SketchySVD

Joel A. Tropp

Computing + Mathematical Sciences
California Institute of Technology
jtropp@cms.caltech.edu

Coauthors: Alp Yurtsever (EPFL), Volkan Cevher (EPFL);
Yiming Sun (Cornell), Yang Guo (UWisc), Charlene Luo (Columbia), Madeleine Udell (Cornell)

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Building Community

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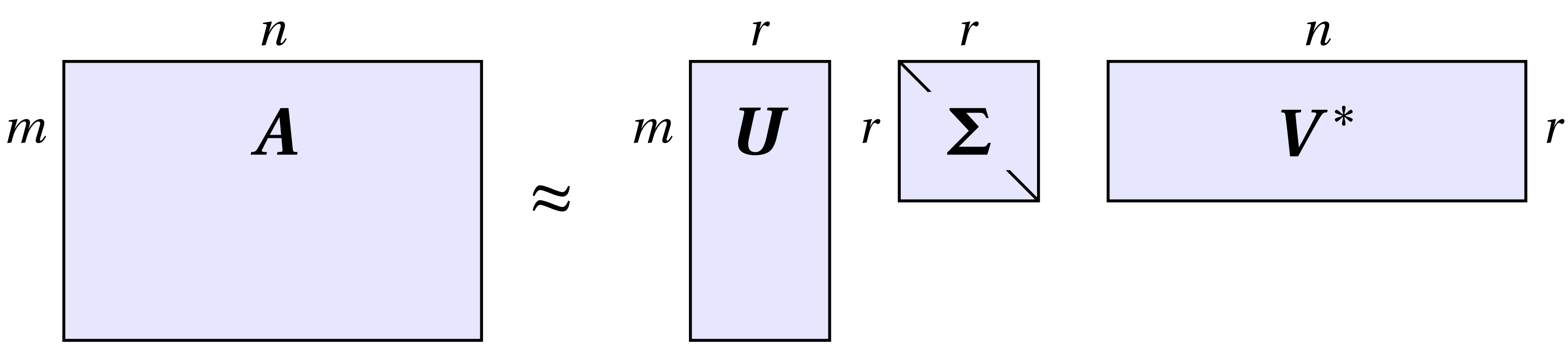
Cincinnati, Ohio, USA

Co-Chairs: Gitta Kutyniok, Ali Pinar, Joel A. Tropp

The Famous Truncated SVD

Truncated Singular Value Decomposition (TSVD)



- $\boldsymbol{U}, \boldsymbol{V}$ have orthonormal columns and $\boldsymbol{\Sigma}$ is nonnegative diagonal
- Approximately $r(m+n)$ degrees of freedom

Interpretation: r-truncated SVD = optimal rank-r approximation

Applications:

- Least-squares computations (linear regression)
- Principal component analysis (orthogonal regression; total least squares)
- Summarization, data reduction, visualization, ...

A Paean to the Truncated SVD

"[Truncated SVD] is one of the few methods that has solid foundations and can be trusted, provided that the computations are correct. Having something reliable in machine learning is worth its weight in gold — there are almost no gold standards in the field, precluding rapid progress. Think of what happens to machine learning when the routine for matrix–vector multiplication doesn't always work right. You can't debug any code, much less a big system consisting of many algorithms thrown together."

–Nemo

Modern Numerical Linear Algebra

What’s Wrong with Classical TSVD Algorithms?

- Nothing... when the matrices are small and fit in core memory

Climate Change:

- Medium- to large-scale data (Megabytes+)
- New architectures (multi-core, distributed, data centers, ...)
- **Today:** New data presentations (dynamic, off-core, streaming)

Engineering:

- Theoretically, we already know how to do streaming TSVD, but...
- Current “algorithms” are not ready for implementation
- For scientific applications, high accuracy is essential!
- **Today:** First practical algorithms for streaming TSVD

Streaming Linear Algebra

The Turnstile Model:

$$\boldsymbol{A} \quad = \quad \boldsymbol{H}_1 + \boldsymbol{H}_2 + \boldsymbol{H}_3 + \boldsymbol{H}_4 + \cdots$$

- Huge input matrix $\boldsymbol{A}$ is presented as a sum of innovations $\boldsymbol{H}_i$
- Must discard each innovation $\boldsymbol{H}_i$ after it is processed
- **Goal:** Without storing $\boldsymbol{A}$ in full, return TSVD after seeing all updates

Applications:

- Scientific simulation and data collection
- One-pass approximation of matrix stored out-of core
- Large-scale semidefinite programming algorithms

Sources: Muthukrishnan 2008; Woolfe et al. 2008; Clarkson & Woodruff 2009; HMT 2011; Woodruff 2014; TYUC 2016–2019; ....

Randomized Linear Sketches

$$\text{sketch} \quad = \quad \mathcal{L}(\boldsymbol{A}) \quad = \quad \sum_i \mathcal{L}(\boldsymbol{H}_i)$$

- Select a **linear** map $\mathcal{L}$ without reference to $\boldsymbol{A}$
- Sketch is much smaller than input matrix
- Use **randomness** so sketch works for an arbitrary input
- **[LNW14] Essentially the only way to handle the turnstile model!**

Examples:

- Left multiply: $\mathcal{L}(\boldsymbol{A}) = \boldsymbol{\Upsilon}\boldsymbol{A}$
- Right multiply: $\mathcal{L}(\boldsymbol{A}) = \boldsymbol{A}\boldsymbol{\Omega}^*$
- Select some entries: $\mathcal{L}(\boldsymbol{A}) = \{a_{ij} : (i, j) \in E\}$

Sources: Alon et al. 1996; Sarlós 2006; Muthukrishnan 2008; Woolfe et al. 2008; Clarkson & Woodruff 2009; HMT 2011; Mahoney 2012; Woodruff 2014; Li et al. 2014; Drineas & Mahoney 2016; TYUC 2016–2019; ....

