–Pastur law (of $\mathbf{X}^\mathsf{T}\mathbf{X}/p$) as $\varepsilon \to 1$ and semicircle law as $\varepsilon \to 0$, a "mixed" of behavior in the sense of *free additive convolution* [Voi86].

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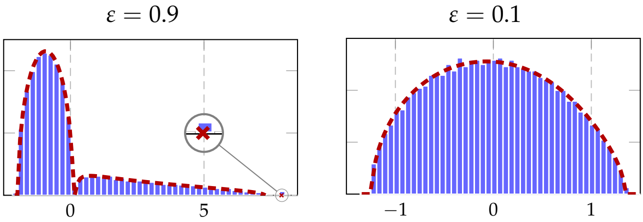

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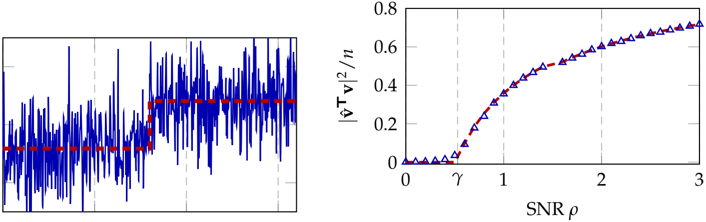

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Outline

Non-uniform "compressed" spectral clustering: method

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$$\mathbf{K} = \left\{ f(\mathbf{x}_i^\mathsf{T}\mathbf{x}_j/\sqrt{p})/\sqrt{p} \right\}_{i,j=1}^{n} \tag{5}$$

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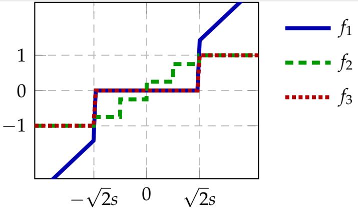

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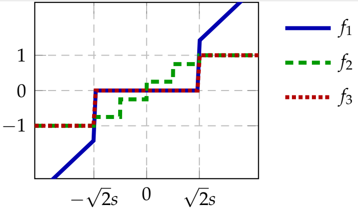

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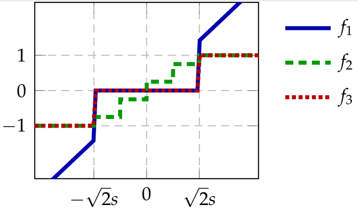

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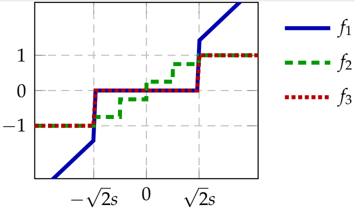

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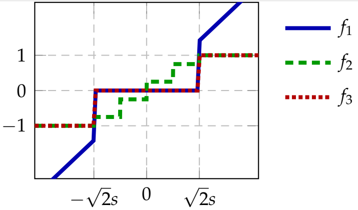

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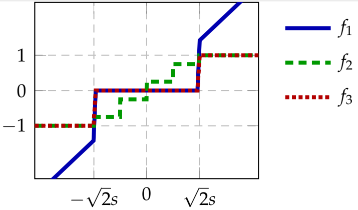

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- truncation threshold $s > 0$
- number of information bits M

Compressed kernel matrix: intuition

Object of interest

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$$\mathbf{K} = \left\{ f(\mathbf{x}_i^\mathsf{T}\mathbf{x}_j/\sqrt{p})/\sqrt{p} \right\}_{i,j=1}^{n} \tag{6}$$

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Notations

For each f and $\xi \sim \mathcal{N}(0,1)$, define the (generalized) moments

$$a_0 = \mathbb{E}[f(\xi)] = 0, \quad a_1 = \mathbb{E}[\xi f(\xi)], \quad \sqrt{2}a_2 = \mathbb{E}[\xi^2 f(\xi)], \quad \nu = \mathbb{E}[f^2(\xi)] \geq a_1^2 + a_2^2. \tag{7}$$

