PRINCIPAL COMPONENT REGRESSION WITHOUT PRINCIPAL COMPONENT ANALYSIS

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[1]Stanford, [2]MIT, [3]Microsoft Reseach

RESOURCES

Paper, slides, and template code available at

chrismusco.com

OUR WORK

Simple, robust algorithms for principal component regression.

PRINCIPAL COMPONENT REGRESSION

Principal Component Regression (PCR) =

Principal Component Analysis (unsupervised)

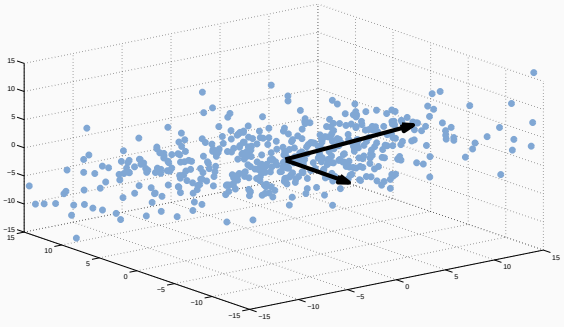
+

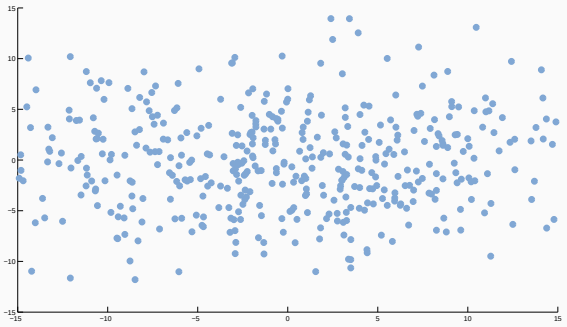
Linear Regression (supervised)

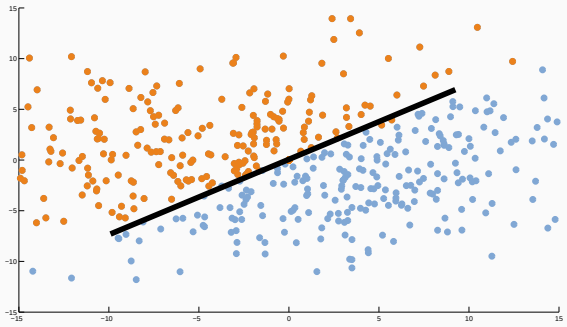
OUR APPROACH: SKIP THE DIMENSIONALITY REDUCTION

PCA

Regression







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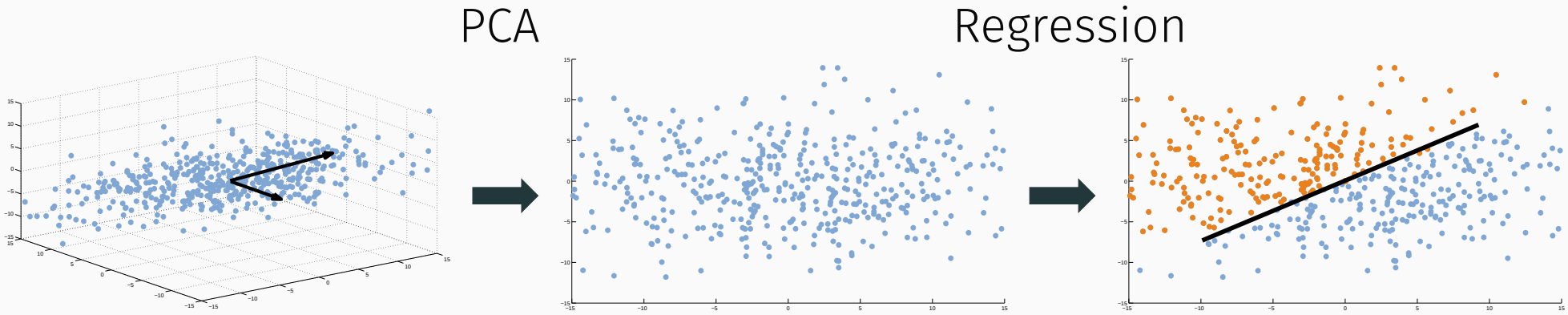
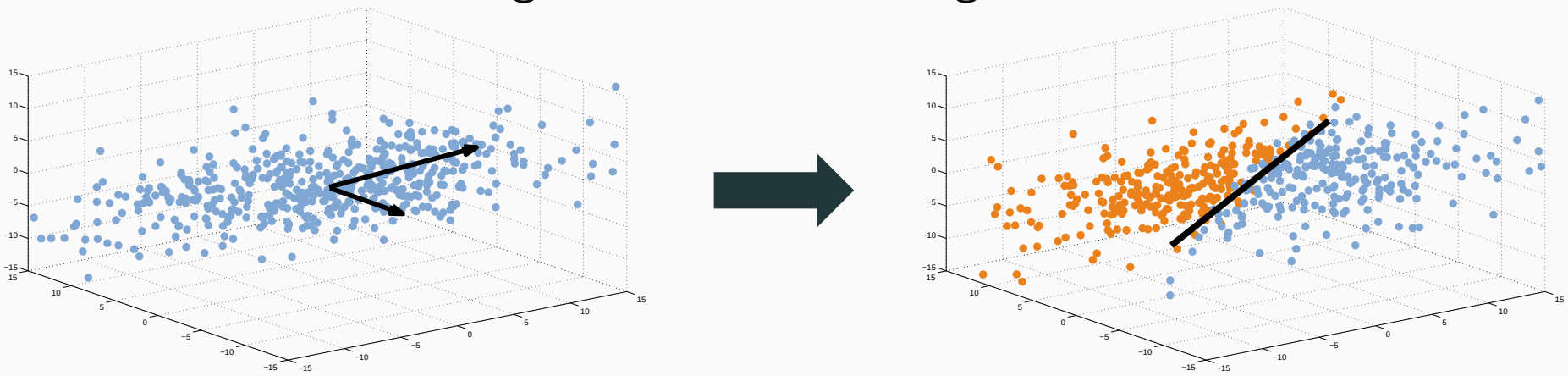


Regression is cheap (fast iterative or stochastic methods).

PCA is a major computational bottleneck.

OUR APPROACH: SKIP THE DIMENSIONALITY REDUCTION

Single-shot iterative algorithm



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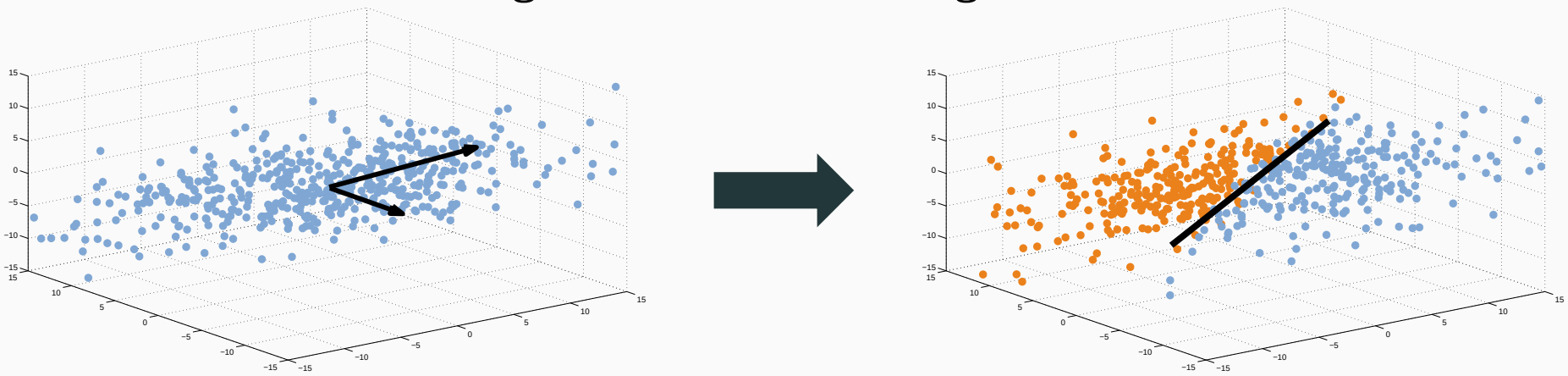

Final algorithm just uses a few applications of any fast, black-box regression routine.