Overview of SketchySVD

Sketch *est Omnis Divisa in Partes Tres*

- Let $\boldsymbol{A} \in \mathbb{C}^{m \times n}$ be an input matrix (presented in turnstile model)

- Fix sketch size parameters (k, s) with $r \le k \le s \ll \min\{m, n\}$
- Draw linear dimension reduction maps independently at random:

$$\boldsymbol{\Upsilon} : \mathbb{C}^m \to \mathbb{C}^k \quad \text{and} \quad \boldsymbol{\Omega} : \mathbb{C}^n \to \mathbb{C}^k$$

$$\boldsymbol{\Phi} : \mathbb{C}^m \to \mathbb{C}^s \quad \text{and} \quad \boldsymbol{\Psi} : \mathbb{C}^n \to \mathbb{C}^s$$

- **Co-range and range sketches:**

$$\boldsymbol{X} = \boldsymbol{\Upsilon} \boldsymbol{A} \in \mathbb{C}^{k \times n} \quad \text{and} \quad \boldsymbol{Y} = \boldsymbol{A} \boldsymbol{\Omega}^* \in \mathbb{C}^{m \times k}$$

- **Core sketch:**

$$\boldsymbol{Z} = \boldsymbol{\Phi} \boldsymbol{A} \boldsymbol{\Psi}^* \in \mathbb{C}^{s \times s}$$

Sources: J. Caesar ca. 50 BCE; Vempala et al. 1998–2000; Drineas et al. 2004–2006; Martinsson et al. 2004–2012; Sarlós 2006; Woolfe et al. 2008; Clarkson & Woodruff 2009, 2011; Boutsidis et al. 2011, 2016; HMT 2011; Nelson et al. 2012–2015; Woodruff 2014; Gu 2015; Cohen et al. 2015; Upadhyay 2016; TYUC 2016–2019....

The SKETCHYSVD Procedure

1. Use range sketches $\boldsymbol{X}, \boldsymbol{Y}$ to find orthonormal $\boldsymbol{Q} \in \mathbb{C}^{m \times k}$ and $\boldsymbol{P} \in \mathbb{C}^{n \times k}$ where

$$\boldsymbol{A} \quad \approx \quad \boldsymbol{Q}\boldsymbol{Q}^* \boldsymbol{A}\boldsymbol{P}\boldsymbol{P}^*$$

2. Use core sketch $\boldsymbol{Z} \in \mathbb{C}^{s \times s}$ to find core approximation $\boldsymbol{C} \in \mathbb{C}^{k \times k}$ such that

$$\boldsymbol{C} \quad \approx \quad \boldsymbol{Q}^* \boldsymbol{A}\boldsymbol{P}$$

3. For $r \leq k$, apply classical or randomized TSVD algorithm to form

$$[\![\boldsymbol{C}]\!]_r \quad = \quad \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^*$$

4. Obtain approximate r-truncated SVD $\hat{\boldsymbol{A}}_r$ in factored form:

$$\begin{aligned} \hat{\boldsymbol{A}}_r \quad &:= \quad (\boldsymbol{Q}\boldsymbol{U})\boldsymbol{\Sigma}(\boldsymbol{P}\boldsymbol{V})^* \quad = \quad \boldsymbol{Q}[\![\boldsymbol{C}]\!]_r\boldsymbol{P}^* \\ &\approx \quad \boldsymbol{Q}\boldsymbol{C}\boldsymbol{P}^* \quad \approx \quad \boldsymbol{Q}\boldsymbol{Q}^*\boldsymbol{A}\boldsymbol{P}\boldsymbol{P}^* \quad \approx \quad \boldsymbol{A} \end{aligned}$$

Sources: Vempala et al. 1998–2000; Drineas et al. 2004–2006; Martinsson et al. 2004–2012; Sarlós 2006; Woolfe et al. 2008; Clarkson & Woodruff 2009; Boutsidis et al. 2011, 2016; HMT 2011; Mahoney 2012; Nelson et al. 2012–2015; Woodruff 2014; Gu 2015; Cohen et al. 2015; Upadhyay 2016; TYUC 2016–2019....

SketchySVD: Pseudocode

Input: Sketch size parameters; input matrix $\boldsymbol{A} \in \mathbb{C}^{m \times n}$ as a turnstile stream

Output: Rank-r approximation $\hat{\boldsymbol{A}}_r = \boldsymbol{U\Sigma V}^*$

function INITIALIZE(m, n, k, s) ▷ Set up the sketch
  Draw random dimension reduction maps $\boldsymbol{\Upsilon}, \boldsymbol{\Omega}, \boldsymbol{\Phi}, \boldsymbol{\Psi}$
  $\boldsymbol{X} \leftarrow \boldsymbol{0}$ and $\boldsymbol{Y} \leftarrow \boldsymbol{0}$ and $\boldsymbol{Z} \leftarrow \boldsymbol{0}$
function LINEARUPDATE($\boldsymbol{H}$) ▷ Process $\boldsymbol{A} \leftarrow \boldsymbol{A} + \boldsymbol{H}$
  $\boldsymbol{X} \leftarrow \boldsymbol{X} + \boldsymbol{\Upsilon H}$
  $\boldsymbol{Y} \leftarrow \boldsymbol{Y} + \boldsymbol{H\Omega}^*$
  $\boldsymbol{Z} \leftarrow \boldsymbol{Z} + \boldsymbol{\Phi H \Psi}^*$
function SKETCHYSVD(r) ▷ Compute r-truncated SVD
  $\boldsymbol{Q} \leftarrow$ `economy_qr`$(\boldsymbol{Y})$ ▷ Basis for range
  $\boldsymbol{P} \leftarrow$ `economy_qr`$(\boldsymbol{X}^*)$ ▷ Basis for co-range
  $\boldsymbol{C} \leftarrow ((\boldsymbol{\Phi Q}) \backslash \boldsymbol{Z}) / (\boldsymbol{\Psi P})$ ▷ Core matrix
  $(\boldsymbol{U}, \boldsymbol{\Sigma}, \boldsymbol{V}) \leftarrow$ `randsvd`$(\boldsymbol{C}; r)$ ▷ Use [HMT11]
  $\boldsymbol{U} \leftarrow \boldsymbol{QU}$ and $\boldsymbol{V} \leftarrow \boldsymbol{PV}$ ▷ Consolidate unitary factors
  return $(\boldsymbol{U}, \boldsymbol{\Sigma}, \boldsymbol{V})$

SketchySVD: Analysis

Theorem 1 (TYUC 2018). **Assume**

- *The input matrix* $\boldsymbol{A} \in \mathbb{C}^{m \times n}$ *and the sketch parameters satisfy* $s \geq 2k$
- *The dimension reduction maps are independent complex standard normal*

Then *SketchySVD computes a rank-*k *approximation* $\hat{\boldsymbol{A}}_k$ *for which*

$$\mathbb{E} \left\| \boldsymbol{A} - \hat{\boldsymbol{A}}_k \right\|_{\mathrm{F}}^2 \quad \leq \quad \frac{s}{s-k} \quad \cdot \quad \min_{\varrho < k} \; \frac{k+\varrho}{k-\varrho} \cdot \left\| \boldsymbol{A} - [\![\boldsymbol{A}]\!]_\varrho \right\|_{\mathrm{F}}^2$$

In particular, when $k = (1+\varepsilon^{-1})r$ *and* $s = (1+\varepsilon^{-1})k$ *for* $\varepsilon \in (0,1]$,

$$\mathbb{E} \left\| \boldsymbol{A} - \hat{\boldsymbol{A}}_k \right\|_{\mathrm{F}}^2 \quad \leq \quad (1+5\varepsilon) \cdot \left\| \boldsymbol{A} - [\![\boldsymbol{A}]\!]_r \right\|_{\mathrm{F}}^2$$

- **Key Fact:** Approximation exploits spectral decay
- Related results hold for rank-r approximation + with high probability

Source: HMT 2011; Gu 2015; TYUC 2016–2019.