"Compressed" spectral clustering: performance analysis

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f	a_1	ν
f_1	$\operatorname{erfc}(s) + 2se^{-s^2}/\sqrt{\pi}$	$\operatorname{erfc}(s) + 2se^{-s^2}/\sqrt{\pi}$
f_2	$\sqrt{\frac{2}{\pi}} \cdot 2^{1-M}(1 + e^{-s^2} + \sum_{k=1}^{2^{M-2}-1} 2e^{-\frac{k^2 s^2}{4^{M-2}}})$	$1 - \frac{2^M - 1}{4^{M-1}} \operatorname{erf}(s) - \sum_{k=1}^{2^{M-2}-1} \frac{k \operatorname{erf}(ks \cdot 2^{2-M})}{2^{2M-5}}$
f_3	$e^{-s^2}\sqrt{2/\pi}$	$\operatorname{erfc}(s)$

with $\mathbf{a_2 = 0}$, $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$, $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$ error/comple. error function.

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Theorem (Limiting spectral measure)

As $n, p \to \infty$ with $p/n \to c \in (0, \infty)$, the empirical spectral measure $\omega_{\mathbf{K}} = \frac{1}{n} \sum_{i=1}^n \delta_{\lambda_i(\mathbf{K})}$ of $\mathbf{K}$ converges to a deterministic limit ω, uniquely defined through its Stieltjes transform $m(z) = \int (t-z)^{-1} \omega(dt)$ solution to

$$z = -\frac{1}{m(z)} - \frac{\nu - a_1{}^2}{c} m(z) - \frac{a_1{}^2 m(z)}{c + a_1 m(z)}. \quad (9)$$

"Compressed" spectral clustering: attention!

Theorem (Informative spike and a phase transition)

For $a_1 > 0$ and $a_2 = 0$, similarly define $F(x) = x^4 + 2x^3 + \left(1 - \frac{c\nu}{{a_1}^2}\right) x^2 - 2cx - c$ *and* $G(x) = \frac{a_1}{c}(1+x) + \frac{a_1}{x} + \frac{\nu - {a_1}^2}{a_1} \frac{1}{1+x}$ *and let γ be the largest real solution to $F(\gamma) = 0$. Then,*

$$\hat{\lambda} \to \lambda = \begin{cases} G(\rho), & \rho > \gamma \\ G(\gamma), & \rho \leq \gamma \end{cases}, \quad \frac{1}{n} |\hat{\mathbf{v}}^\mathsf{T} \mathbf{v}|^2 \to \alpha = \begin{cases} \frac{F(\rho)}{\rho(1+\rho)^3}, & \rho > \gamma \\ 0, & \rho \leq \gamma \end{cases} \tag{10}$$

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Remark (Spurious non-informative spikes)

If $\mathbf{a_2 \neq 0}$, then there may be *up to two* **non-informative** eigenvalues (with eigenvectors containing only random noise) on the *left or right* of the main bulk.

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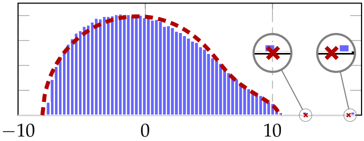

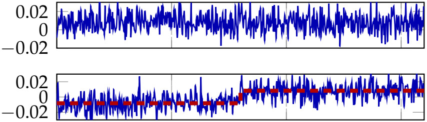

“Compressed” spectral clustering: practical implications

Corollary (Performance of spectral clustering)

Let $a_1 > 0, a_2 = 0$, and let $\hat{\mathcal{C}}_i = \operatorname{sign}([\hat{\mathbf{v}}]_i)$ be the estimate of the underlying class $\mathcal{C}_i$ of the datum $\mathbf{x}_i$, with the convention $\hat{\mathbf{v}}^\mathsf{T}\mathbf{v} \geq 0$, for $\hat{\mathbf{v}}$ the top eigenvector of $\mathbf{K}$. Then, the misclassification rate satisfies $\frac{1}{n}\sum_{i=1}^n \delta_{\hat{\mathcal{C}}_i \neq \mathcal{C}_i} \to \frac{1}{2}\operatorname{erfc}(\sqrt{\alpha/(2-2\alpha)})$, as $n, p \to \infty$, for α the limit of the eigenvector alignment $\frac{1}{n}|\hat{\mathbf{v}}^\mathsf{T}\mathbf{v}|^2$.

