Understanding Trainable Sparse Coding with Matrix Factorization

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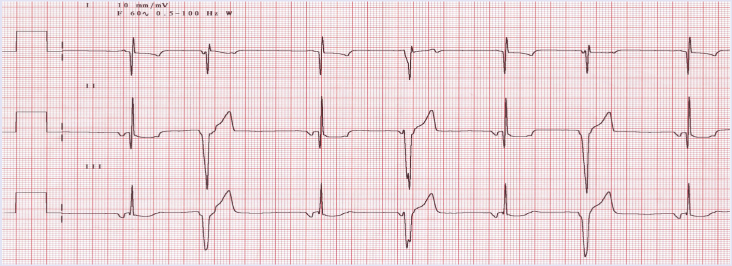
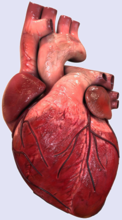
Plan

Plan

1. Physiological signals
2. End-to-end Approaches for Time Series
3. Post-training for Deep Learning
4. Adaptive Iterative Soft Thresholding
5. Numerical Experiments

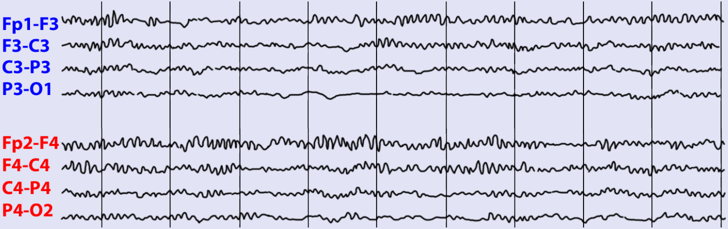
ECG



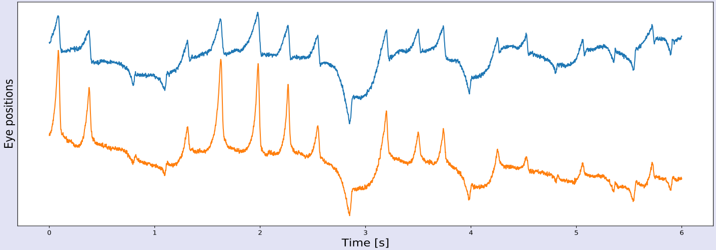


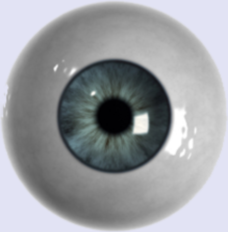
Physiological signals

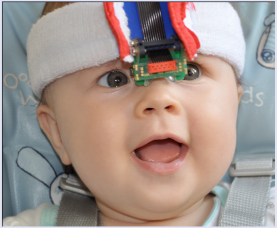
EEG



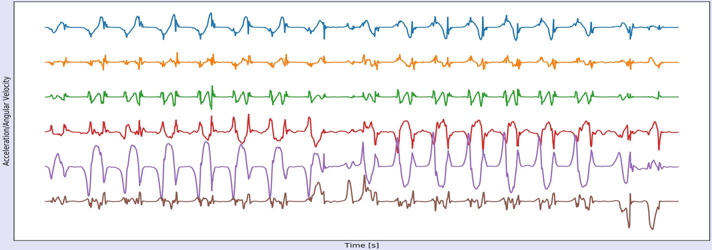
Oculometric signals

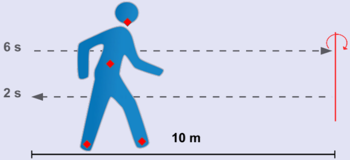




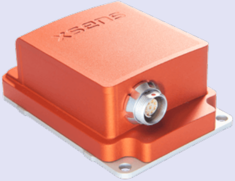


Accelerometers





4×



Statistical analysis for Time Series

- Failure of the vectorial distances
  - Alignment issues, different lengths

    (can be solved with DTW)
  - "Curse of dimensionality"
- Different approaches which can be classified in 2 categories:
  - Model based methods:
    feature extraction + vectorial method, ...
  - Data driven methods
    End-to-end model, Neural networks, ...