Resource Usage with Sparse Maps, $s = 2k$

Storage:

- Dimension reduction maps: $O(m+n)$
- Sketches: $O(k(m+n))$

Arithmetic:

- Linear update: Depends on structure of update (cheap!)
- SKETCHYSVD: $O(k^2(m+n))$
  - Computation of range and co-range: $O(k^2(m+n))$
  - Computation of core: $O(k(m+n)+k^3)$
  - Truncated SVD of core: $O(k^3)$
  - Consolidation: $O(k^2(m+n))$

Communication:

- One pass over data

Sources: Charikar et al. 2002; Cormode & Muthukrishnan 2005; Sarlós 2006; Woolfe et al. 2008; Clarkson & Woodruff 2009, 2011; HMT 2011; Nelson et al. 2012–2015; Meng & Mahoney 2013; Cohen 2015; TYUC 2016–2019....

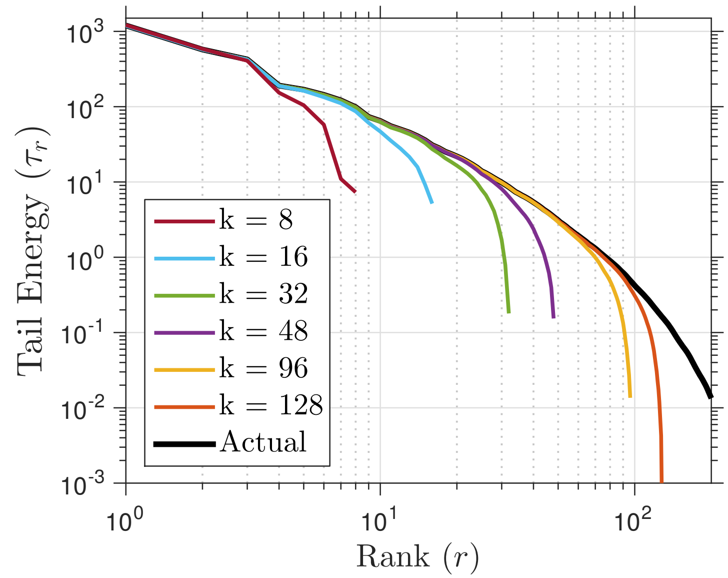
Empirical Performance

Important Things I'm Not Going to Show You

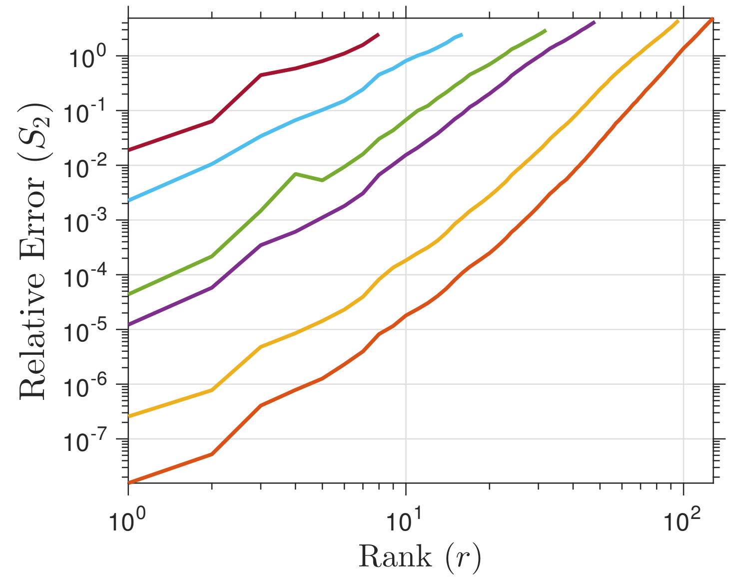
- SKETCHYSVD is insensitive to the choice of dimension reduction map
- Theory gives parameter choices (k, s) that are nearly optimal in practice
- SKETCHYSVD beats earlier techniques for synthetic and real data
- Methodology for estimating errors and selecting the truncation rank r
- Sampling distribution of approximation error and error estimator
- Other structured approximations via re-factorization or matrix nearness
- Extension to low-rank Tucker approximation of a tensor

Sources: HMT 2011; TYUC 2016–2019; SGLTU 2018–2019.

Why Truncate?



(A) Tail Energy $\tau_r(\hat{\boldsymbol{A}}_k)$



(B) Error in Rank-r Truncation $\hat{\boldsymbol{A}}_r$

$$\tau_{r+1}(\boldsymbol{M}) = \|\boldsymbol{M} - [\![\boldsymbol{M}]\!]_r\|_{\mathrm{F}}$$

