Optimal prediction in the linearly transformed spiked model

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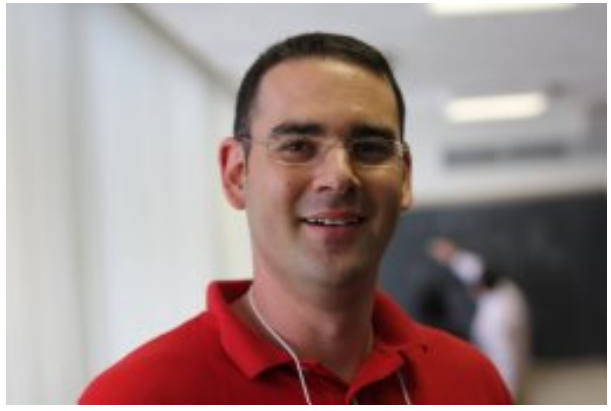
July 31, 2017

Collaborators

(a) William Leeb.
Princeton PACM



(b) Amit Singer.
Princeton Math+PACM

arxiv.org/abs/1611.10333, to be updated very soon

Linearly transformed spiked model

- Model $Y_i = A_i X_i + \varepsilon_i$, $i = 1, \ldots, n$
- Observe
  - $Y_i \in \mathbb{R}^{q_i}$, $A_i \in \mathbb{R}^{q_i \times p}$
  - Y_i: linear transform of unobserved signal of interest $X_i \in \mathbb{R}^p$
- Goal: recover X_i
  - "spiked" signal, lies on unknown low dimensional space
- Information loss:
  - Sampling noise ε_i
  - Transformation A_i: $q_i < p$
- Commutative case: $A_i^\top A_i$ diagonal

Examples

I Standard spiked model

II Cryo-Electron Microscopy (Cryo-EM)

III Missing data

Example I: Standard spiked model

- $Y_i = X_i + \varepsilon_i$, $i = 1, \ldots, n$, so $A_i = I_p$
  - $X_i \in \mathbb{R}^p$ signal, lies on unknown low dimensional space
  - $\varepsilon_i \in \mathbb{R}^p$ noise
- Well studied under high-dimensional asymptotics: e.g., Johnstone (2001); Baik et al. (2005); Baik and Silverstein (2006); Paul (2007); Nadakuditi and Edelman (2008); Nadler (2008); Bai and Ding (2012); Bai and Yao (2012); Benaych-Georges and Nadakuditi (2012); Onatski (2012); Onatski et al. (2013, 2014); Nadakuditi (2014); Gavish and Donoho (2014); Johnstone and Onatski (2015); Hachem et al. (2015); Yao et al. (2015); Donoho et al. (2017).

Example II: Cryo-EM

- Mapping the structure of molecules without crystallizing them
- Imaging of heterogeneous samples, with mixtures of molecules or multiple conformations