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Given: $\mathbf{A}$, $\mathbf{b}$

Solve: $\mathbf{x}^* = \arg\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$

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Given: $\mathbf{A}$, $\mathbf{b}$, λ

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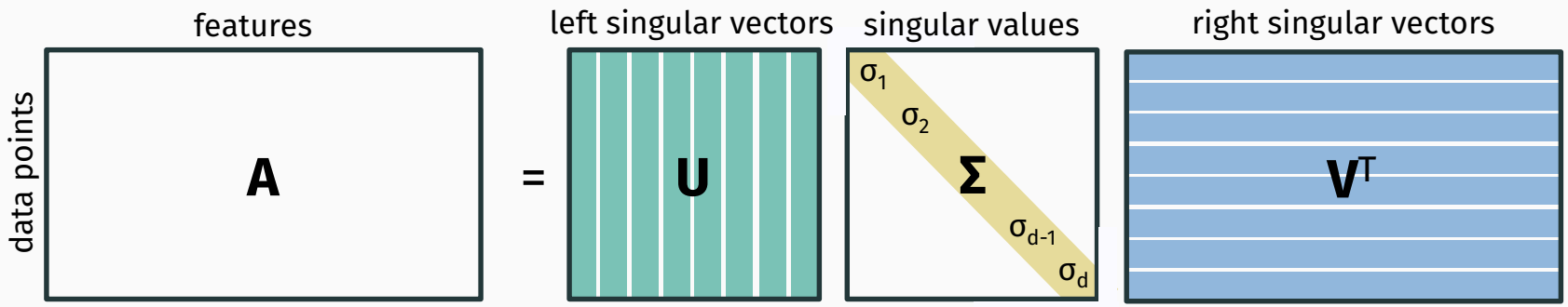

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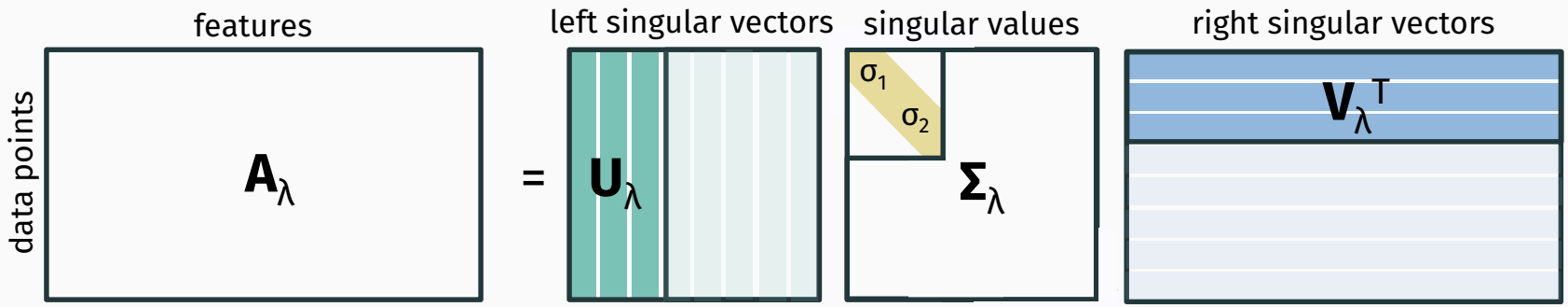
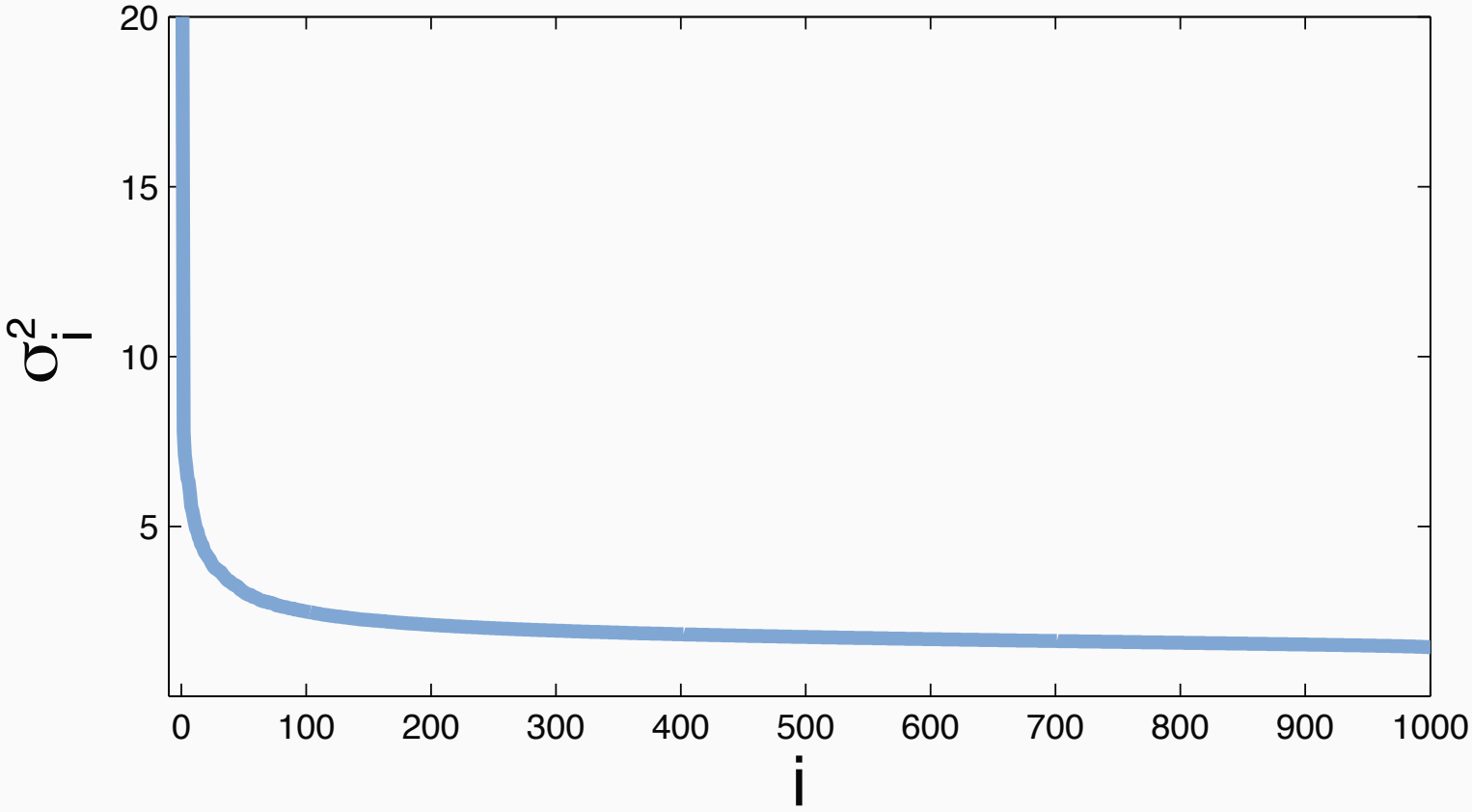