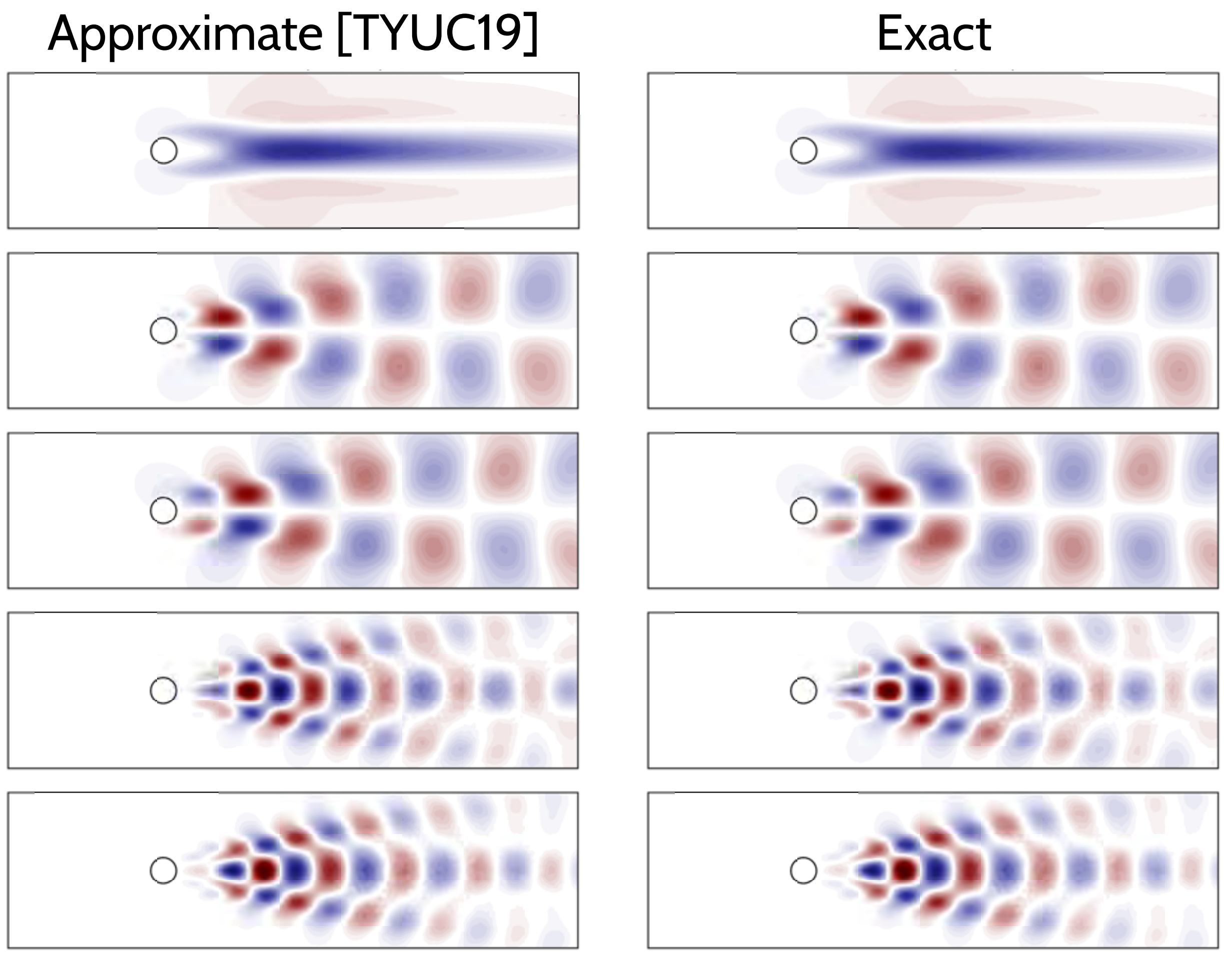
$$\operatorname{relerr}(\hat{\boldsymbol{A}}) = \frac{\|\boldsymbol{A} - \hat{\boldsymbol{A}}\|_{\mathrm{F}}}{\tau_r(\boldsymbol{A})} - 1$$

Comments: `StreamVel` Data: $m = 10,738$; $n = 5,001$; 430 MB. Algorithm: Sparse maps; $s = 2k+1$.

Reconstruction of von Kármán Street

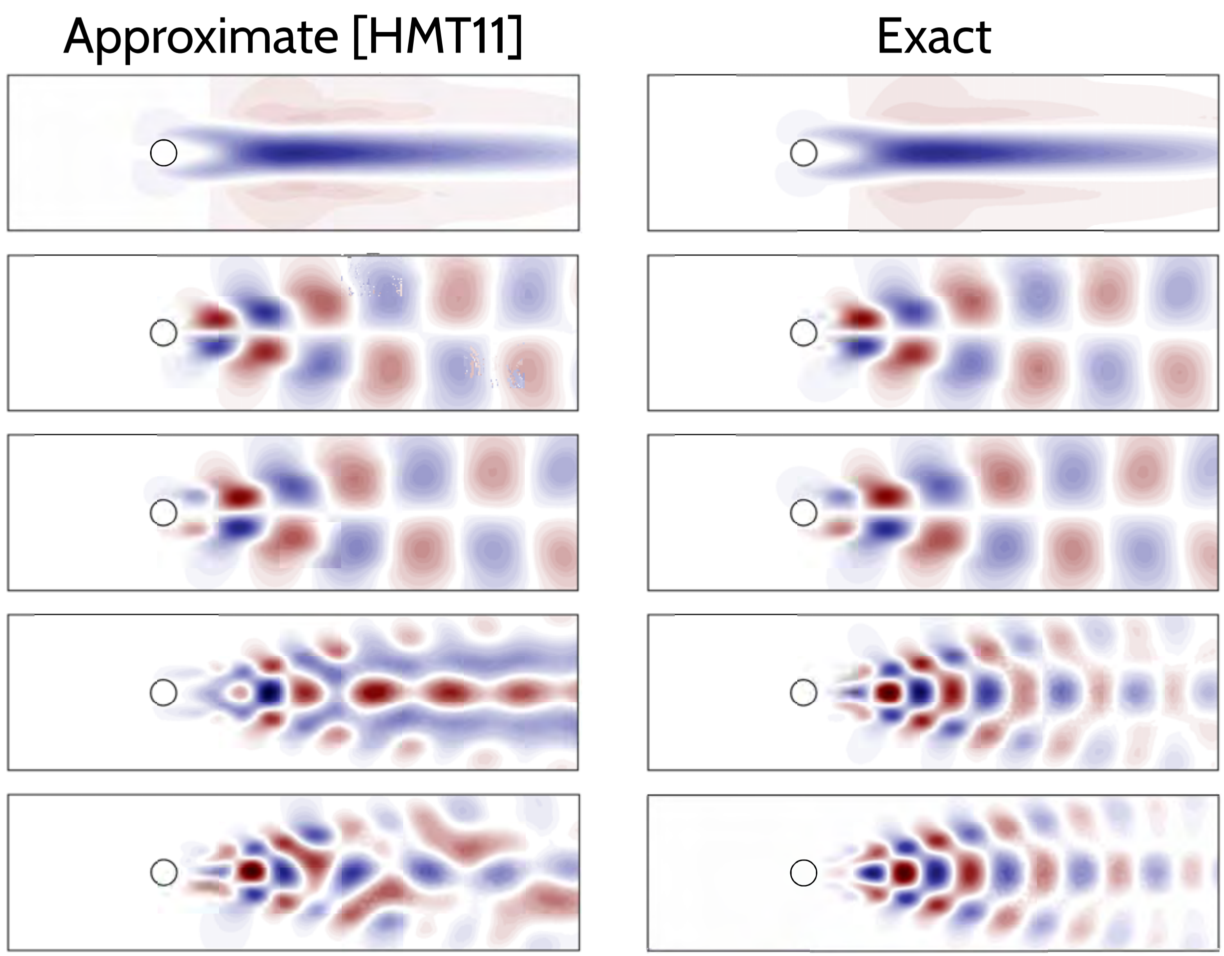
Comments: Data: $m = 10,738$; $n = 5,001$; 430 MB. Algorithm: Sparse maps; rank $r = 5$; storage $T = 48(m+n)$. Compression: $71\times$.

