Applications of Random Matrices in Spectral Computations and Machine Learning

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This talk

Viewpoint:

use randomness to “transform” the data

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use randomness to "transform" the data

- Random Projections
- Fast Spectral Computations
- Sampling in Kernel PCA

The Setting

Input: Set S of n points in $\mathbf{R}^d$ — d is "too big"

Output: Set S' of n points in $\mathbf{R}^k$ which is "like" S — k is "affordable/right"

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Solution 1: Compute the SVD of $A = UDV^T$

Solution 2: Compute? Naah.. Flip coins to form $P \in \mathbf{R}^{d \times k}$

Output: AP

The Johnson-Lindenstrauss lemma

JL-lemma: For every set S of n points in $\mathbf{R}^d$ and every $\epsilon > 0$ there exists $f : \mathbf{R}^d \to \mathbf{R}^k$, where $k = O(\epsilon^{-2} \log n)$, such that for all pairs $u, v \in S$

$$(1-\epsilon)|u-v|^2 \leq |f(u) - f(v)|^2 \leq (1+\epsilon)|u-v|^2 \ .$$

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Algorithm:

Projecting onto a random hyperplane (subspace) of dimension

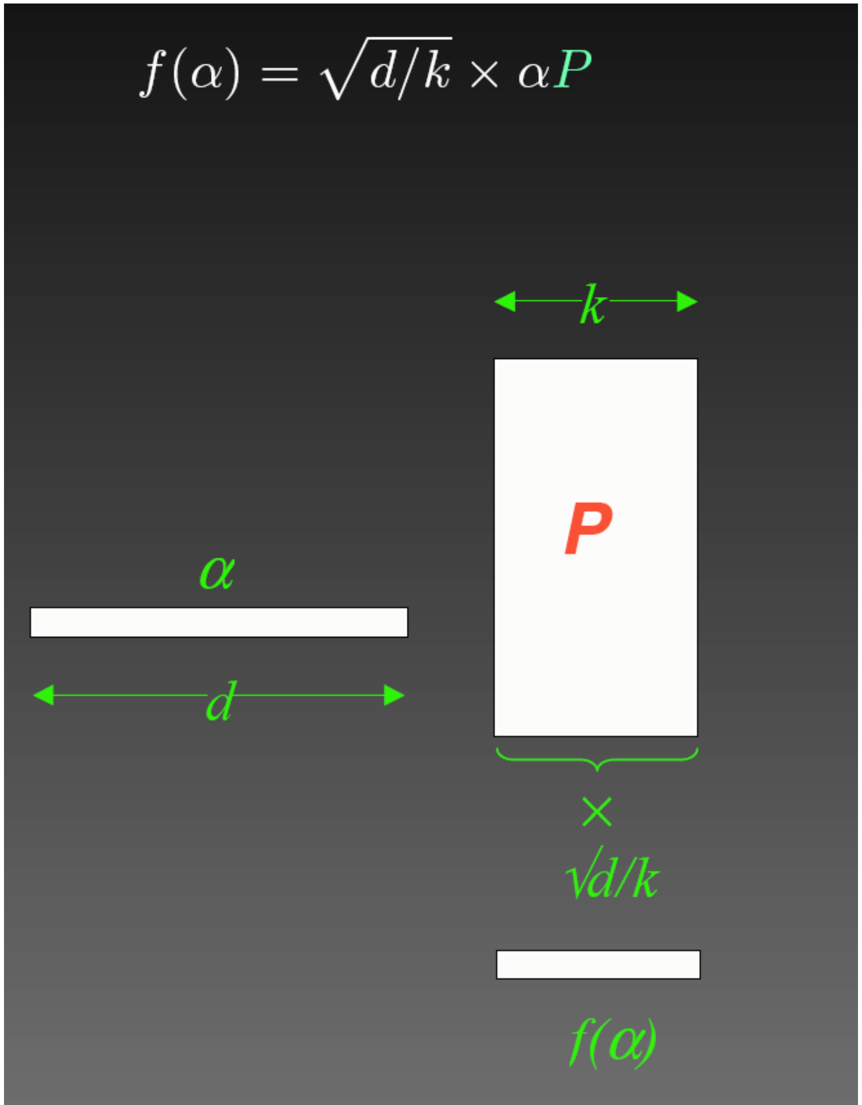
$$k = \frac{4 + 2\beta}{\epsilon^2/2 - \epsilon^3/3} \log n$$

succeeds with probability $1 - 1/n^\beta$

Applications

- Approximation algorithms [Charikar'02]
- Hardness of approximation [Trevisan '97]
- Learning mixtures of Gaussians [Arora, Kannan '01]
- Approximate nearest-neighbors [Kleinberg '97]
- Data-stream computations [Alon et al. '99, Indyk '00]
- Min-cost clustering [Schulman '00]
- ….
- Information Retrieval (LSI) [Papadimitriou et al. '97]

How to pick a random hyperplane



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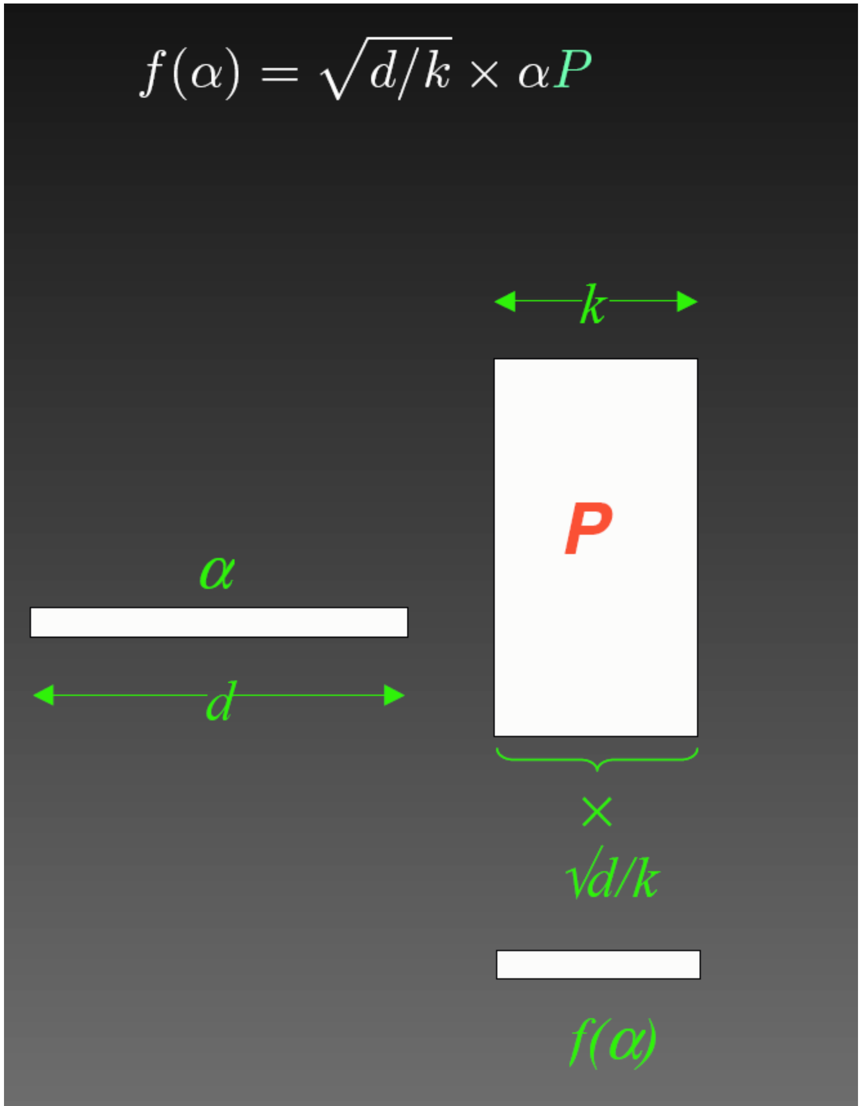