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Plan

Neural Networks:

- Raw signal as input,

  No feature-engineering

- Internally select the data representation,

  Adaptive

- Representation adapted to the task,

  Performant

- Simple training algorithms,

  Scalable

Split between risk error 3 terms:

[Bottou and Bousquet, 2008]

- Approximation error: Universal approximation,
  [Hornik, 1991]
- Estimation error: Generalization bound,
  [Kawaguchi et al., 2017]
- Optimization error: Learning convexification,
  [Haeffele and Vidal, 2017]

Main drawback:

Lack of interpretability. It is often seen as a black box.

How can we bring interpretability in the internal representation?

Task-driven Dictionary Learning:

[Mairal et al., 2012]

- Raw signal as input,

  No feature-engineering

- Representation adapted to the task,

  Performant

- Complex training algorithms,

  ~~Scalable~~

- Highlight local structures,

  Interpretable

Can we study the links between these two models to bring more interpretability in neural networks?

Plan

Paper with J. Audiffren: arxiv:1611.04499

Use the idea to split the representation learning and the task resolution:

- *Post-training* step: only train the last layer,
- Easy problem: this problem is often convex,
- Link with kernel: close form solution for optimal last layer.
- Experiments: consistent performance boost with multiple architecture.

Plan

The LASSO or sparse coding problem is defined as

$$\underset{z}{\operatorname{argmin}}\, F(z) := \underbrace{\|x - Dz\|_2^2}_{E(z)} + \lambda \|z\|_1 \ , \tag{1}$$

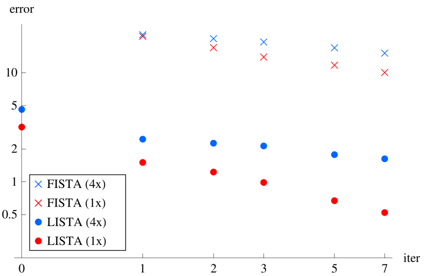
where $x \in \mathbb{R}^P$, $D \in \mathbb{R}^{P \times K}$ and $z \in \mathbb{R}^K$.

(1) can be rewritten as a proximal problem for the B-norm

$$\underset{z}{\operatorname{argmin}}\, \underbrace{(y - z)^\mathsf{T} B (y - z)}_{E(z)} + \lambda \|z\|_1 \quad \Big(= F(z)\Big)$$

where $B = D^\mathsf{T} D$ is the Gram matrix of D and $y = D^\dagger x$.

Accelerate the LASSO resolution using a neural network.



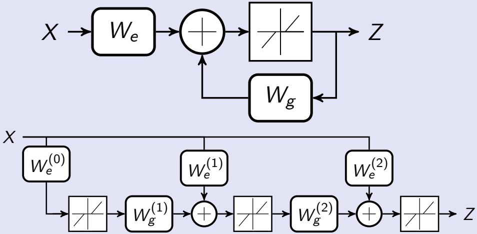


Figure: Adapted from [Gregor and Lecun, 2010]

Link dictionary learning model and sparse representation.

Why does it work?

ISTA (1/2) [Daubechies et al., 2004, Beck and Teboulle, 2009]

Surrogate function F_q associated with point $z^{(q)}$:

$$F_q(z) = E(z^{(q)}) + \langle B(z^{(q)} - y), z - z^{(q)} \rangle + \frac{\|B\|_2}{2} \|z - z^{(q)}\|_2^2 + \lambda \|z\|_1 \ ,$$

Properties

This surrogate function satisfies

1. $F_q(z^{(q)}) = F(z^{(q)})$
2. for all z, $F_q(z) \geq F(z)$,
3. solving $\operatorname{argmin}_z F_q(z)$ is computationally efficient.

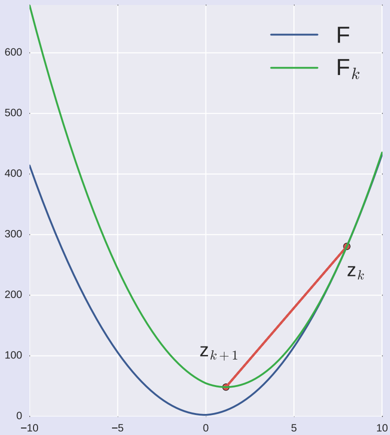
ISTA (2/2)

Iterative procedure: proximal splitting

$$z^{(q+1)} = \operatorname*{argmin}_z F_q(z)$$
$$= \operatorname*{prox}_{\lambda\|\cdot\|_1}\left(z^{(q)} - \frac{1}{L}\nabla E(z^{(q)})\right) \quad (2)$$

Properties

1. z^* is a fix point of (2),
2. Efficient computation for $z^{(q+1)}$ as the problem is separable,
3. Convergence in $\mathcal{O}\left(\frac{1}{q}\right)$ in general.