Left Singular Vectors of von Kármán Street



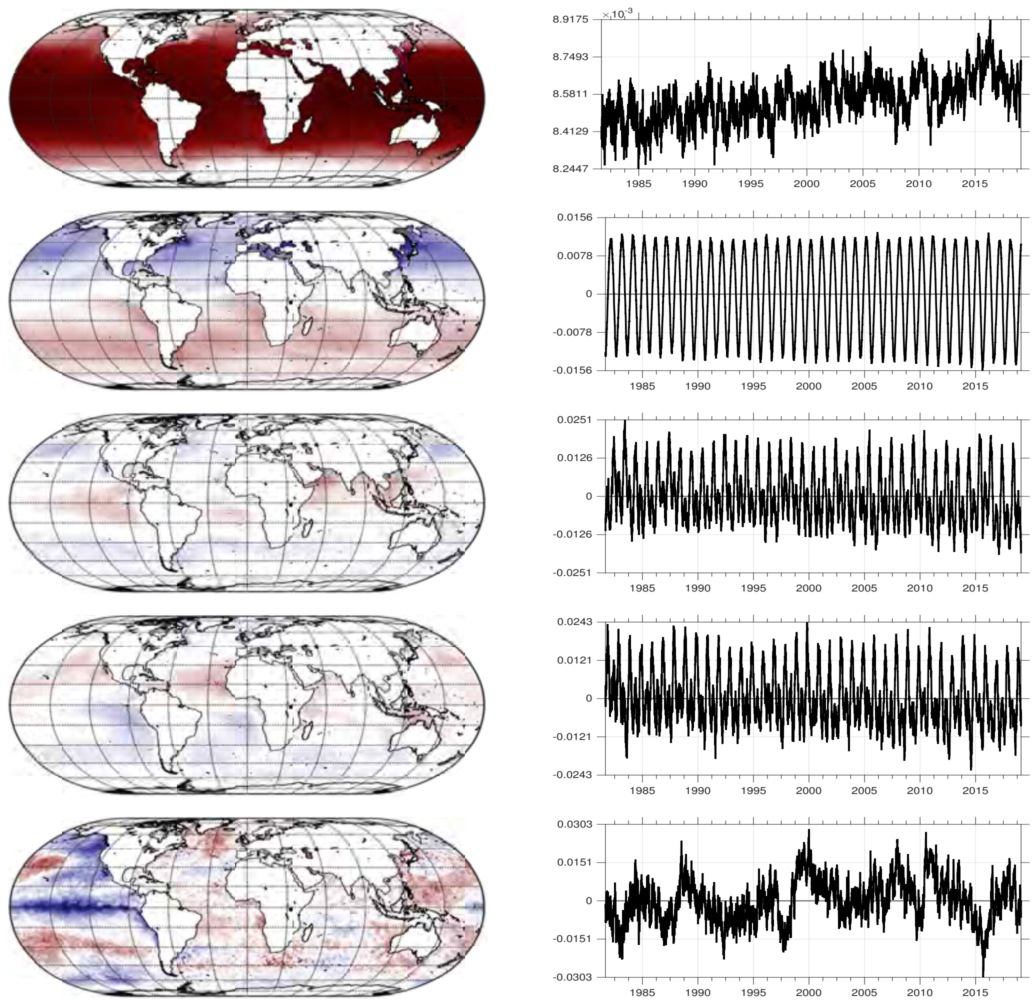
Comments: Data: $m = 10{,}738$; $n = 5{,}001$; 430 MB. Algorithm: Sparse maps; rank $r = 5$; storage $T = 48(m+n)$. Compression: $71\times$.

Left Singular Vectors of von Kármán Street



Comments: Data: $m = 10,738$; $n = 5,001$; 430 MB. Algorithm: Sparse maps; rank $r = 5$; storage $T = 48(m + n)$. Compression: $71\times$.

Singular Vectors of Sea Surface Temperature Data



Spatiotemporal Avg.

Austral / Boreal

Madden–Julian Osc.

Madden–Julian Osc.

La Niña / El Niño

Comments: Data: $m = 691{,}150$; $n = 13{,}670$; 75 GB. Algorithm: Sparse maps; $k = 48$; $s = 839$. Compression ratio: $222\times$.

Contributions

1. The first practical TSVD algorithms for streaming data
2. Rigorous *a priori* error bounds and parameter recommendations
3. *A posteriori* error estimation and methodology for rank truncation
4. Extensions to low-rank Tucker approximation for tensors
5. Validation on applications in scientific computing and optimization

To learn more...

E-mail: `jtropp@cms.caltech.edu`

Web: `http://users.cms.caltech.edu/~jtropp`

Papers:

- Halko, Martinsson, & Tropp, "Finding structure with randomness: Probabilistic algorithms for computing approximate matrix decompositions," *SIREV*, 2011.
- Tropp, Yurtsever, Udell, & Cevher, "Sketchy decisions: Low-rank matrix optimization with optimal storage," AISTATS 2017.
- Tropp, Yurstever, Udell, & Cevher, "Practical sketching algorithms for low-rank matrix approximation," *SIMAX*, 2017.
- Tropp, Yurtsever, Udell, & Cevher, "Fixed-rank approximation of a positive-semidefinite matrix from streaming data," *NeurIPS*, 2017.
- Tropp, Yurtsever, Udell, & Cevher, "Streaming low-rank matrix approximation with an application to scientific simulation," arXiv cs.NA 1902.08651.
- Sun, Guo, Tropp, & Udell, "Tensor random projections for low-memory dimension reduction," *NeurIPS Relational Databases Workshop*, 2018.
- Sun, Guo, Luo, Tropp, & Udell, "Low-rank Tucker approximation of a tensor from streaming data." Coming soon!
- Cevher, Tropp, & Yurtsever, "Scalable semidefinite programming." Coming soon!