- Take $P(i,j) = r_{ij}$ where the $\{r_{ij}\}$ are independent $N(0,1)$ random variables
- $P \leftarrow \mathrm{Orthonormalize}(P)$

[Indyk Motwani 99]

[Johnson Lindenstrauss 82]

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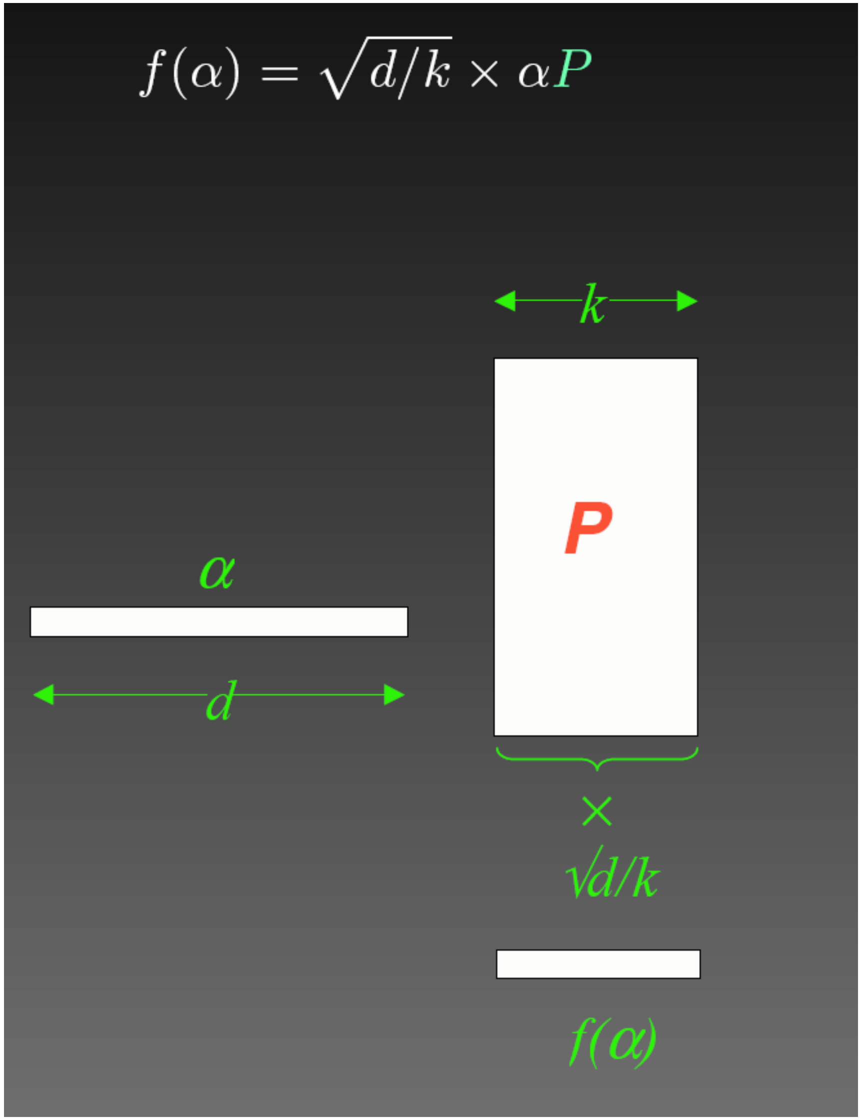

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Intuition:

- Each column of *P* points to a uniformly random direction in $\mathbf{R}^d$.