Cryo-EM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Summary
Precise knowledge of the structure of macromolecules in the cell is essential for understanding how they function. Structures of large macromolecules can now be obtained at near-atomic resolution by averaging thousands of electron microscope images recorded before radiation damage accumulates. This is what Amunts et al. have done in their research article on page 1485 of this issue (1), reporting the structure of the large subunit of the mitochondrial ribosome at 3.2 Å resolution by electron cryo-microscopy (cryo-EM). Together with other recent high-resolution cryo-EM structures (2–4) (see the figure), this achievement heralds the beginning of a new era in molecular biology, where structures at near-atomic resolution are no longer the prerogative of x-ray crystallography or nuclear magnetic resonance (NMR) spectroscopy.
Science
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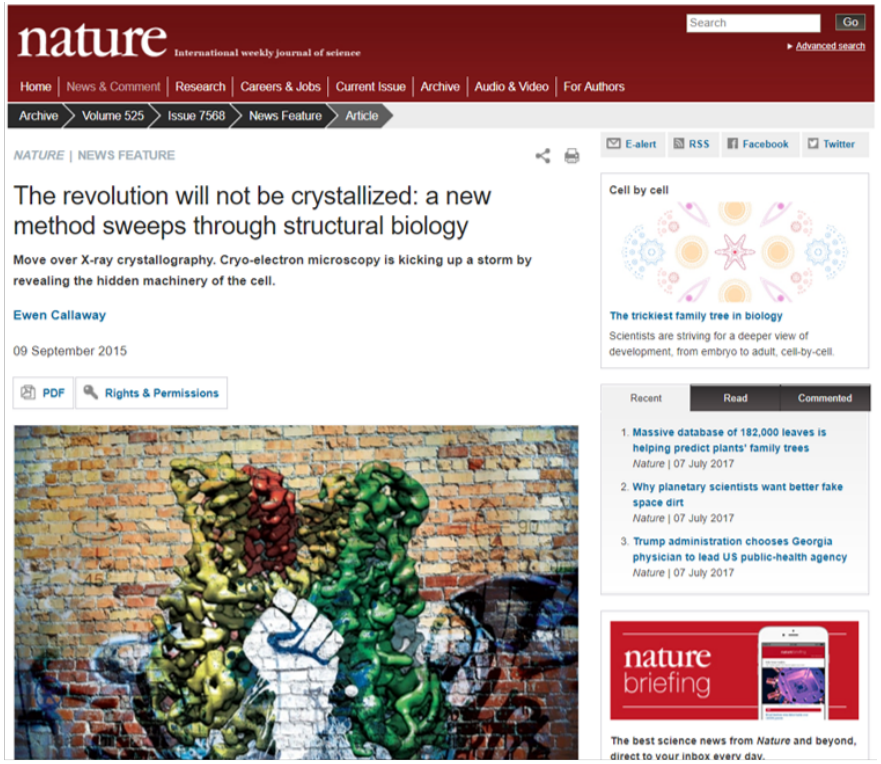
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The end of 'blob-ology': single-particle cryo-electron microscopy (cryo-EM) is now being used to solve macromolecular structures at high resolution.
Subject terms: Cryoelectron microscopy
The three-dimensional structure of a protein or protein complex provides crucial insights into its biological function. As a structure-determination technique, cryo-EM has played second fiddle to the higher-resolution approaches of X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy. This is rapidly changing, however, thanks to recent technical advances that now allow near-atomic-resolution structures to be solved using cryo-EM. The time is right to celebrate single-particle cryo-EM as our Method of the Year.
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Deconvolution in cryo-EM

- **Goal:** Estimate unfiltered projections X_i from

$$Y_i = A_i X_i + \varepsilon_i, \quad i = 1, \ldots, n.$$

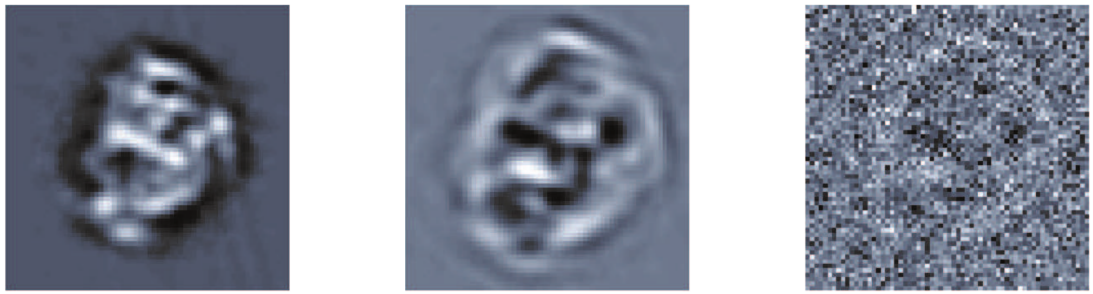


Figure : From left to right: X_i. $A_i X_i$. $A_i X_i + \varepsilon_i$

- A_i blurring convolution operator. Ill-conditioned. Diagonalized by Fourier Transform.