Singular values of **A**



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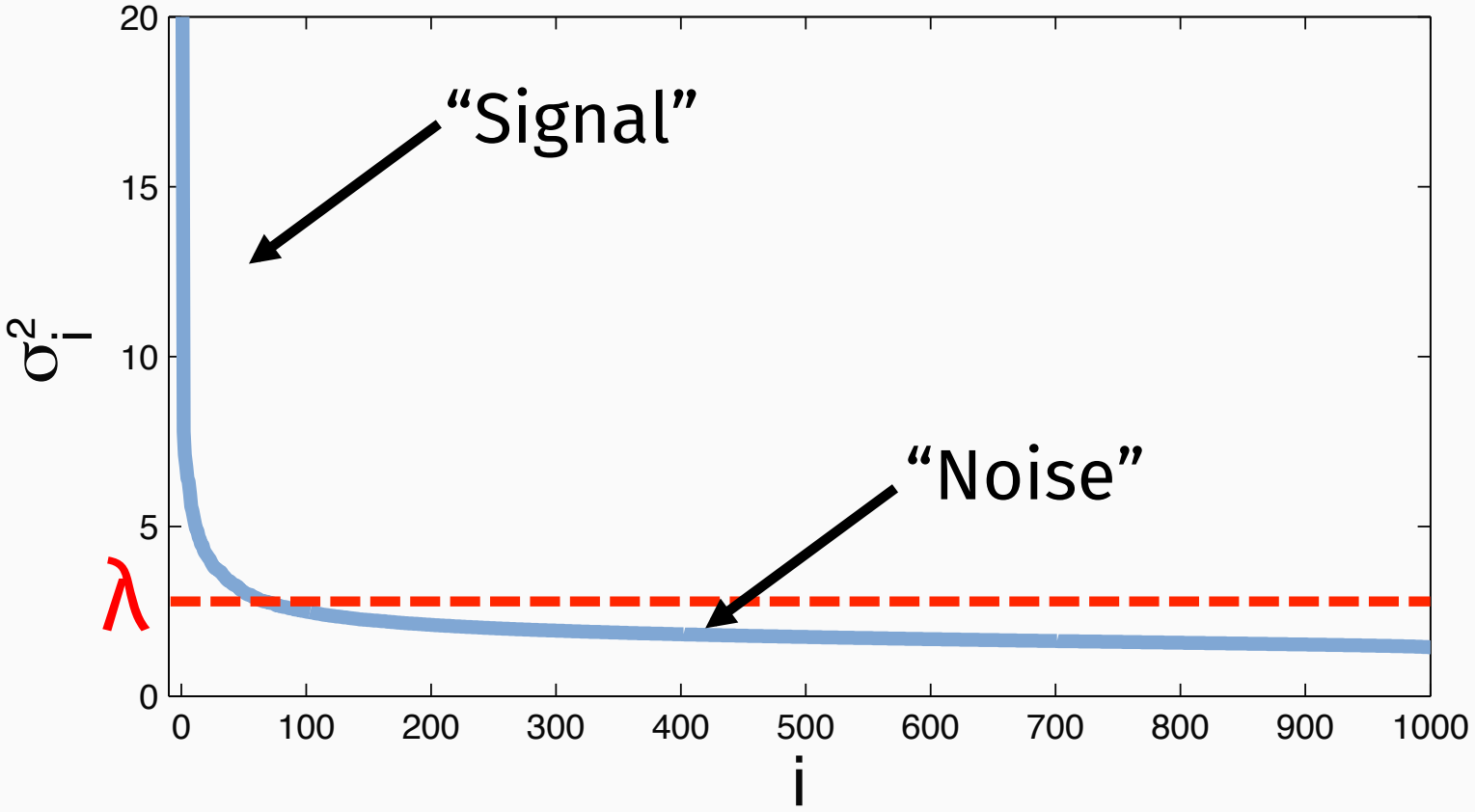
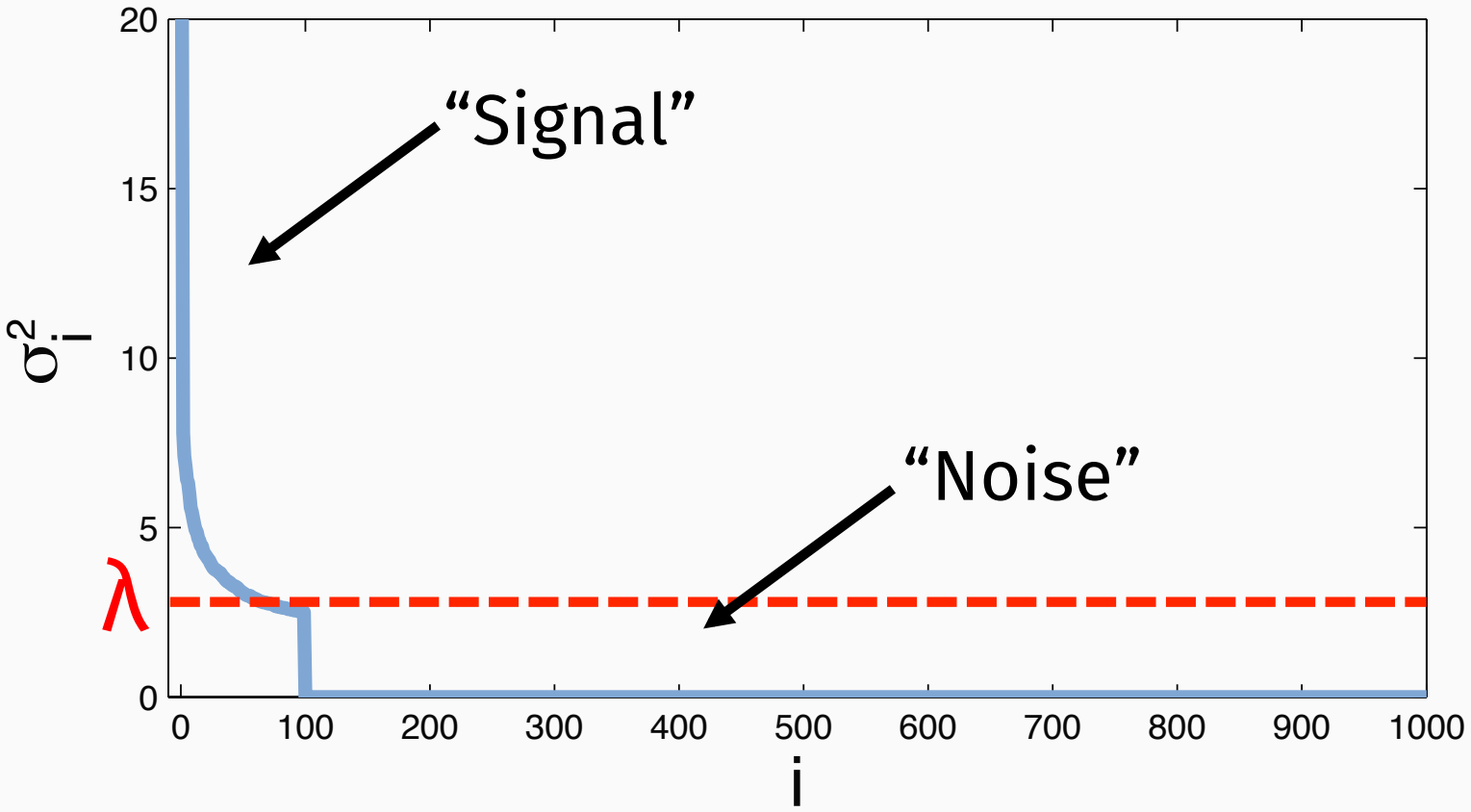


Singular values of $\mathbf{A}_\lambda$



Principal Component Regression (PCR):

Goal: $\mathbf{x}^* = \arg\min_{\mathbf{x}} \|\mathbf{A}_\lambda \mathbf{x} - \mathbf{b}\|^2$

Solution: $\mathbf{x} = (\mathbf{A}_\lambda^T \mathbf{A}_\lambda)^{-1} \mathbf{A}_\lambda^T \mathbf{b}$

What's the computational cost?