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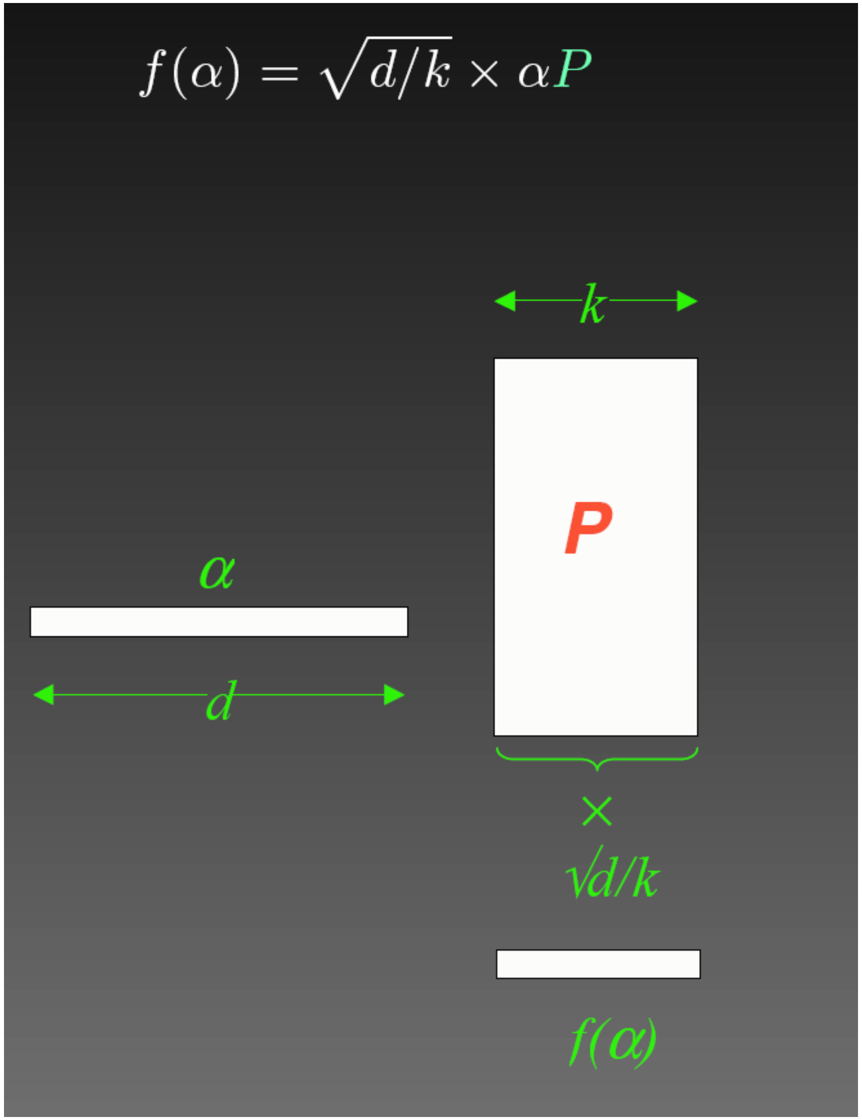

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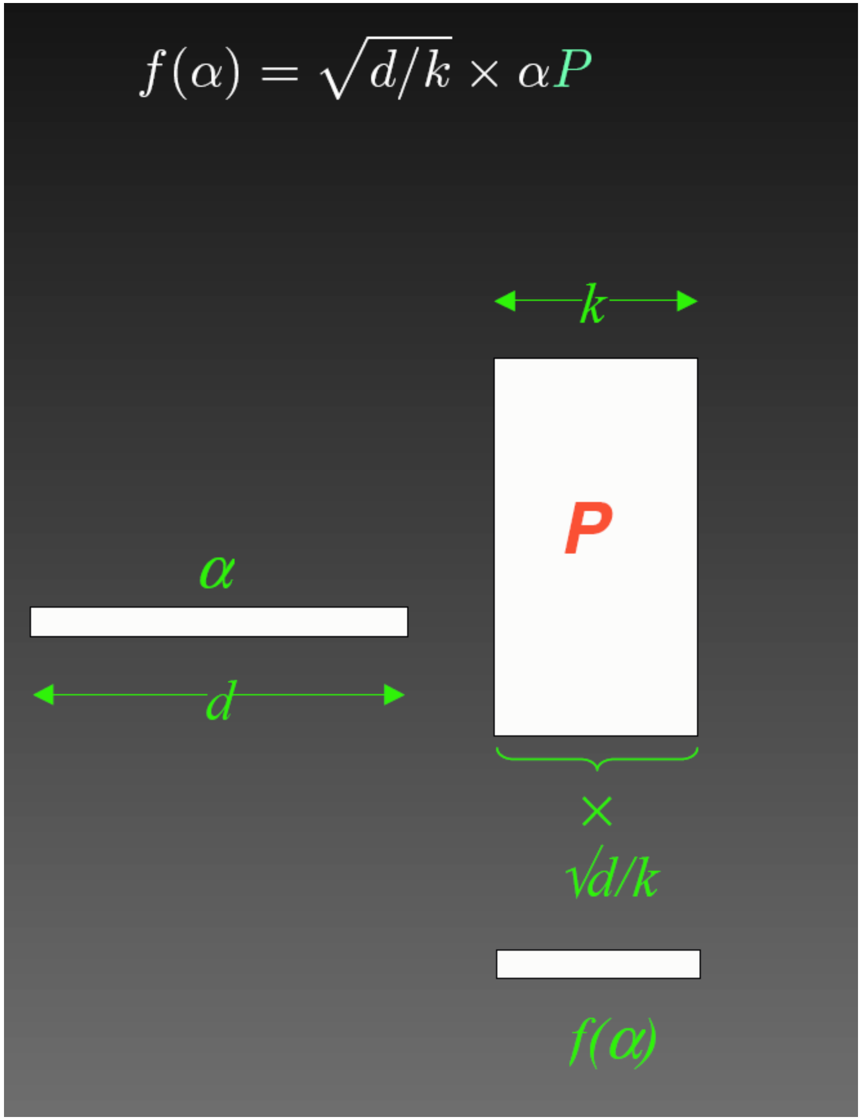

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- $|\alpha P|^2$ is the average estimate
  (since we take the sum)

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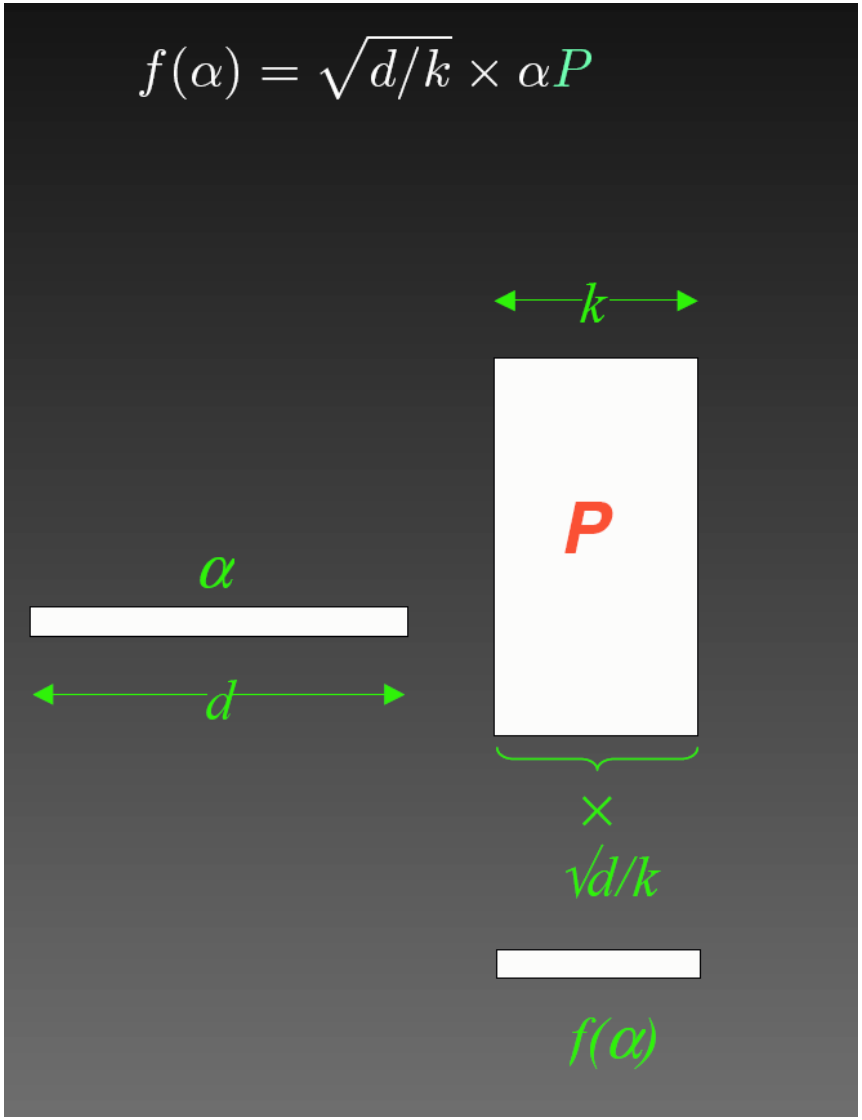