- Deconvolution arises in other imaging problems too

Other applications to cryo-EM

- Ab-initio 3D reconstruction
- Heterogeneity

Example III: Missing data

- $Y_i = A_i X_i + \varepsilon_i$
- A_i are coordinate-selection operators.
  - k-th row of A_i selects coordinate $l_i(k)$: $A_i(k, l) = \delta_{k, l_i(k)}$
  - $A_i^\top A_i$ diagonal, 1-s for observed entries, 0-s otherwise
- High-noise matrix completion.
  - Most prior work designed for low-noise scenarios. (Candès and Recht, 2009; Candès and Tao, 2010; Keshavan et al., 2009, 2010; Koltchinskii et al., 2011; Negahban and Wainwright, 2011; Recht, 2011; Rohde et al., 2011; Jain et al., 2013)

Goals

- Develop general methods for observations of the form $Y_i = A_i X_i + \varepsilon_i$
- Task: Predict X_i.
- Desired properties:
  1. Applicable to big data.
  2. Weak distributional assumptions. (moments)
  3. Robust to high levels of noise.
  4. Statistical guarantees. (optimality)

Our approach/methodology

1. Random effects models: Best Linear Predictor (BLP, BLUP) (Searle et al., 2009)
2. Estimate unknown coefficients: Empirical BLP.
3. Equivalent to singular value shrinkage of a new of random matrix model.
4. RMT: Characterize spectrum.
5. "Normalize" to use optimal shrinkers (Nadakuditi, 2014; Gavish and Donoho, 2014).

1. Random effects models: Best Linear Predictor (BLP).

- "Spike" X_i: $X_i = \sum_{k=1}^{r} \ell_k^{1/2} z_{ik} u_k$, where $z_{ik} \dot{\sim} (0,1)$, $\ell_1 > \ldots > \ell_r > 0$, and $|u_k| = 1$.
- BLP $\hat{X}_i^B = LY_i$ minimizes $\mathbb{E}|\hat{X}_i^B - X_i|^2$
- $L = \mathrm{Cov}\,[X_i, Y_i]\,\mathrm{Cov}\,[Y_i, Y_i]^{-1} = \Sigma_X A_i^\top (A_i \Sigma_X A_i^\top + \Sigma_\varepsilon)^{-1}$
- Under conditions (see paper) show $\mathbb{E}|\hat{X}_i^B - \hat{X}_i^0|^2 \to 0$, where

$$\hat{X}_i^0 = \sum_{k=1}^{r} \tau_k u_k u_k^\top A_i^\top Y_i$$

for some $\tau_k > 0$.

2. Estimate unknown coefficients: Empirical BLP.

- BLP $\hat{X}_i^0 = \sum_{k=1}^{r} \tau_k u_k u_k^\top A_i^\top Y_i$
- u_k, τ_k parameters, must be estimated.
- $$\hat{X}_i = \sum_{k=1}^{r} \eta_k \hat{u}_k \hat{u}_k^\top A_i^\top Y_i$$

  where $\hat{u}_k$ are eigenvectors of cov mx of $A_i^\top Y_i$.
- Goal: find optimal η_k

3. Equivalence to singular value shrinkage.

- By exchangeability,

$$\mathbb{E}|\hat{X}_i - X_i|^2 = \frac{1}{n}\mathbb{E}|\hat{X} - X|^2,$$

  where $X = (X_1, \ldots, X_n)^\top$, $\hat{X} = (\hat{X}_1, \ldots, \hat{X}_n)^\top$.
- Backprojected data $B = (A_1^\top Y_1, \ldots, A_n^\top Y_n)^\top = \sum_{k=1}^m \sigma_k \cdot \hat{u}_k \hat{v}_k^\top$,

$$\hat{X} = \sum_{k=1}^r \eta_k \sigma_k \cdot \hat{u}_k \hat{v}_k^\top$$

  is singular value shrinkage estimate.
- Thus, asy optimal η_k are determined by asy spectrum of B (e.g. Nadakuditi, 2014; Gavish and Donoho, 2014).