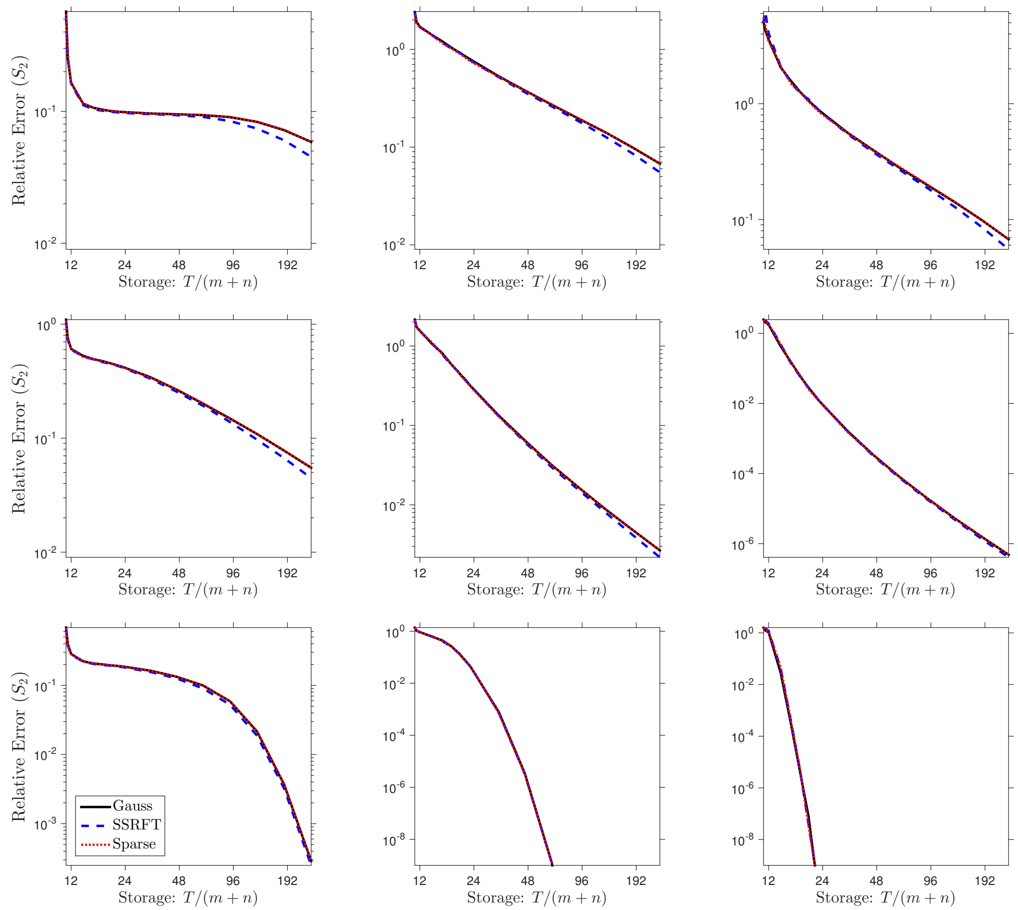
Supplementary Materials

Insensitivity to Dimension Reduction Map

LowRankHiNoise
LowRankMedNoise
LowRankLowNoise

PolyDecaySlow
PolyDecayMed
PolyDecayFast

ExpDecaySlow
ExpDecayMed
ExpDecayFast



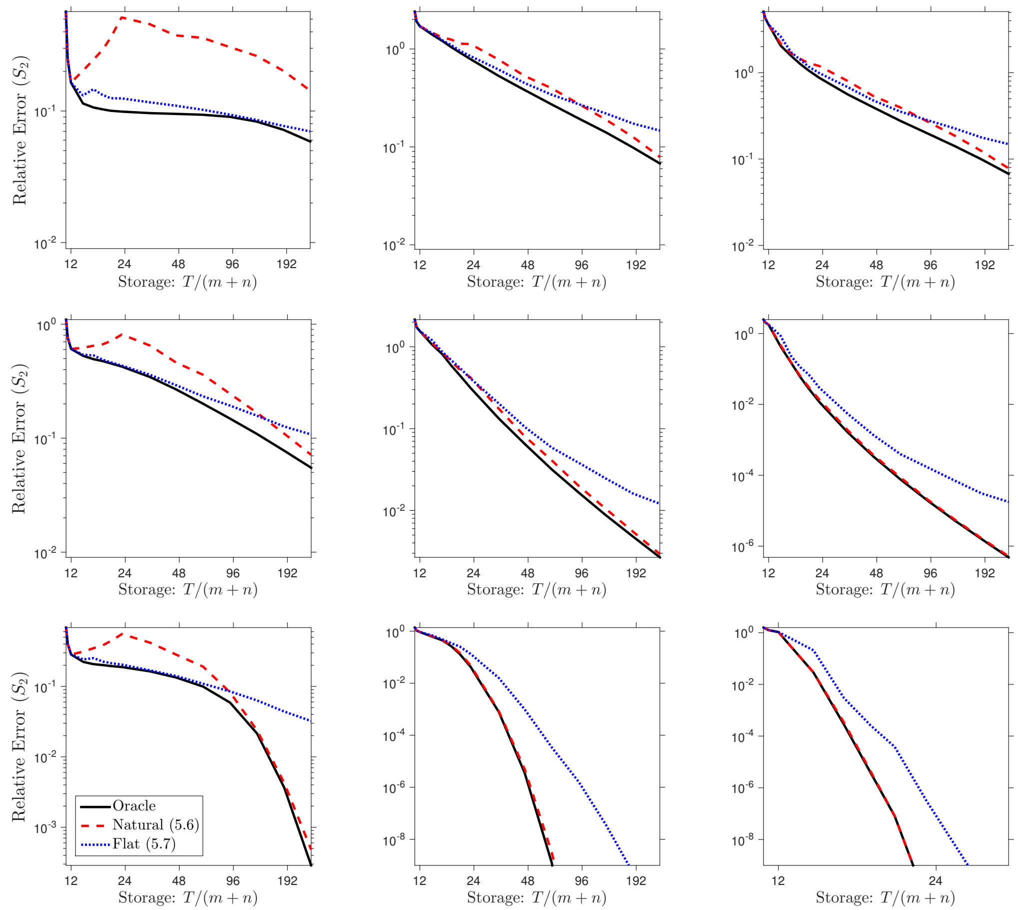
Comments: Effective rank $R = 10$, approximation rank $r = 10$, Schatten 2-norm.