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- Estimators are "equal"
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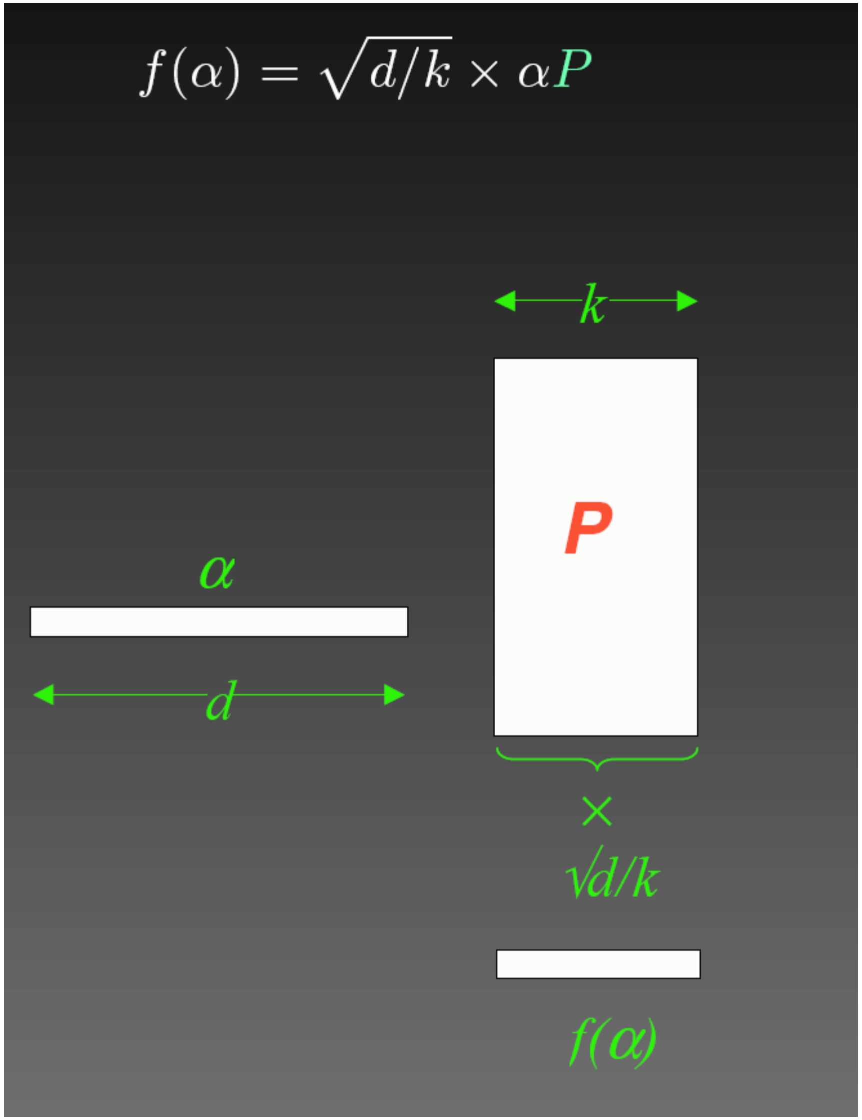

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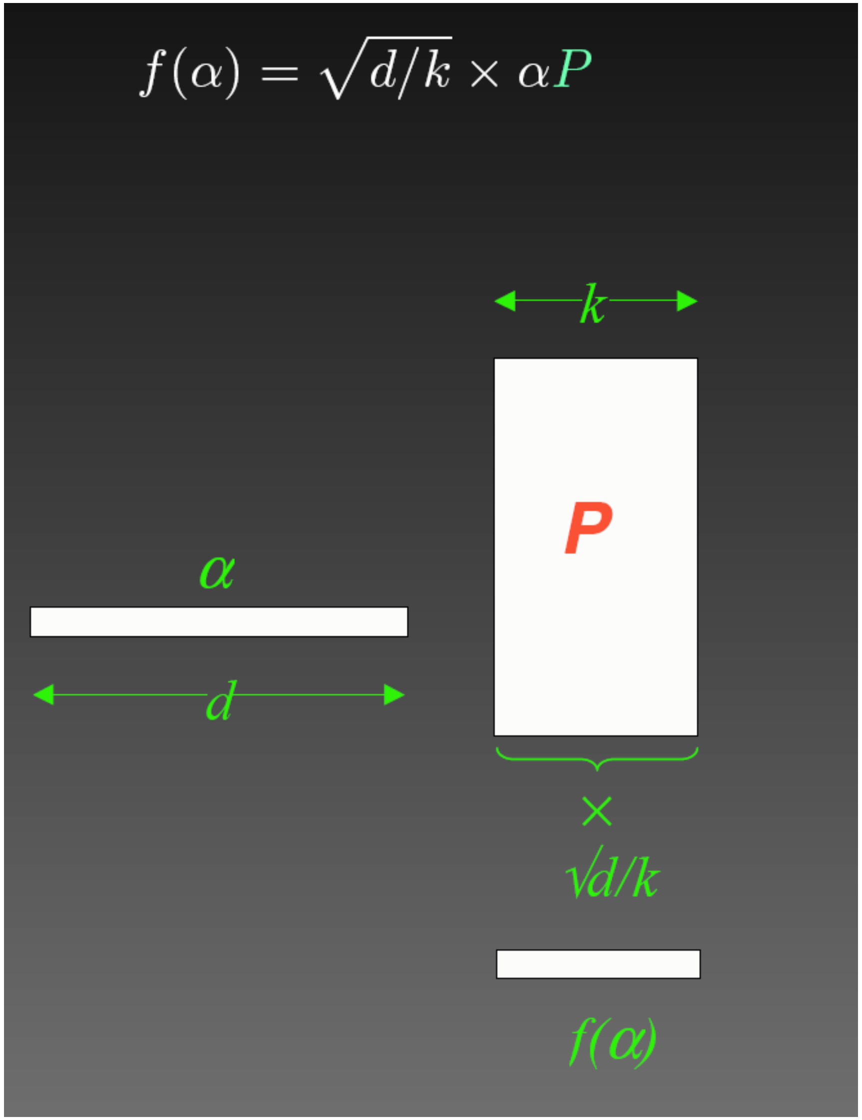