Cost of computing A_λ (PCA):

$$\approx O(\mathrm{nnz}(\mathbf{A})k + dk^2).$$

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NAIVE PCR RUNTIME

Cost of computing $\mathbf{A}_\lambda$ (PCA):

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For PCR, k is large, κ is small ($\mathbf{A}_\lambda$ is well conditioned).

Goal: Remove bottleneck dependence on k

Reason for hope?

Optimistic observation: PCA computes too much information.

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Don't need to compute $\mathbf{A}_\lambda$ (which incurs a k dependence) as long as we can apply it to a *single vector* efficiently.

REASON FOR HOPE?

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Why not $\mathbf{A}_\lambda$?

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There's an algorithm that approximately applies $\mathbf{A}_\lambda^T$ *to any vector* $\mathbf{b}$ *using* $\approx \log(1/\epsilon)$ *well conditioned linear system solutions.*

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$$\text{PCR in} \approx O(\text{nnz}(\mathbf{A}) \cdot \sqrt{\kappa}) \text{ time.}$$

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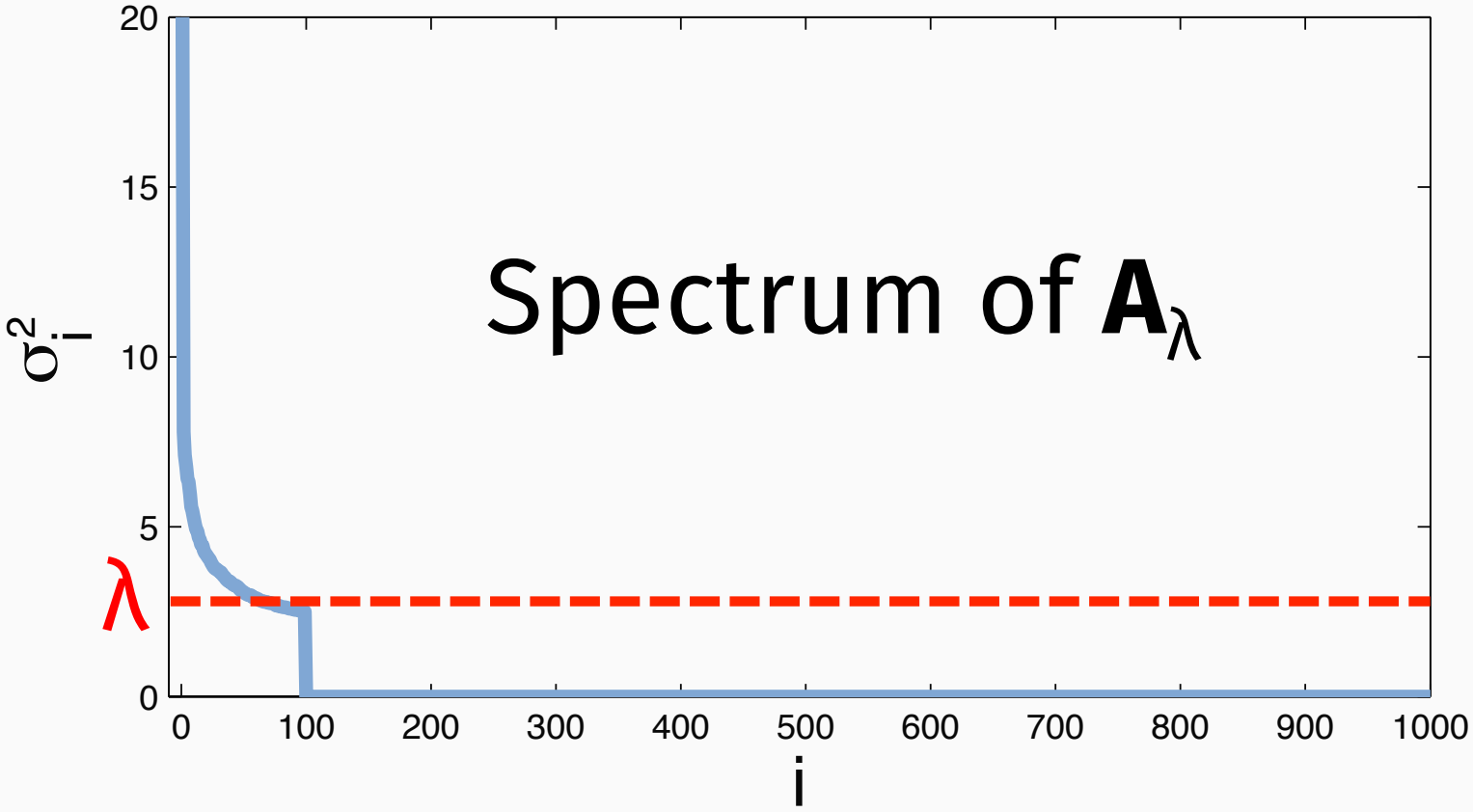
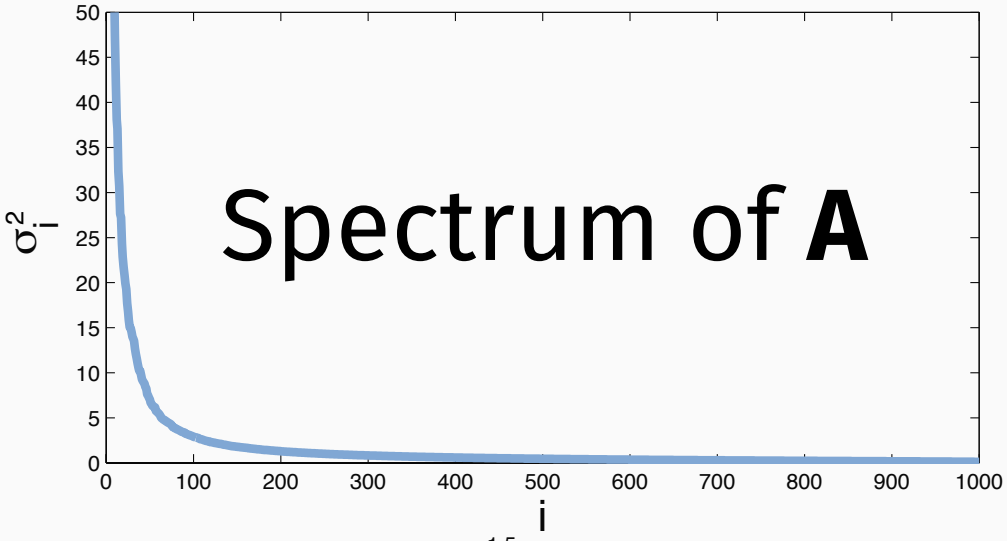
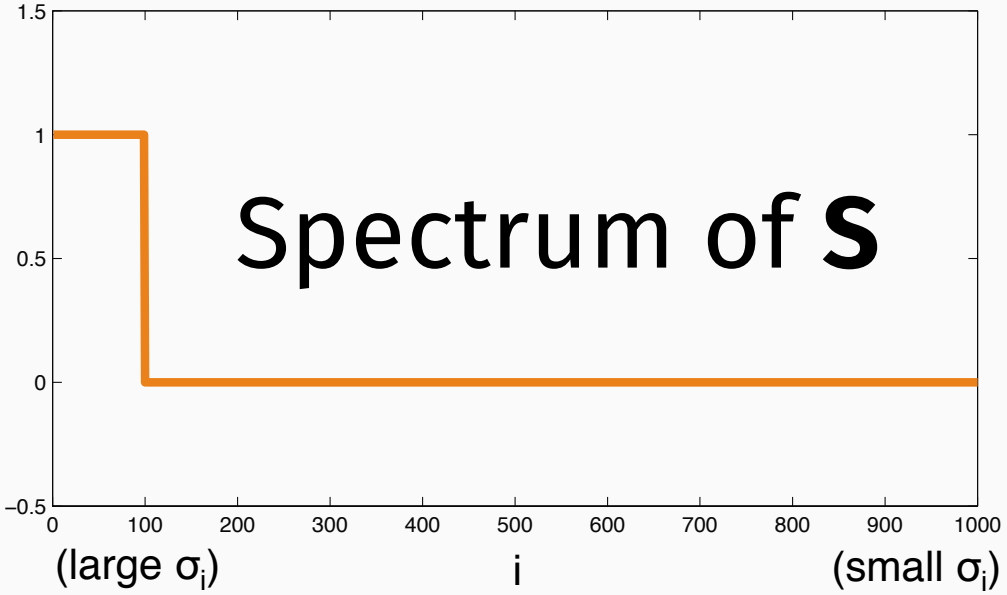