Performance with Theoretical Parameter Choices

LowRankHiNoise
LowRankMedNoise
LowRankLowNoise

PolyDecaySlow
PolyDecayMed
PolyDecayFast

ExpDecaySlow
ExpDecayMed
ExpDecayFast



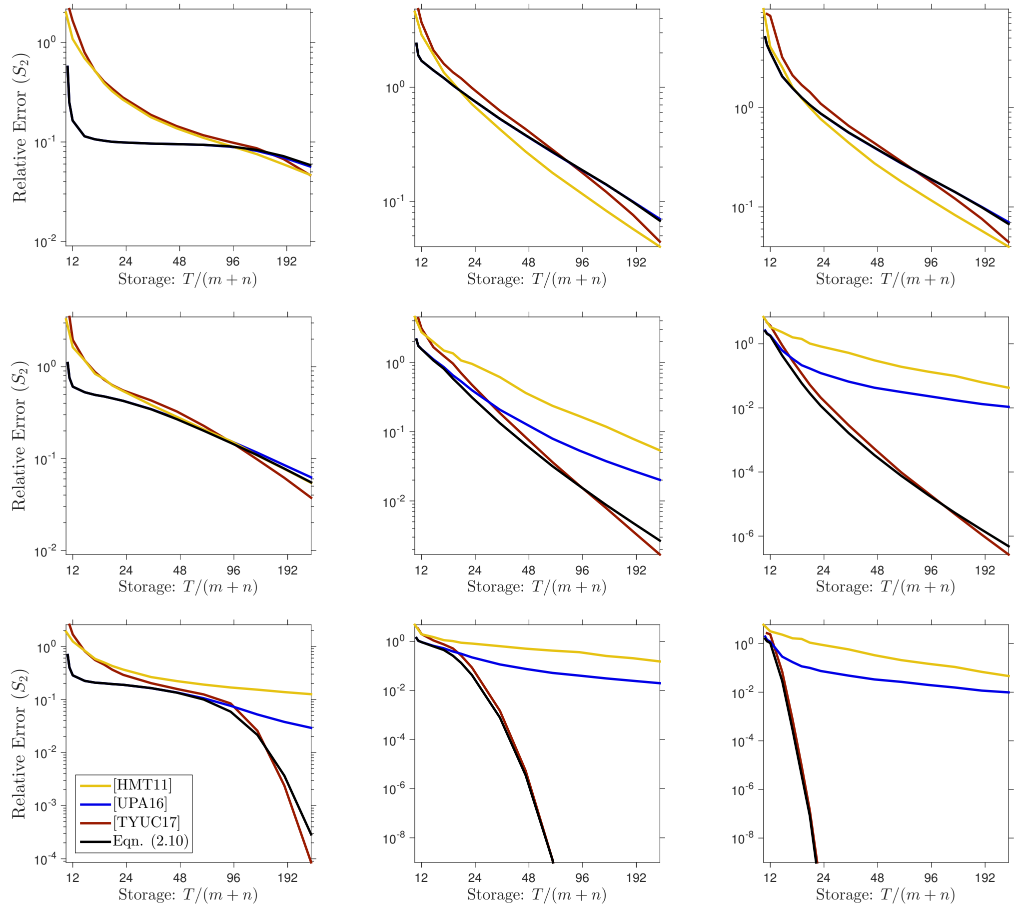
Comments: Gaussian maps, effective rank $R = 10$, approximation rank $r = 10$, Schatten 2-norm.

Method Comparison: Synthetic Data

LowRankHiNoise
LowRankMedNoise
LowRankLowNoise

PolyDecaySlow
PolyDecayMed
PolyDecayFast

ExpDecaySlow
ExpDecayMed
ExpDecayFast

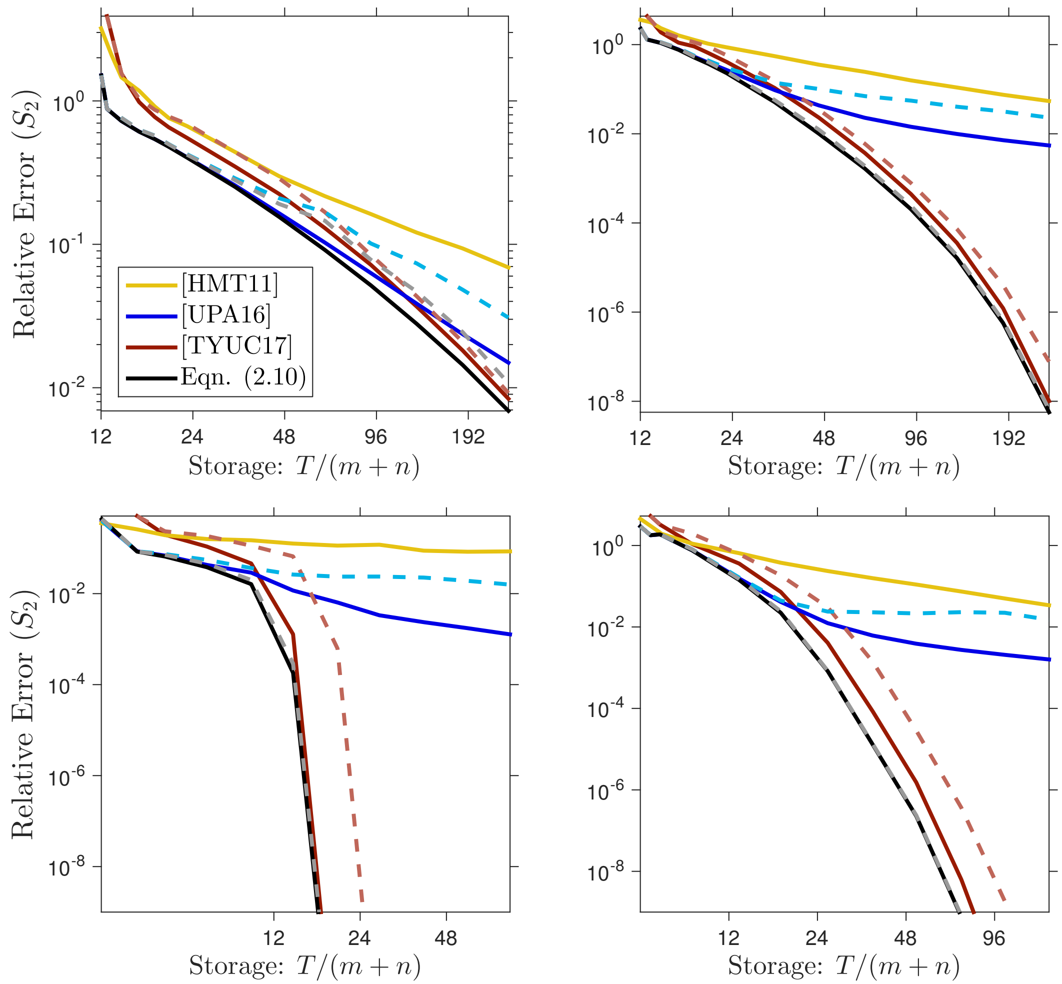


Comments: Gaussian maps, effective rank $R = 10$, oracle parameters, approximation rank $r = 10$, Schatten 2-norm.)

Method Comparison: Real Data

`MinTemp`
$m = 19,264$
$n = 7,305$
$r = 10$

`StreamVel`
$m = 10,738$
$n = 5,001$
$r = 10$



`MaxCut`
$n = 2,000$
$r = 1$

`PhaseRetrieval`
$n = 25,921$
$r = 5$

Comments: Sparse maps, Schatten 2-norm. Solid lines are errors with oracle parameters; dashed lines are *a priori* parameter choices.