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$\boxed{\text{Same thing!}}$

Orthonormality: Take #1

Random vectors in high-dimensional Euclidean space

are very nearly orthonormal.

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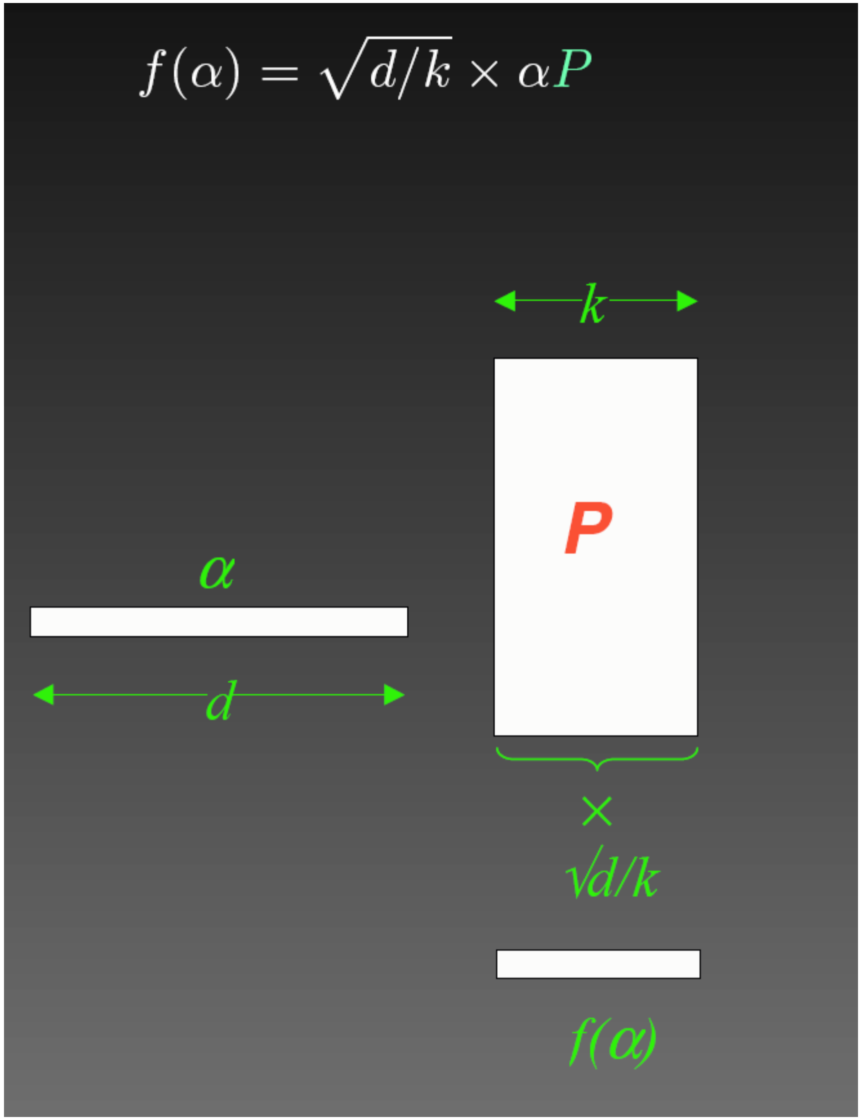
Do they have to be uniformly random?

Is the Gaussian distribution magical?

JL with binary coins



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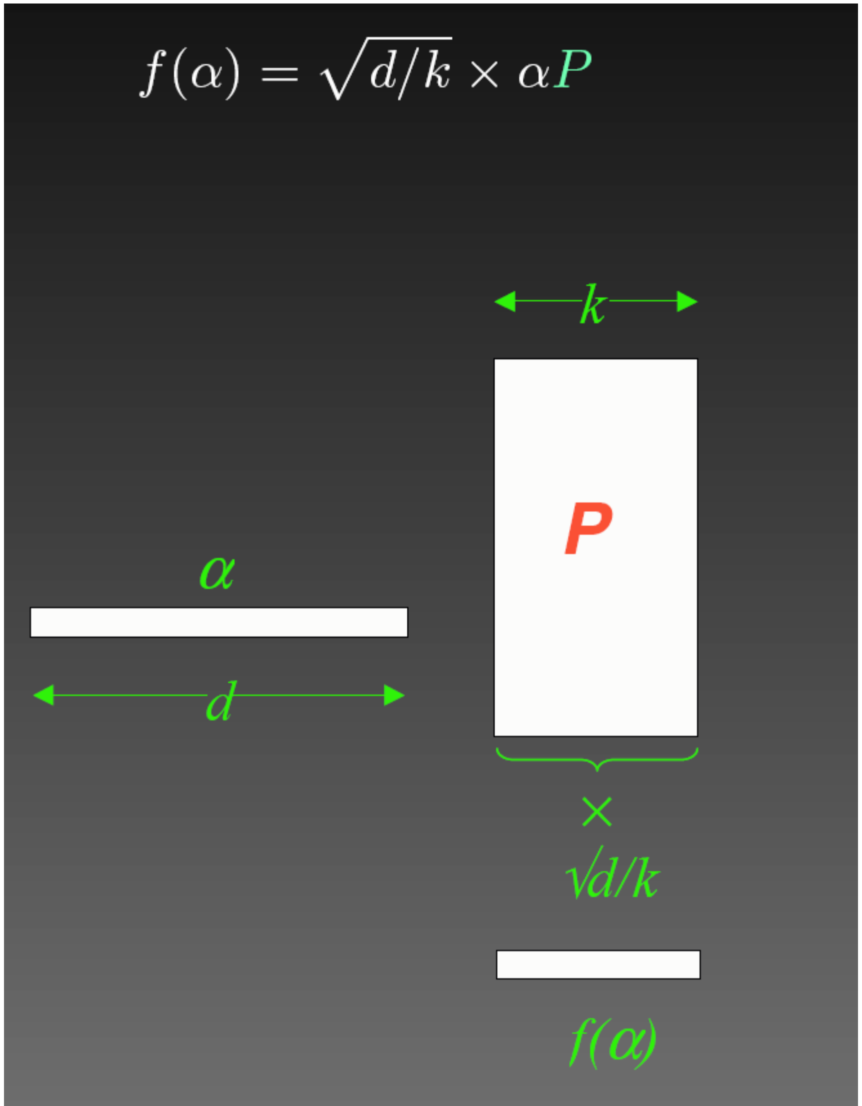