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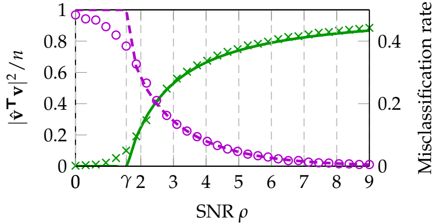

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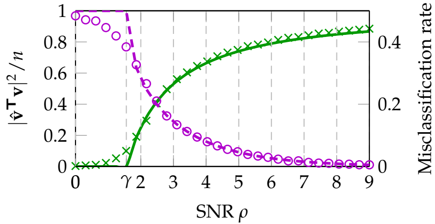

Remark (Optimality of linear $f(t) = t$)

Both phase transition point γ and misclassification rate grow with ν/a_1^2, the linear $f(t) = t$ with minimal $\nu/a_1^2 = 1$ is *optimal* in: **(i)** *smallest* SNR ρ or *largest* ratio p/n to observe a spike, and **(ii)** upon existence, reaching *lowest* classification error rate.

Uniform versus non-uniform sparsification

Comparison between uniform (Bernoulli) sparsification and "selective" non-uniform sparsification $f_1(t) = t \cdot 1_{|t|>\sqrt{2}s}$. **Same** performance with **different** *level of sparsity*:

$$\varepsilon_{\text{unif}} = \operatorname{erfc}(s) + 2se^{-s^2}/\sqrt{\pi} > \operatorname{erfc}(s) = \varepsilon_{\text{selec}} \tag{11}$$

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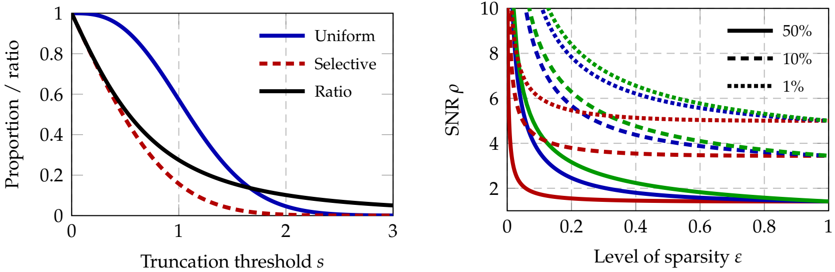
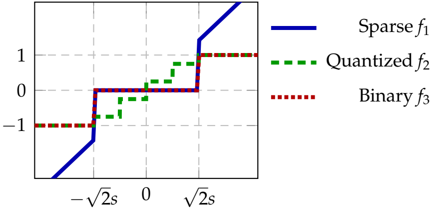


Figure: **(Left)** Proportion of non-zero entries with uniform versus selective sparsification f_1 and their ratio, as a function of the truncation threshold s. **(Right)** Comparison of 1%, 10% error and phase transition (i.e., 50% error) curves between subsampling (**green**), uniform (**blue**) and selective sparsification f_1 (**red**), as a function of sparsity level ε and SNR ρ, for $c = 2$.

Optimally quantized spectral clustering



Tuning parameters:

- truncation threshold $s > 0$
- number of information bits M

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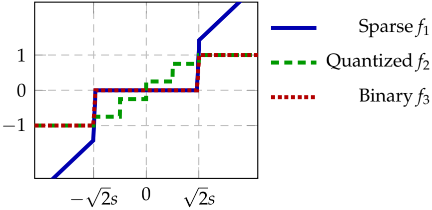

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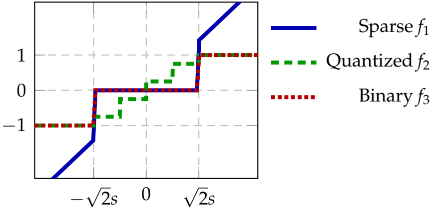