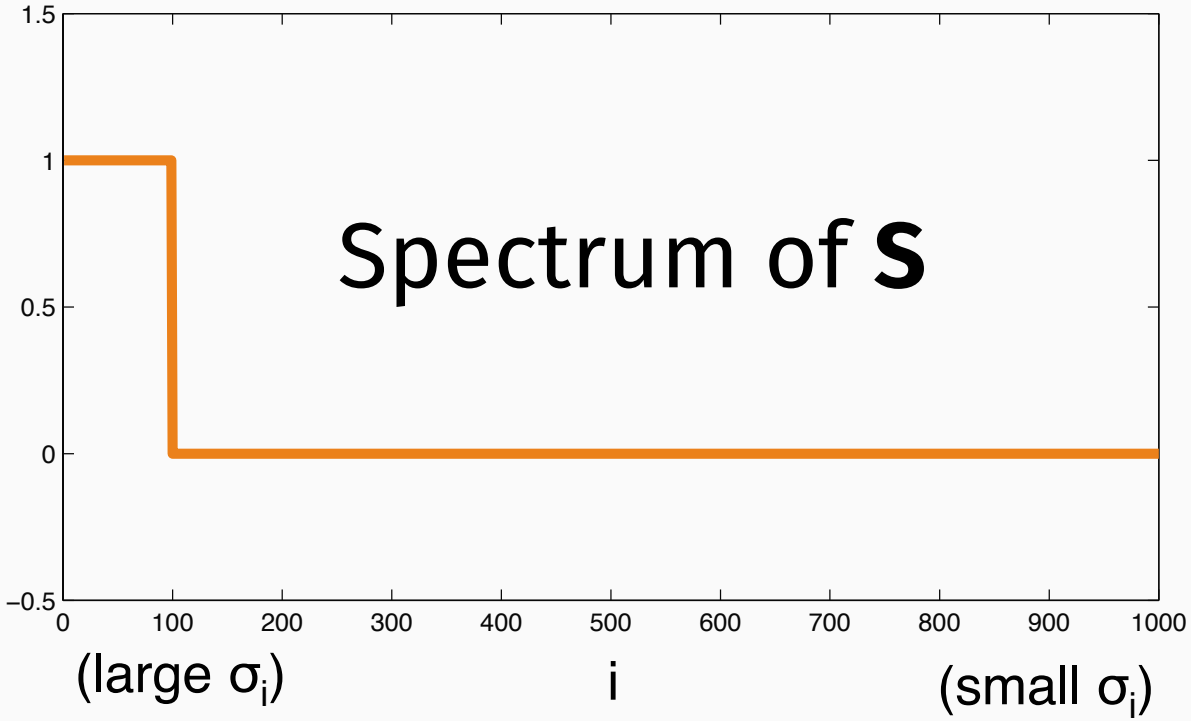
DECOMPOSING MATRIX



$$\mathbf{A}_\lambda^T = \mathbf{S}\mathbf{A}^T$$



$$A_\lambda^T b = S A^T b$$



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- **Tremblay, Puy, Gribonval, Vandergheynst**: "Compressive Spectral Clustering" ICML 2016.

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Claim:

$$\mathbf{R} = (\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{A}$$
coarsely approximates $\mathbf{S}$.

Singular values of S:

$$\sigma_i(\mathsf{S}) = \begin{cases} 1 & \text{if } \sigma_i^2(\mathsf{A}) \geq \lambda, \\ 0 & \text{if } \sigma_i^2(\mathsf{A}) < \lambda. \end{cases}$$

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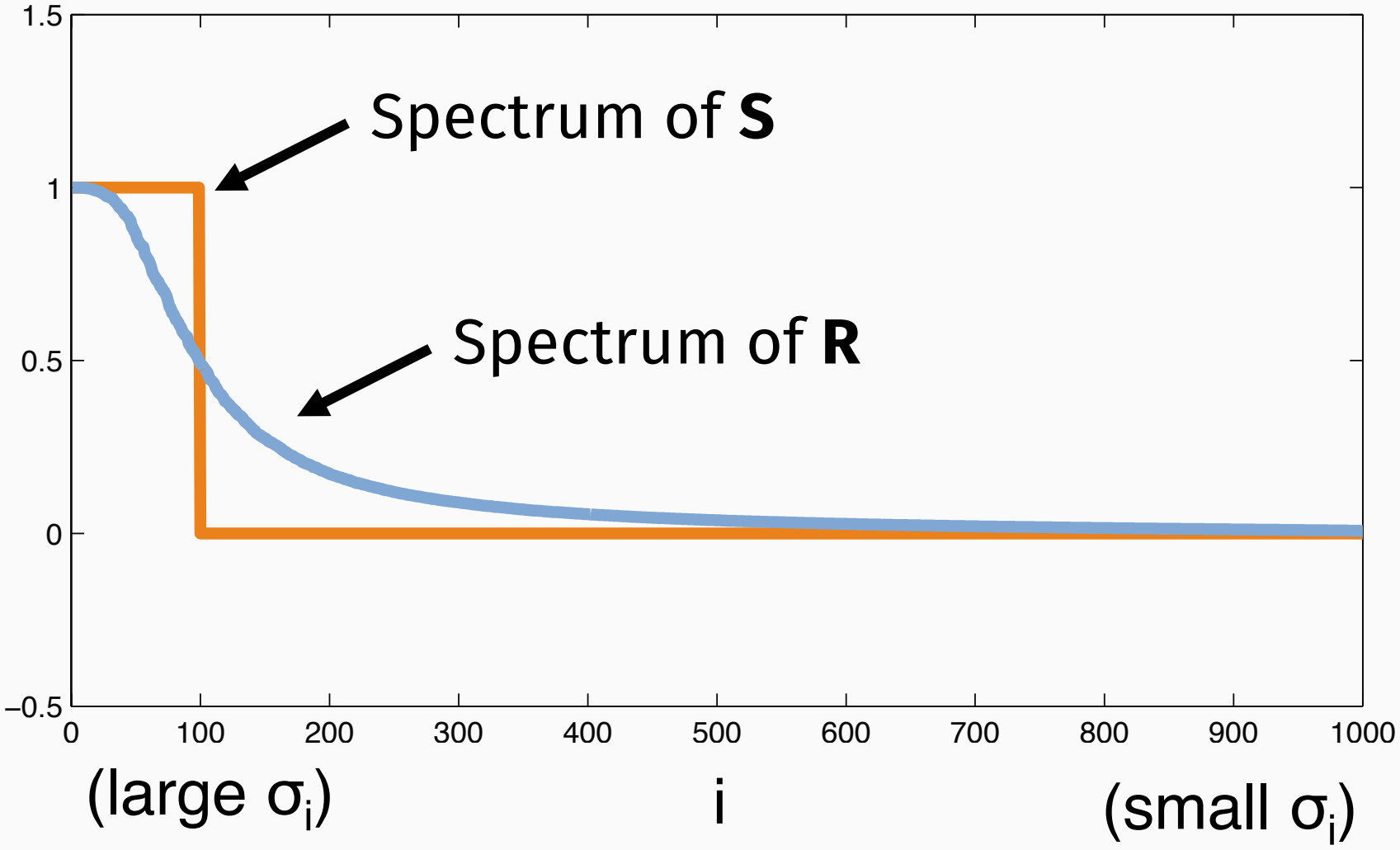
$$\sigma_i(\mathbf{R}) = \frac{\sigma_i^2(\mathbf{A})}{\sigma_i^2(\mathbf{A}) + \lambda} \approx \begin{cases} 1 & \text{if } \sigma_i^2(\mathbf{A}) >> \lambda, \\ 0 & \text{if } \sigma_i^2(\mathbf{A}) << \lambda. \end{cases}$$