4. RMT: Characterize spectrum.

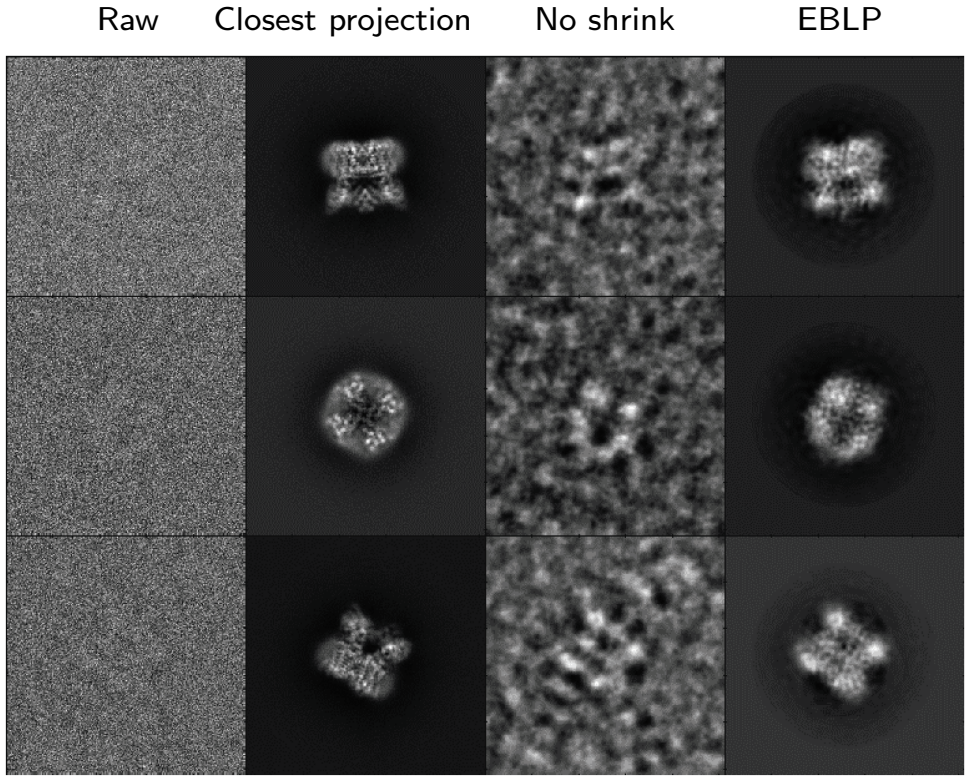
- Remains to find asy spectrum of $B = (A_1^\top Y_1, \ldots, A_n^\top Y_n)^\top$
- Non-standard random matrix model.
- $A_i^\top Y_i = A_i^\top A_i X_i + A_i^\top \varepsilon_i$.
  - Dependence between signal and noise.
  - General moment assumptions on X_i, A_i, ε_i, no invariance.
- Follow approach of Benaych-Georges and Nadakuditi (2012); extend "deterministic equivalents" tools of Bai et al. (2007).

5. "Normalize".

- Almost done... But optimal shrinkage coefficients η_k depend on $|\mathbb{E}[A_i^\top A_i]u_k|^2$, not clear how to estimate consistently.
- Normalize: $\hat{M}^{-1/2} A_i^\top Y_i$, where $\hat{M} = n^{-1} \sum_{i=1}^n A_i^\top A_i$. Everything goes through.

Results: Experimental data - TRPV1

Bhamre, Zhang, Singer (*Journal of Structural Biology, 2016*)