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Benefits:

- Much faster in practice
- Only $\pm$ operations (no $*$)
- Fewer random bits
- Derandomization
- Slightly smaller(!) k

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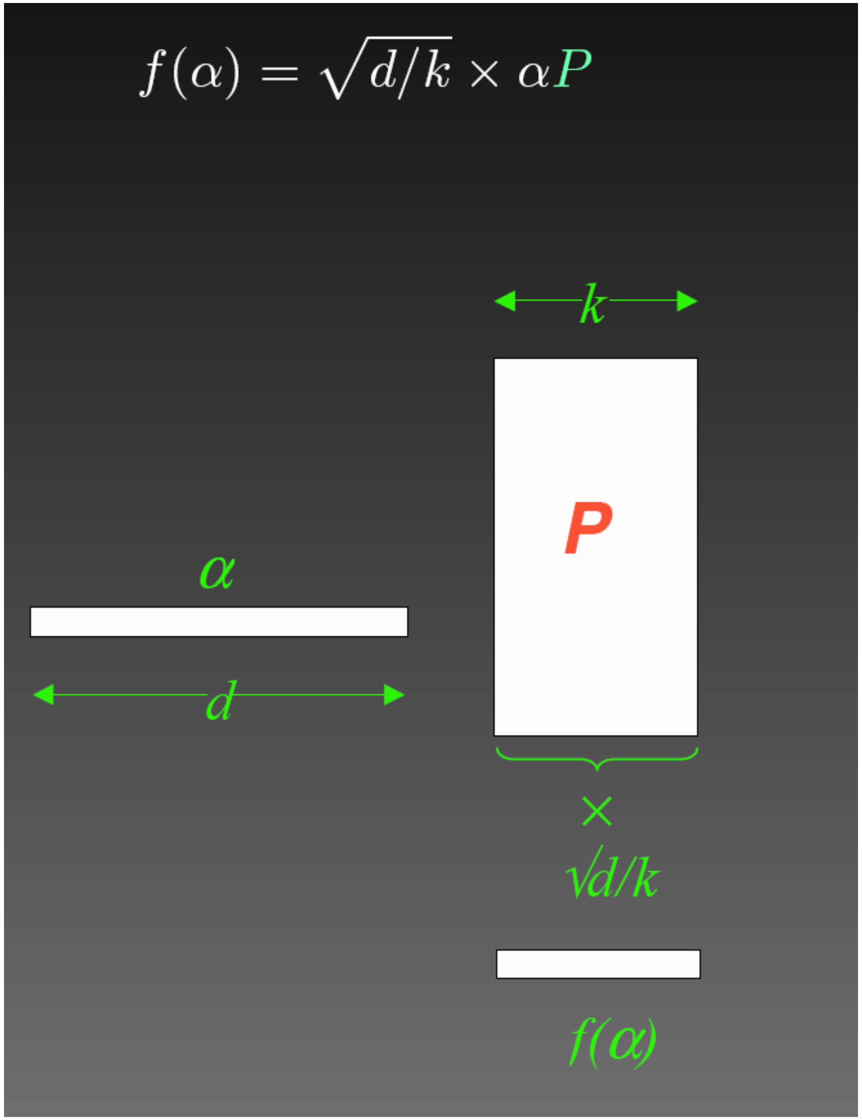

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- Preprocessing with a randomized FFT

[Ailon, Chazelle '06]

$$O\left(d \log d + \min\{d\varepsilon^{-2} \log n, \varepsilon^{p-4} \log^{p+1} n\}\right)$$

Let's at least

look at the data

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Spectral Norm: $$\|A\|_2 = \max_{\|x\|=1} \|Ax\|$$

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For any matrix A, there is a well defined matrix A_k that is the "best" rank k approximation to A for many norms.

For any rank k matrix B,
$$\|A - A_k\|_2 \leq \|A - B\|_2$$
$$\|A - A_k\|_F \leq \|A - B\|_F$$

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A_k is the maximizer of $\|AP\|$ over all projections P into $\mathbf{R}^k$

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- Synthesize a new candidate by combining the rows of A according to their enthusiasm for x:

$$x \leftarrow \frac{A^T y}{||A^T y||} \in \mathbf{R}^d$$

(This is power iteration on $A^T A$. Also known as PCA.)

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- Project A on subspace orthogonal to x and repeat

PCA for Denoising

- Assume that we perturb the entries of a matrix A by adding independent Gaussian noise $N(0, \sigma)$

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- **Intuition**:
  - The perturbation vectors are nearly orthogonal
  - No small subspace accommodates many of them

Rigorously

Lemma: For any matrices A and $\widehat{A}$

$$\|A - \widehat{A}_k\|_2 \;\leq\; \|A - A_k\|_2 + 2\|A - \widehat{A}\|_2$$

Rigorously

Lemma: For any matrices A and $\widehat{A}$

$$||A - \widehat{A}_k||_2 \ \leq \ ||A - A_k||_2 + 2||A - \widehat{A}||_2$$

Theorem [Füredi Komlos] Let R be an $n \times d$ random matrix whose entries are independent random variables with mean 0 and variance at most σ^2. Then with [very] high probability,

$$||R||_2 \leq 4\sigma\sqrt{n}$$

Perspective: For any fixed x we have $||Rx||_2 \sim \sigma\sqrt{n}$ w.h.p.