A FIRST APPROXIMATION



FINAL STEP

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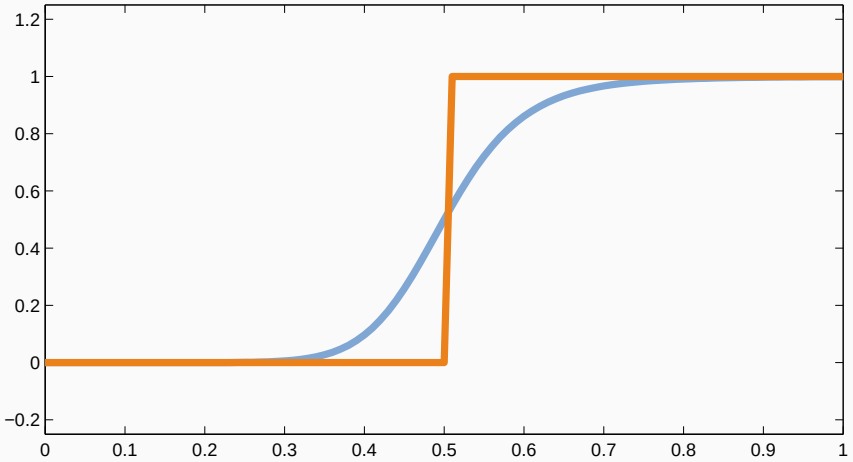

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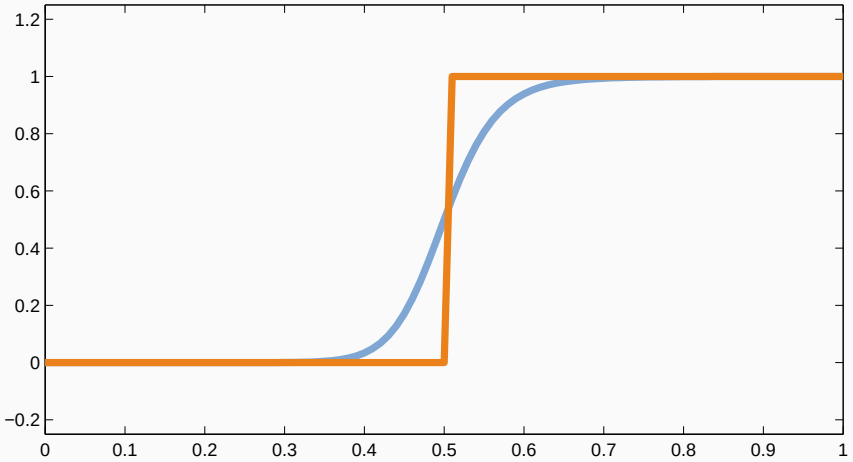

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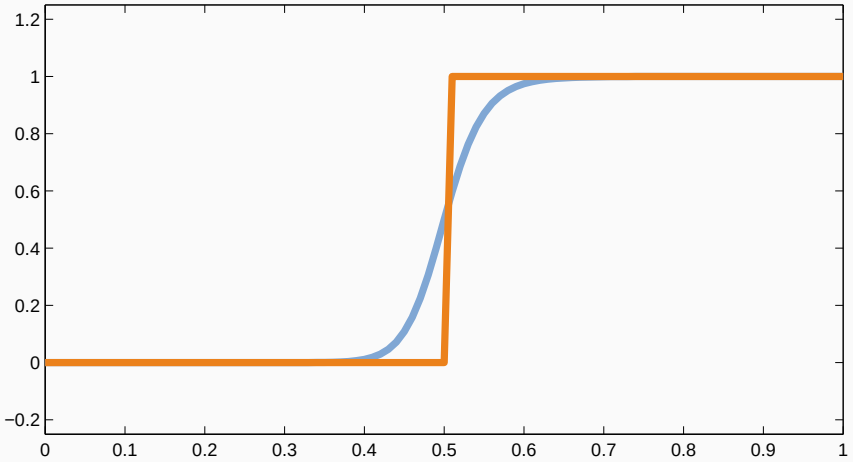

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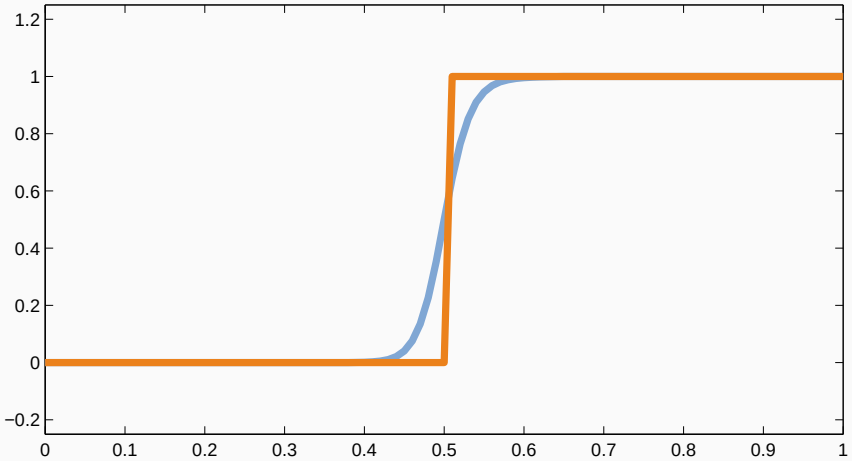

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FINAL ALGORITHM

1. Compute $\mathbf{R}\mathbf{A}^T\mathbf{b}$, $\mathbf{R}^2\mathbf{A}^T\mathbf{b}$, $\ldots$ $\mathbf{R}^{O(\log 1/\epsilon)}\mathbf{A}^T\mathbf{b}$.