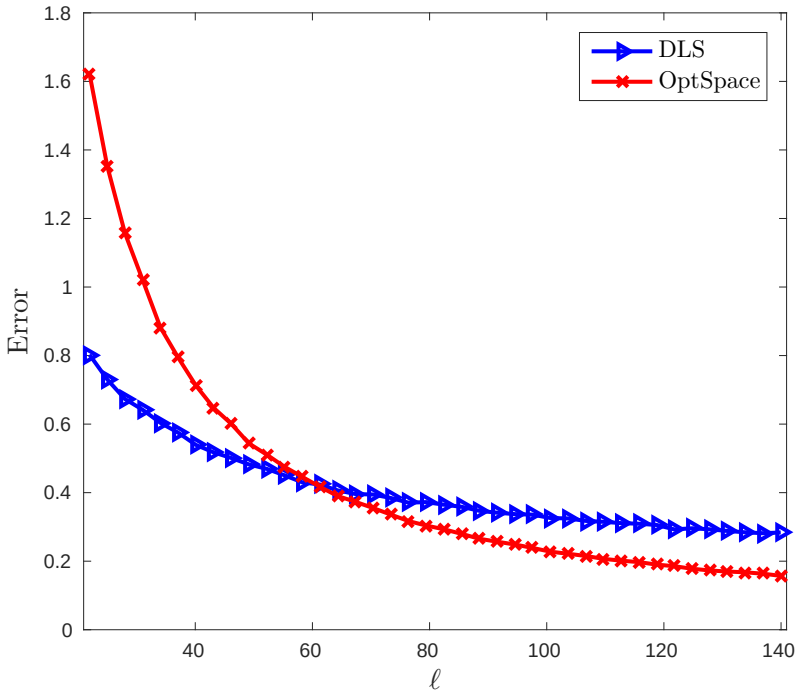


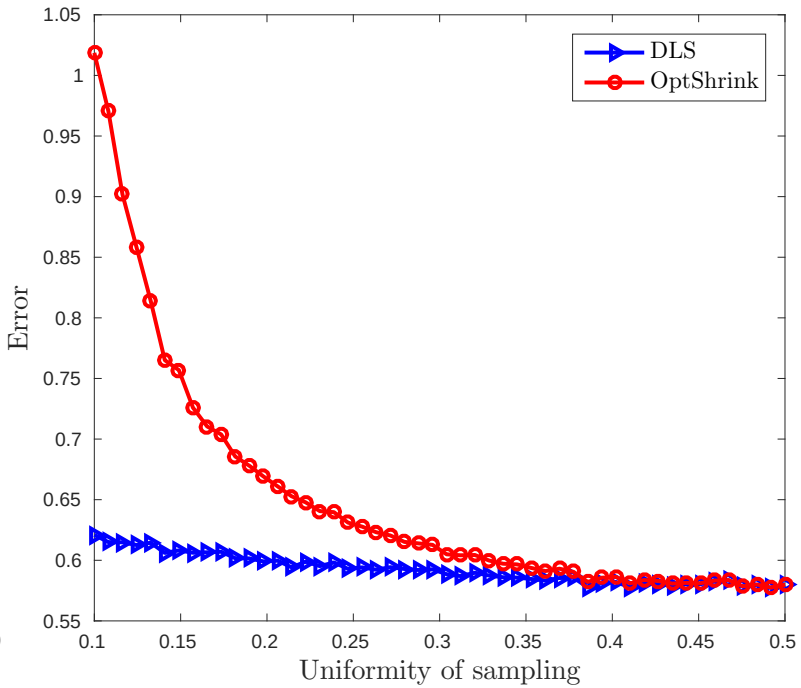
- TRPV1, K2 direct electron detector
- 35645 motion corrected, picked particle images of 256×256 pixels belonging to 935 defocus groups (Liao et al., Nature 2013)

Results: matrix completion

- We test our shrinkage method to other scalable matrix completion methods.

D, Leeb, Singer (*arXiv 2016*)





- Left: Comparison with OptSpace (Keshavan et al., 2009) for different SNRs. Our method outperforms in the high-noise regime.
- Right: Comparison with OptShrink (Nadakuditi, 2014) for different sampling uniformity levels. Our method outperforms OptShrink when the data is unevenly sampled across the rows of the matrix.

Conclusion

- Linearly transformed spiked model: $Y_i = A_i X_i + \varepsilon_i$, $i = 1, \ldots, n$
- Broad applicability: Image processing, Cryo-EM, Missing data
- EBLP Methods for predicting X_i: fast, weak assumptions, robust to noise, guarantees
- Key technical result: spectrum of backprojected data.

slides available at github.com/dobriban

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