Why does it work?

- **Guaranteed descent**

  The construction of the next point guarantees the cost function is decreasing:

$$F(z^{(q+1)}) \leq F_q(z^{(q+1)}) \leq F_q(z^{(q)}) = F(z^{(q)})$$

- **Efficient computation:**

  With the isotropic quadratic form $\frac{L}{2}\boldsymbol{I}_K$, the function F_q is separable. The computation are linear in K .

Toward an adaptive procedure

We define $Q_S(u,v) = \frac{1}{2}(u-v)^\mathsf{T} S(u-v) + \lambda\|u\|_1$.

ISTA:

$$\begin{aligned} F_q(z) &= E(z^{(q)}) + \langle B(z^{(q)}-y), z - z^{(q)}\rangle + Q_{L\boldsymbol{I}_K}(z, z^{(q)}) \ , \\ &\to \min_z Q_{L\boldsymbol{I}_K}(z, z^{(q)} - \frac{1}{L}B(z^{(q)}-y)) \end{aligned}$$

$\Longrightarrow$ Replace B with an upperbound $L\boldsymbol{I}_K$

FacNet: For any matrix S diagonal, and A unitary we define :

$$\begin{aligned} \widetilde{F}_q(z) &= E(z^{(q)}) + \langle B(z^{(q)}-y), z - z^{(q)}\rangle + Q_S(Az, Az^{(q)}) \ , \\ &\to \min_z Q_S(Az, Az^{(q)} - S^{-1}AB(z^{(q)}-y)) \end{aligned}$$

$\Longrightarrow$ Replace B with an approximation $A^\mathsf{T} SA$

Can we choose A, S to accelerate the optimization compared to ISTA?

Toward an adaptive procedure

Similar iterative procedure with steps adapted to the problem topology.

$$\widetilde{F_q}(z) = F(z) + (z - z^{(q)})^{\mathsf{T}} R (z - z^{(q)}) + \delta_A(z)$$

Tradeoff between:

- Rotation to align the norm $\|\cdot\|_B$ and the norm $\|\cdot\|_1$, Computation

$$R = A^{\mathsf{T}} S A - B$$

- Deformation of the ℓ_1-norm with the rotation A . Accuracy

$$\delta_A(z) = \lambda \left(\|Az\|_1 - \|z\|_1 \right)$$

One step improvement

Proposition

Suppose that $R = A^\mathsf{T} S A - B \succ 0$ is positive definite, and define

$$z^{(q+1)} = \arg\min_z \widetilde{F_q}(z) \ ,$$

Then

$$F(z^{(q+1)}) - F(z^*) \leq \frac{1}{2}(z^{(q)} - z^*)^\mathsf{T} R (z^{(q)} - z^*) + \delta_A(z^*) - \delta_A(z^{(q+1)}) \ .$$

We are interested in factorization (A, S) for which $\|R\|_2$ and δ_A are small.

Adaptive Iterative Soft thresholding - Convergence rate

Theorem

Let A_q, S_q be the pair of unitary and diagonal matrices corresponding to iteration q, chosen such that $R_q = A_q^{\mathsf{T}} S_q A_q - B \succ 0$. It results that

$$F(z^{(q)}) - F(z^*) \leq \frac{(z^* - z^{(0)})^{\mathsf{T}} R_0 (z^* - z^{(0)}) + 2L_{A_0}(z^{(1)}) \|(z^* - z^{(1)})\|_2}{2q} + \frac{\alpha_q - \beta_q}{2q} \ ,$$

$$\alpha_q = \sum_{i=1}^{q-1} \left(2L_{A_i}(z^{(i+1)}) \|(z^* - z^{(i+1)})\| + (z^* - z^{(i)})^{\mathsf{T}} (R_{i-1} - R_i)(z^* - z^{(i)}) \right) \ ,$$

$$\beta_q = \sum_{i=0}^{q-1} (i+1) \left((z^{(i+1)} - z^{(i)})^{\mathsf{T}} R_i (z^{(i+1)} - z^{(i)}) + 2\delta_{A_i}(z^{(i+1)}) - 2\delta_{A_i}(z^{(i)}) \right) \ ,$$

where $L_A(z)$ denote the local Lipschitz constant of δ_A at z.