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1. $O(\log 1/\epsilon)$ calls to a regression algorithm.
2. Low cost linear combination of vectors.
3. One call to a regression algorithm

NOTE ON PRIOR WORK

In prior work, $\mathbf{S}$ is approximated *directly* using a matrix polynomial. Why not here?

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In prior work, $\mathbf{S}$ is approximated *directly* using a matrix polynomial. Why not here?

- We match polynomial approximation, but can be faster when non-standard regression algorithms are used.
- We give a full end-to-end runtime and stability analysis.

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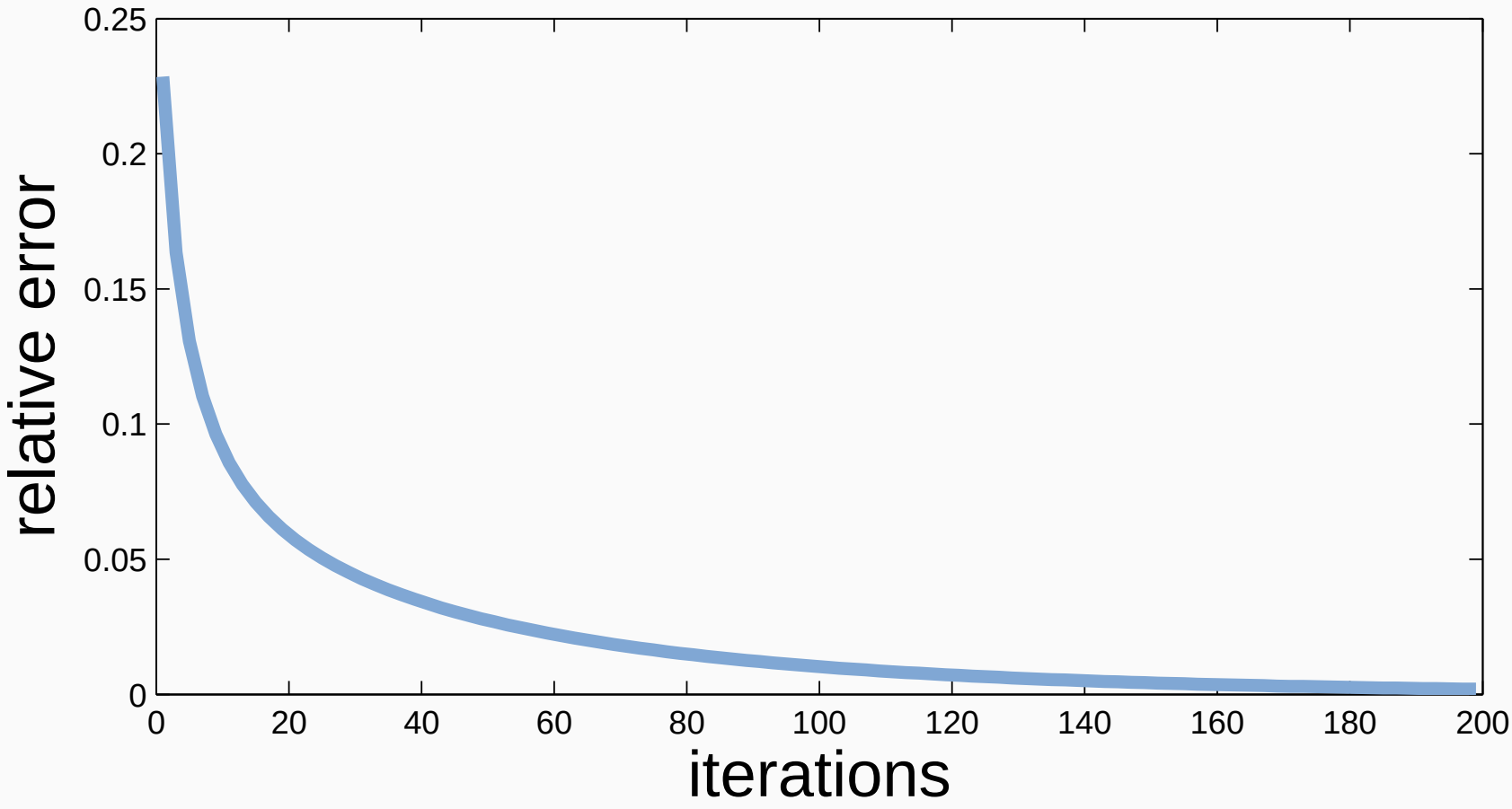
- Recurrence for stable application of symmetric step polynomial.
- More work to make last regression step stable and fast.

But the algorithm itself remains simple!

SAMPLE CODE

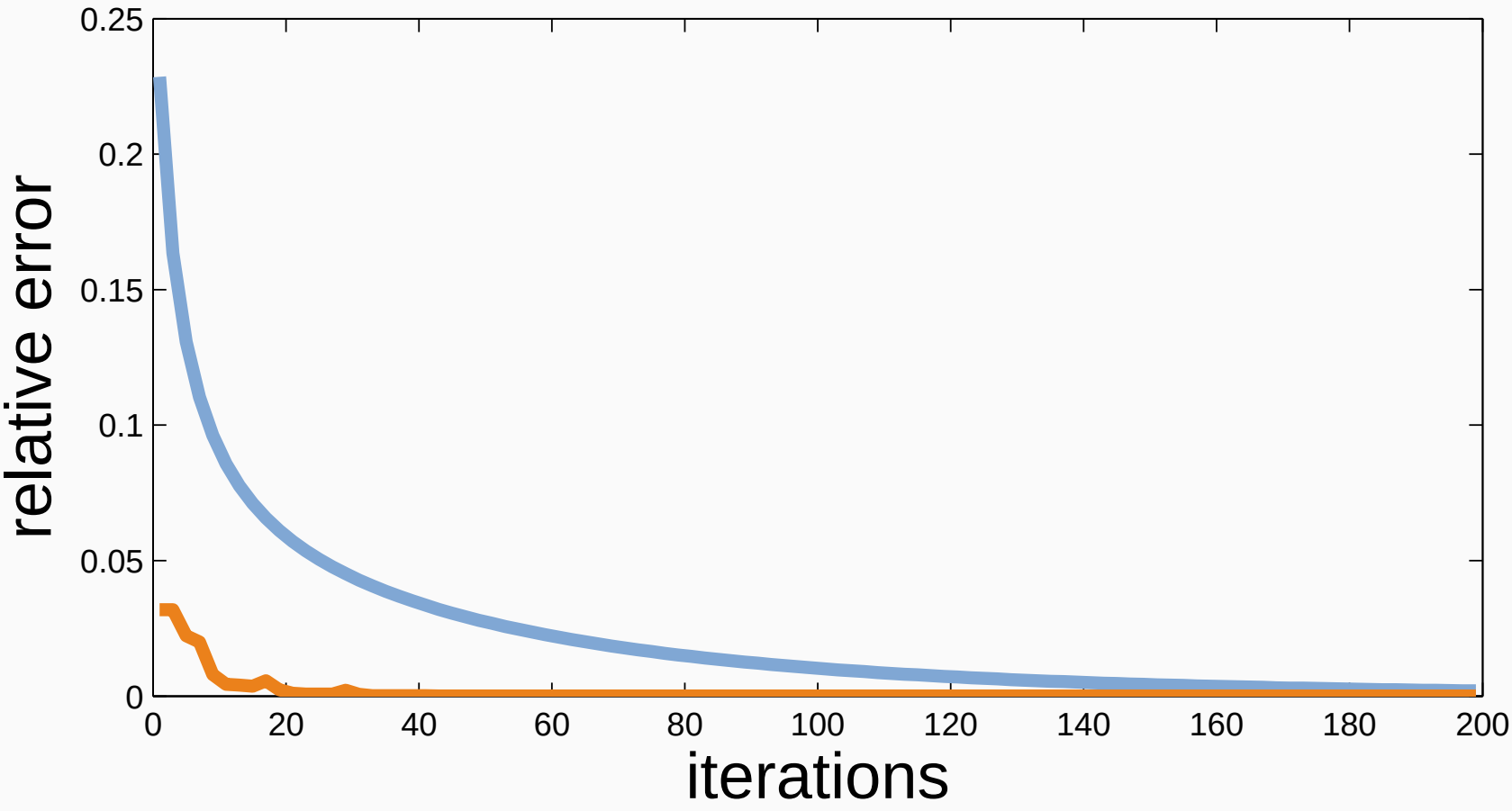
```
function [x,patb] = fpcr(A, b, lambda, iter)
z = A'*b;
pz = ridgeReg(A,A*z,lambda);

w = pz - z/2;
for i = 1:iter
    w = 4*(2*i+1)/(2*i)*ridgeReg(A, ...
        A*(w - ridgeReg(A,A*w,lambda)), lambda);
    pz = pz + 1/(2*i+1)*w;
end
patb = pz;

x = robustReg(A,pz,lambda);
end

function x = robustReg(A,pz,lambda)
    tol = 1e-5; %default
    function y = afun(z,~)
        y = A'*(A*z) + tol*lambda*z;
    end
    [x,~] = pcg(@afun,pz);
end
```