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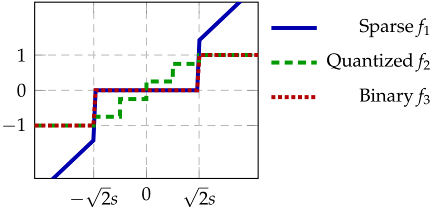

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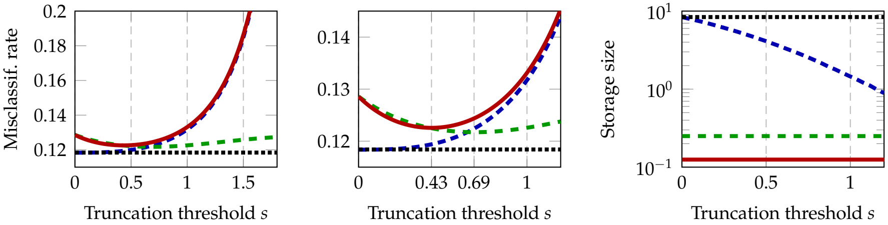

Figure: Clustering performance (**left**, a zoom-in in **middle**) and storage size (MB) **(right)** of f_1 (**blue**), f_2 with $M = 2$ (**green**), f_3 (**red**), and linear $f(t) = t$ (**black**), versus the truncation threshold s, for SNR $\rho = 2$, $c = 1/2$ and $n = 10^3$, with 64 bits per entry for non-quantized matrices.

Experiments on real-world data

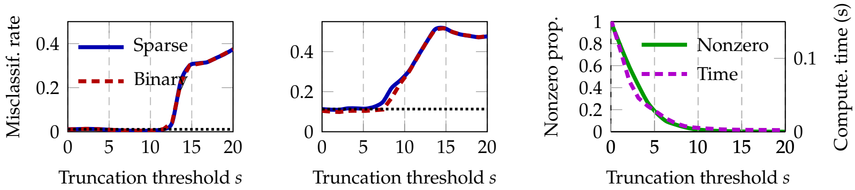

Figure: Clustering performance (**left** and **middle**), proportion of nonzero entries and computational time of the top eigenvector for f_3 (**right**), on the MNIST dataset: digits $(0,1)$ (**left**) and $(5,6)$ (**middle** and **right**) with $n = 2\,048$ and performance of the linear function in **black**.

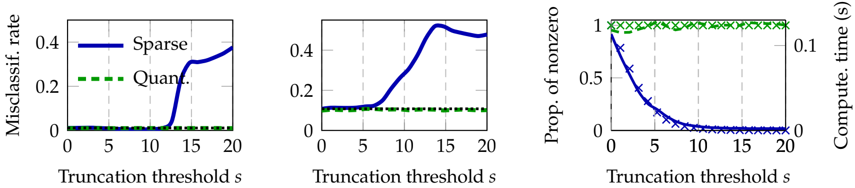

Figure: Clustering performance (**left** and **middle**), proportion of nonzero entries, and computational time of the top eigenvector (**right**, in markers) of sparse f_1 and quantized f_2 with $M = 2$, on the MNIST dataset.

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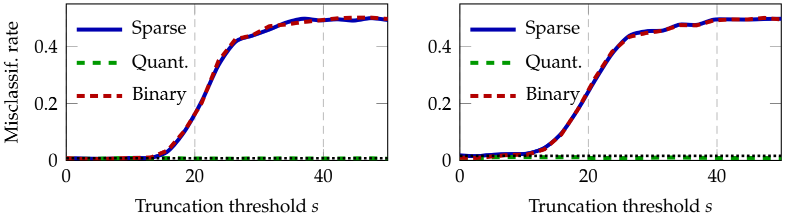

Figure: Clustering performance of sparse f_1, quantized f_2 (with $M = 2$) and binary f_3 as a function of the truncation threshold s on *GoogLeNet* features of the ImageNet datasets: (**left**) class "pizza" versus "daisy" and (**right**) class "hamburger" versus "coffee", for $n = 1\,024$ and performance of the linear function in **black**. Results averaged over 10 runs.

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