Interpretation

- For $A_q = \boldsymbol{I}_K$ and $S_q = \|B\|_2 \boldsymbol{I}_K$, the procedure is equivalent to ISTA, with the same rate of convergence.

- If $\|R_0\|_2 + 2\dfrac{L_{A_0}(z_1)}{\|z^* - z_0\|_2} \leq \dfrac{\|B\|_2}{2}$ and $A_q = \boldsymbol{I}_K$ and $S_q = \|B\|_2 \boldsymbol{I}_K$ for $k > 0$, then the procedure get a head start compare to ISTA

- **Phase transition :**
  The upper bound is improved when $\|R_q\|_2 + 2\dfrac{L_{A_q}(z^{(q+1)})}{\|z^* - z^{(q)}\|_2} \leq \dfrac{\|B\|_2}{2}$, it is thus harder to gain as $\|z^{(q)} - z^*\|_2 \to 0$

Generic Dictionaries

A dictionary $D \in \mathbb{R}^{p \times K}$ is a generic dictionary when its columns D_i are drawn uniformly over the ℓ_2 unit sphere $\mathcal{S}^{p-1}$.

Theorem (Acceleration conditions)

In **expectation over the generic dictionary** D, the factorization algorithm using a diagonally dominant matrix $A \subset \mathcal{E}_\delta$, has better performance for iteration $q+1$ than the normal ISTA iteration – which uses the identity – when

$$\lambda \mathbb{E}_z \left[\|z^{(q+1)}\|_1 + \|z^*\|_1 \right] \leq \sqrt{\frac{K(K-1)}{p}} \underbrace{\mathbb{E}_z \left[\|z^{(q)} - z^*\|_2^2 \right]}_{\substack{\text{expected resolution} \\ \text{at iteration } q}}$$

Corollary (Acceleration conditions)

If the input distribution and the regularization parameter λ verify

$$\frac{\lambda\sqrt{p}}{8} \leq \mathbb{E}_z\left[\|z^*\|_1\right] ,$$

Then for any resolution $\mathbb{E}_z\left[\|z^{(q)} - z^*\|_2\right] = \epsilon > 0$ at iteration q, the performance of our factorization algorithm is better than the performance of ISTA, in expectation over the generic dictionaries.

FacNet can improve the performances compared to ISTA when this is verified.

Plan

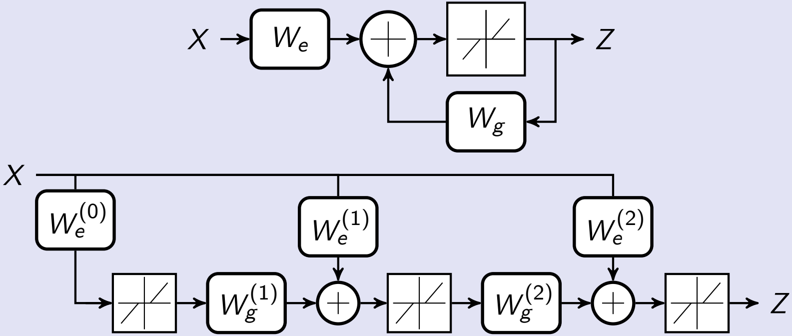


Figure: Network architecture for ISTA/LISTA. LISTA is the unfolded version of the RNN of ISTA, trainable with back-propagation.

If $W_e = \frac{D^\top}{L}$ and $W_g = I - \frac{B}{L}$, this network is exactly 2 iterations of ISTA.

FacNet

Specialization of LISTA

$$z^{(q+1)} = A^{\mathsf{T}} \operatorname*{prox}_{S}(Az^{(q)} - S^{-1}AB(z^{(q)} - y)) \ ,$$

with A unitary and S diagonal.
Same architecture with more constraints on the parameter space:

$$\begin{cases} W_e & = S^{-1}AD^{\mathsf{T}} \\ W_g & = A^{\mathsf{T}} - S^{-1}ABA^{\mathsf{T}} \end{cases}$$

$\Rightarrow$ LISTA can be at least as good as this model.