A Posteriori Error Estimation

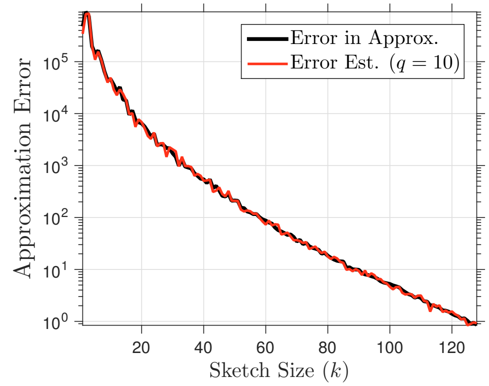
- Fix a sketch size parameter q
- Draw a random Gaussian dimension reduction map $\mathbf{\Theta} \in \mathbb{C}^{m \times q}$
- Maintain an error sketch $\boldsymbol{S} = \mathbf{\Theta}\boldsymbol{A}$
- Given an approximation $\hat{\boldsymbol{A}}$, compute the error estimator

$$\mathrm{err}_2^2(\hat{\boldsymbol{A}}) = \left\| \boldsymbol{S} - \mathbf{\Theta}\hat{\boldsymbol{A}} \right\|_{\mathrm{F}}^2$$

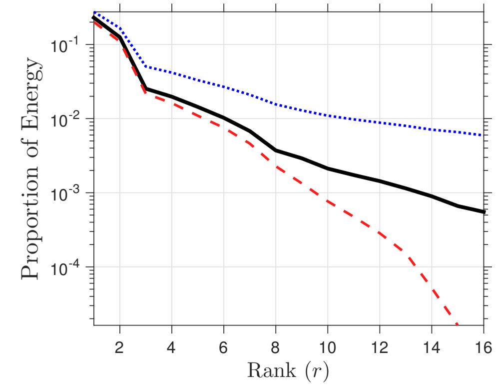
- The error estimator is unbiased and concentrates sharply
- We can also compute an empirical upper bound on the scree curve as

$$\overline{\mathrm{scree}}(r) = \left[\frac{\tau_{r+1}(\hat{\boldsymbol{A}}) + \mathrm{err}_2(\hat{\boldsymbol{A}})}{\mathrm{err}_2(\mathbf{0})} \right]^2.$$

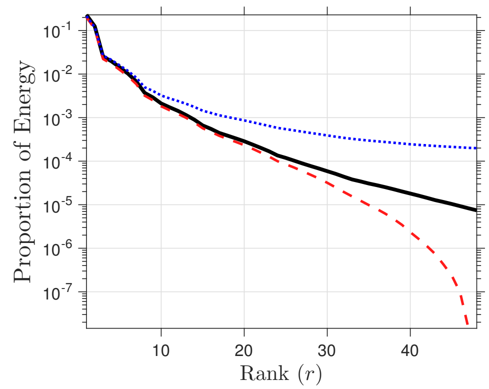
Error Estimates and Empirical Scree Curves



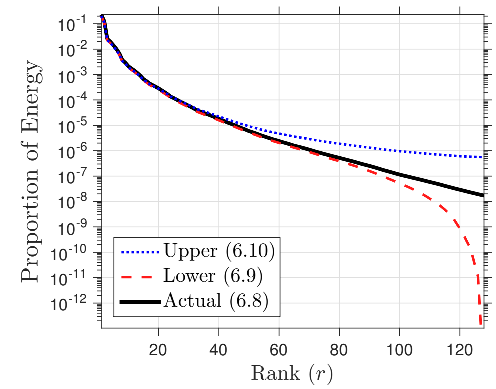
(A) Error Estimates for $\hat{\boldsymbol{A}}$



(B) Scree Plot ($k = 16$)



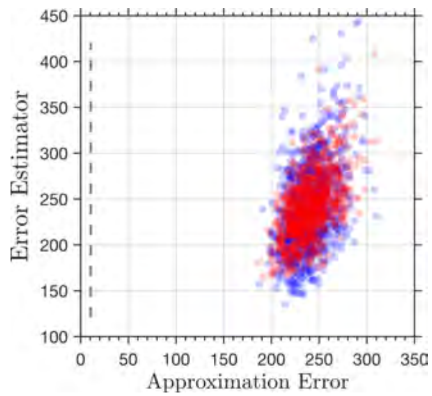
(C) Scree Plot ($k = 48$)



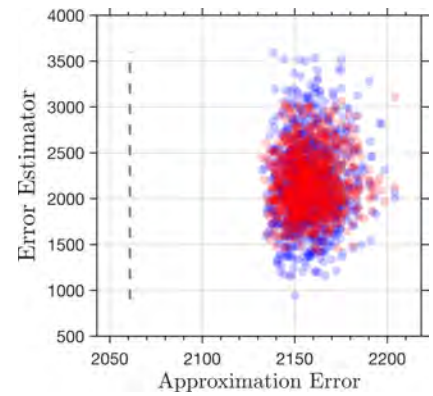
(D) Scree Plot ($k = 128$)

Comments: `StreamVel`, sparse maps, $s = 2k + 1$, $q = 10$.

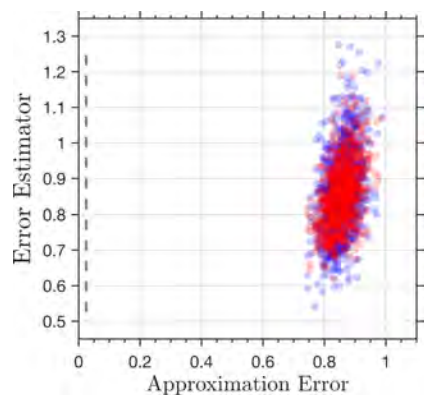
Sampling Distribution of Error and Estimator



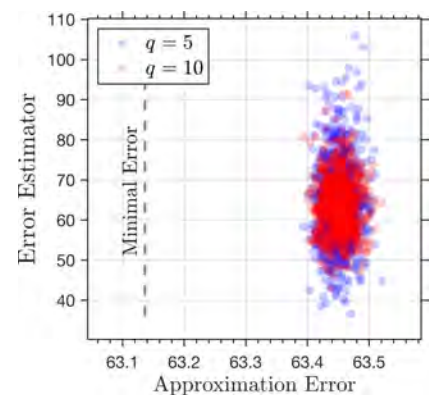
(A) Rank-k Approximation ($k = 48$)



(B) Rank-r Truncation ($k = 48$, $r = 12$)



(C) Rank-k Approximation ($k = 128$)



(D) Rank-r Truncation ($k = 128$, $r = 32$)

Comments: `StreamVel`, sparse maps, $s = 2k + 1$.