Synthetic data (with small spectral gap)



Standard Algorithm

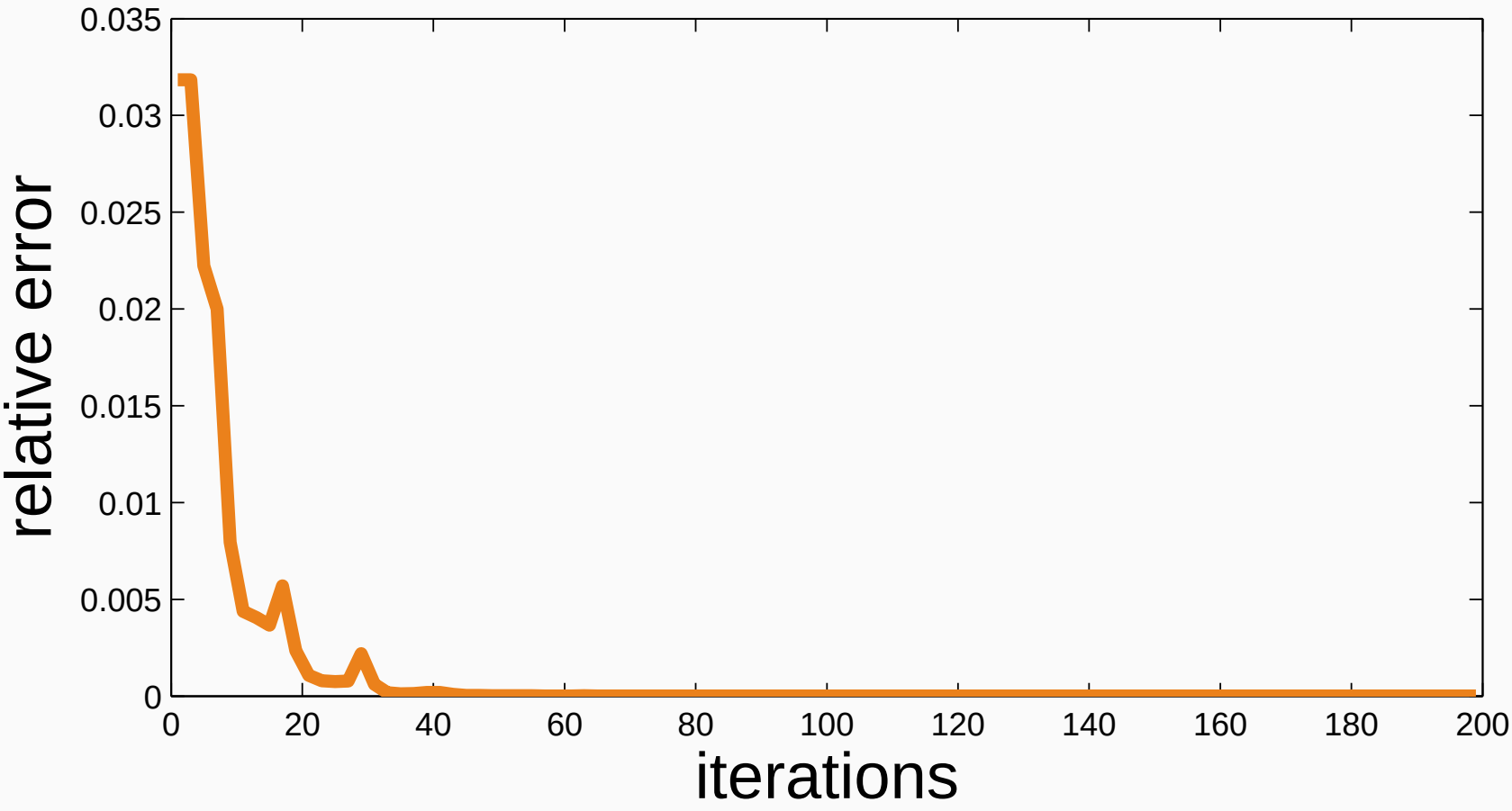
Synthetic data (with small spectral gap)



Standard Algorithm

Krylov Accelerated Algorithm

Synthetic data (with small spectral gap)



Standard Algorithm

Krylov Accelerated Algorithm

Take away: PCR can be computed *without explicit PCA*.

Ridge regression + matrix polynomial = efficient operator access to $\mathbf{A}$'s top principal components.

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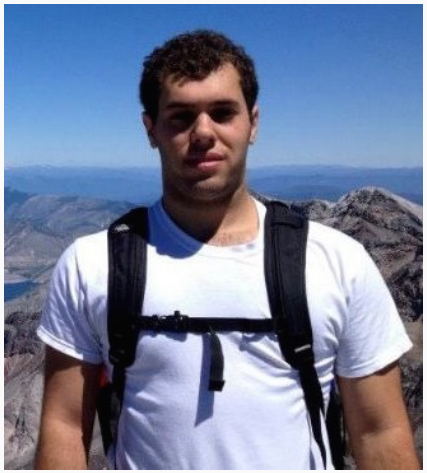
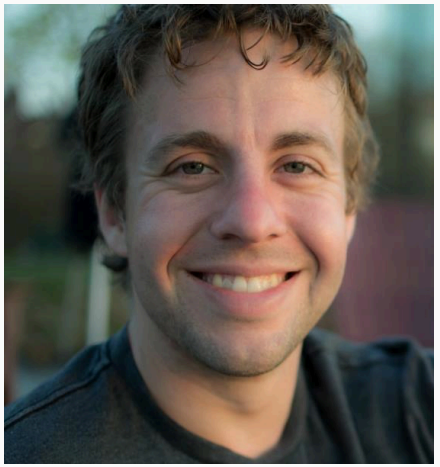
Questions? Joint work with:

Roy Frostig



Cameron Musco



Aaron Sidford