Learned FISTA

The same ideas can also be applied to FISTA to obtain similar procedures:

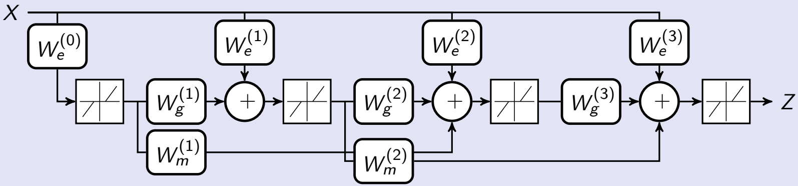


Figure: Network architecture for L-FISTA.

Artificial simulation

Generating Model:

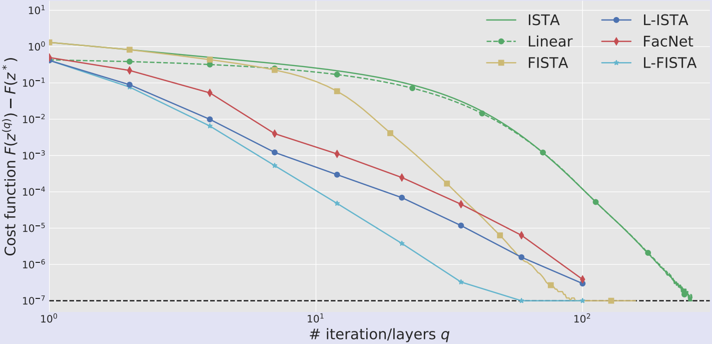
- $D = \left(\frac{d_1}{\|d_1\|_2}, \dots \frac{d_K}{\|d_K\|_2} \right)$ with $d_k \sim \mathcal{N}(0, \boldsymbol{I}_P)$ for all $k \in [\![1, K]\!]$,
- $z = (z_1, \dots z_K)$ are constructed following a bernouilli gaussian:

$$z_k = b_k a_k, \qquad b_k \sim \mathcal{B}(\rho) \text{ and } a \sim \mathcal{N}(0, \sigma \boldsymbol{I}_K)$$

<u>with:</u> $K = 100$, $P = 64$, for the dimension, $\sigma = 10$ and $\lambda = 0.01$

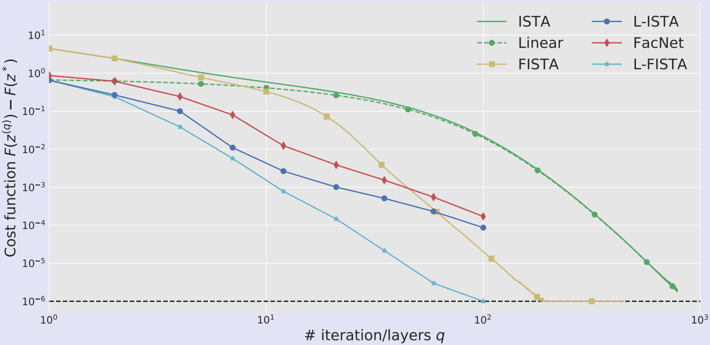
$\Rightarrow$ The sparsity patterns are uniformely distributed.

Artificial simulation



Evolution of the cost function $F(z^{(q)}) - F(z^*)$ with the number of layers/iterations q with a sparse model $\rho = {}^1/_{20}$.

Artificial simulation

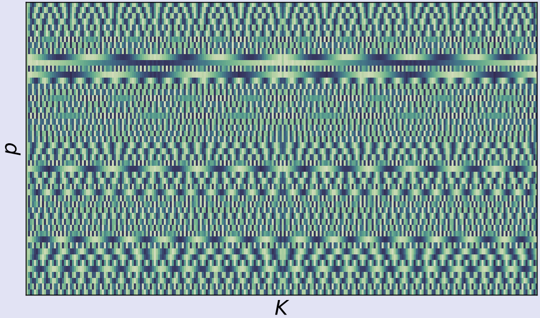


Evolution of the cost function $F(z^{(q)}) - F(z^*)$ with the number of layers/iterations q with a denser model $\rho = {}^1/_4$.

Adversarial dictionary:
$D = \left[d_1 \dots d_K\right] \in \mathbb{R}^{K \times p}$,
with

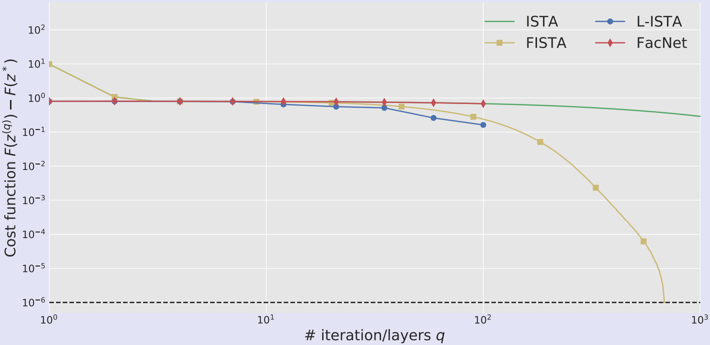
$$d_j = e^{-i\frac{2\pi j \zeta_q}{K}}$$

for a random subset of frequencies $\left\{\zeta_i\right\}_{i \leq m}$



$\Rightarrow$ Eigenvectors of D are far from canonical basis.

Adversarial dictionary



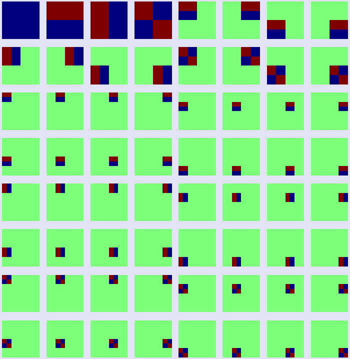
Evolution of the cost function $F(z^{(q)}) - F(z^*)$ with the number of layers/iterations k with n adversarial dictionary.

PASCAL 08

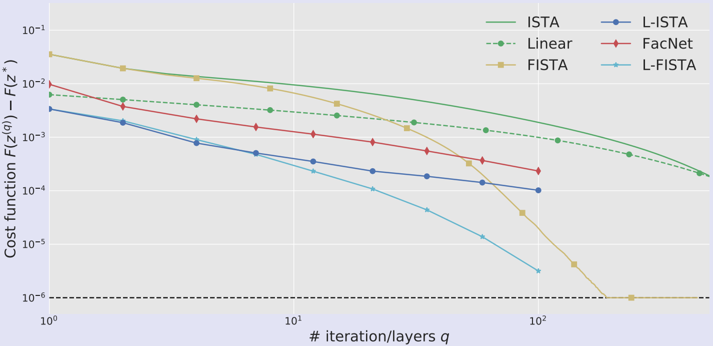
Sparse coding for the PASCAL 08 datasets over the Haar wavelets family.

The sparse coding is performed for patches of size 8×8.

Train over 500 images and test over 100 images.



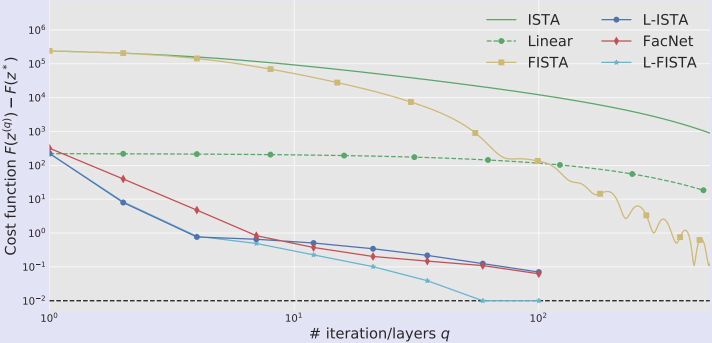
PASCAL 08



Evolution of the cost function $F(z^{(q)}) - F(z^*)$ with the number of layers or the number of iteration q for Pascal VOC 2008.

MNIST

Dictionary D with $K = 100$ atoms learned on 10 000 MNIST samples (17x17) with dictionary learning. LISTA trained with MNIST training set and tested on MNIST test set.



Evolution of the cost function $F(z^{(q)}) - F(z^*)$ with the number of layers or the number of iteration q for MNIST.

Conclusion

- Non asymptotic acceleration is possible :
  Approximate matrix factorization of $B = D^{\mathsf{T}} D$
  - Nearly diagonalize the kernel,
  - ℓ_1-norm nearly invariant by this orthogonal transformation.

- Future work:
  - Improve the factorization formulation:

$$\min_{A^{\mathsf{T}} A = \boldsymbol{I}_K} f(\|DA\|_{1,2}) + \lambda_q \frac{\|A\|_{1,1}}{n} \ ,$$

  - Give generic bounds for sub gaussian D,
  - Link to Sparse PCA.

Questions?

Code: tomMoral/AdaptiveOptim

Paper: https://arxiv.org/abs/1706.01338

More at tommoral.github.io tomMoral

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