Two new ideas

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- Computation-friendly noise:

> **Inject data-dependent noise**

Quantization

Consider the matrix $\widehat{A}$, defined as

$$\widehat{A}_{ij} = \begin{cases} +1 & \text{with probability } 1/2 + A_{ij}/2 \\ \\ -1 & \text{with probability } 1/2 - A_{ij}/2 \end{cases}$$

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- Each entry in $\widehat{A}$ can be represented by a single bit.

Sparsification

Consider the matrix $\widehat{A}$, defined as

$$\widehat{A}_{ij} \;=\; \begin{cases} A_{ij}/p & \text{with probability } p \\[2ex] 0 & \text{with probability } 1-p \end{cases}$$

for some $0 < p < 1$.

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- The expected value of $\widehat{A}_{ij}$ is A_{ij}.
- The variance of each $\widehat{A}_{ij}$ is at most $1/p$.
- $\widehat{A}$ is much sparser than A.

Accelerating spectral computations

- By injecting sparsification/quantization “noise” we can accelerate spectral computations:
  - Fewer/simpler arithmetic operations
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- L2 error can be quadratically better than “Nystrom”

Orthonormality: Take #2

Matrices with independent, 0-mean entries

are

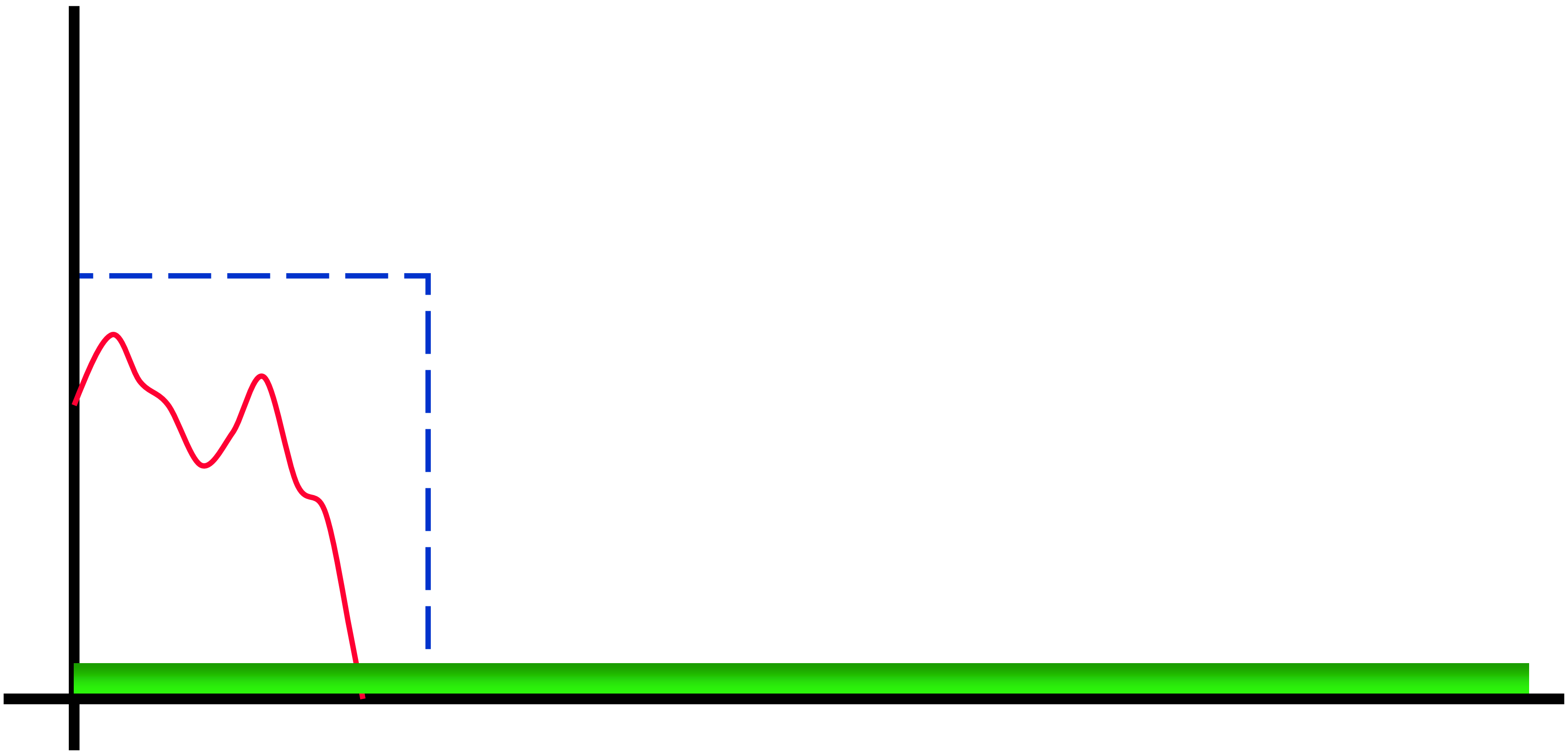
"white noise" matrices

A scalar analogue

A scalar analogue

Crude quantization at extremely high rate

A scalar analogue



Crude quantization at extremely high rate + low-pass filter

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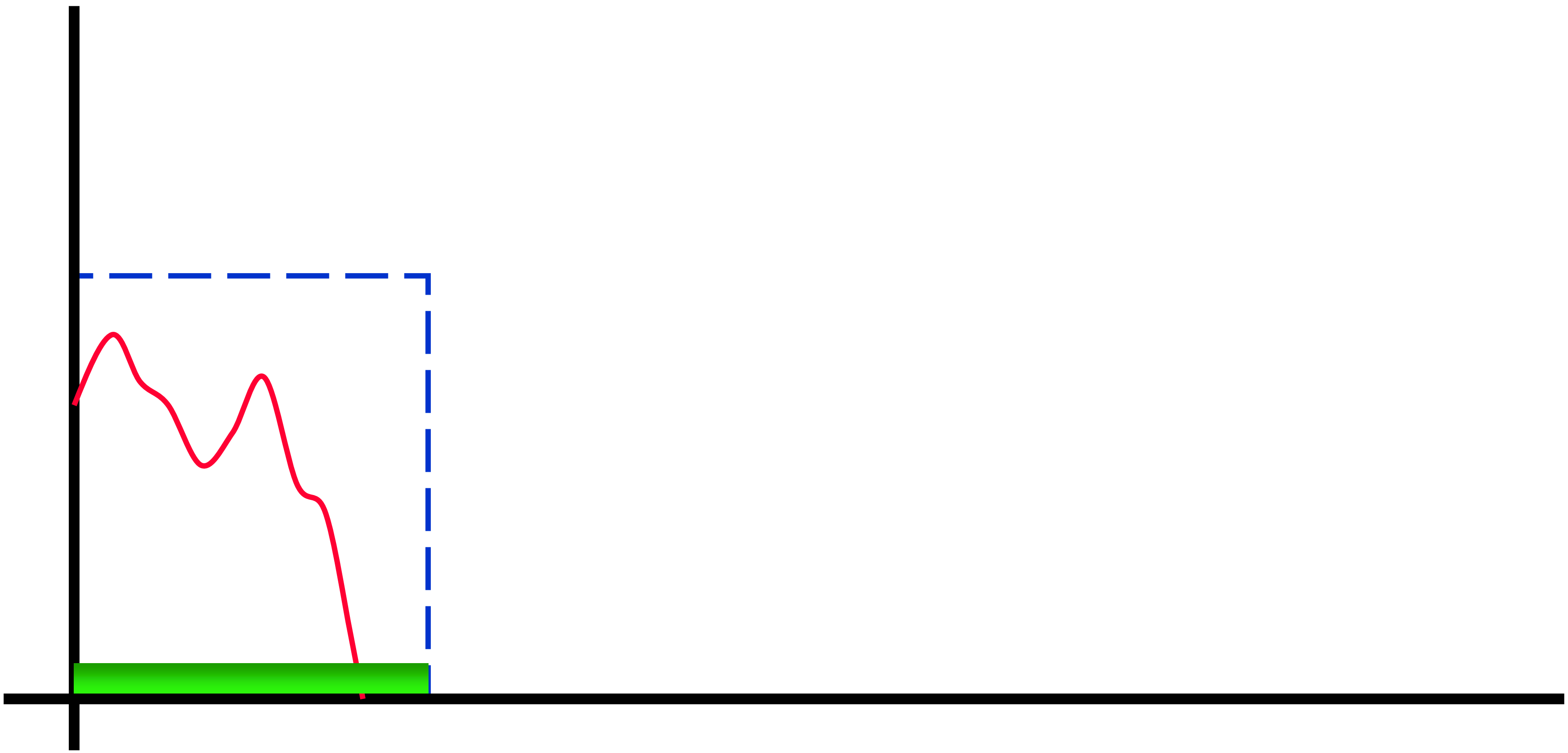

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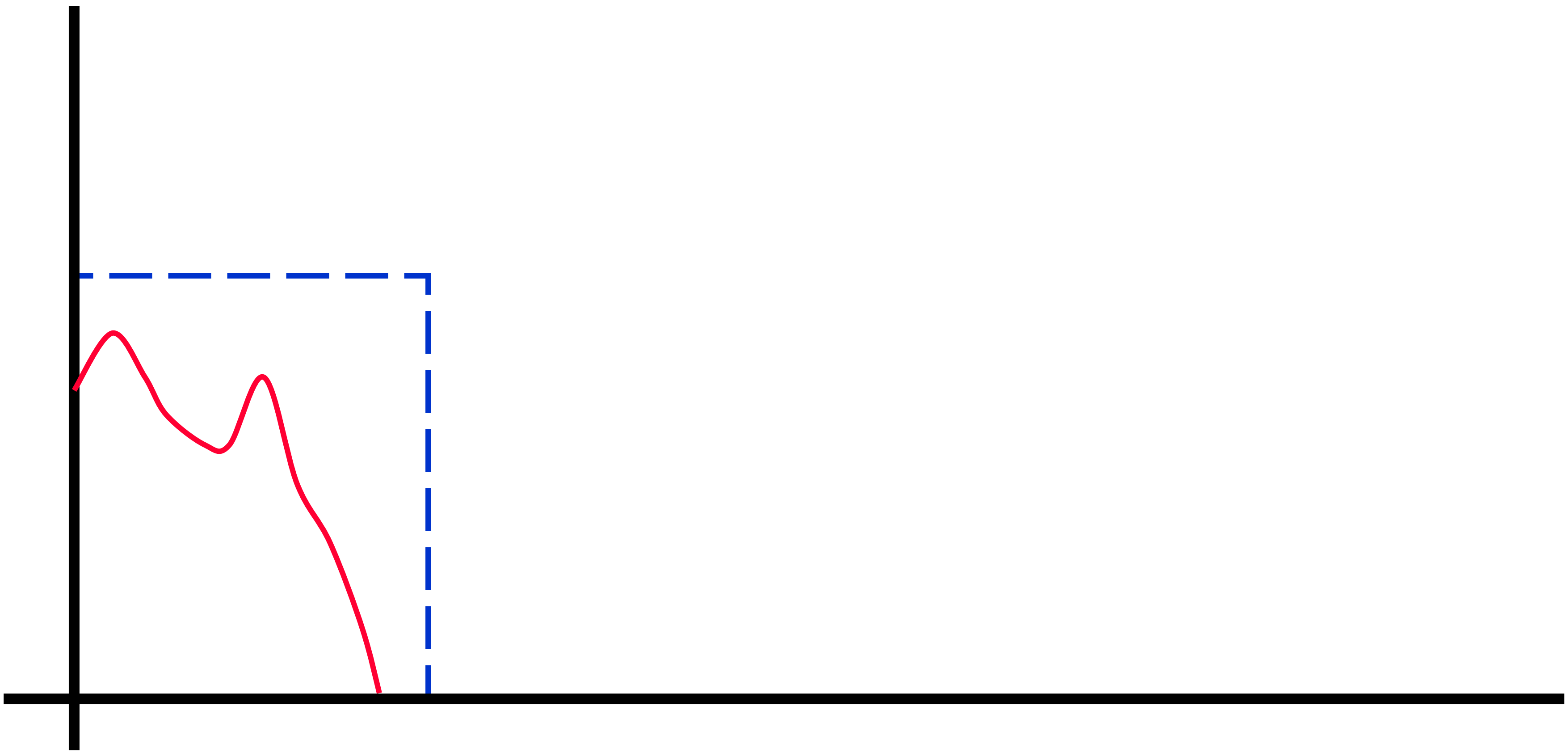

Crude quantization at extremely high rate + low-pass filter = 1-bit CD player ("Bitstream")

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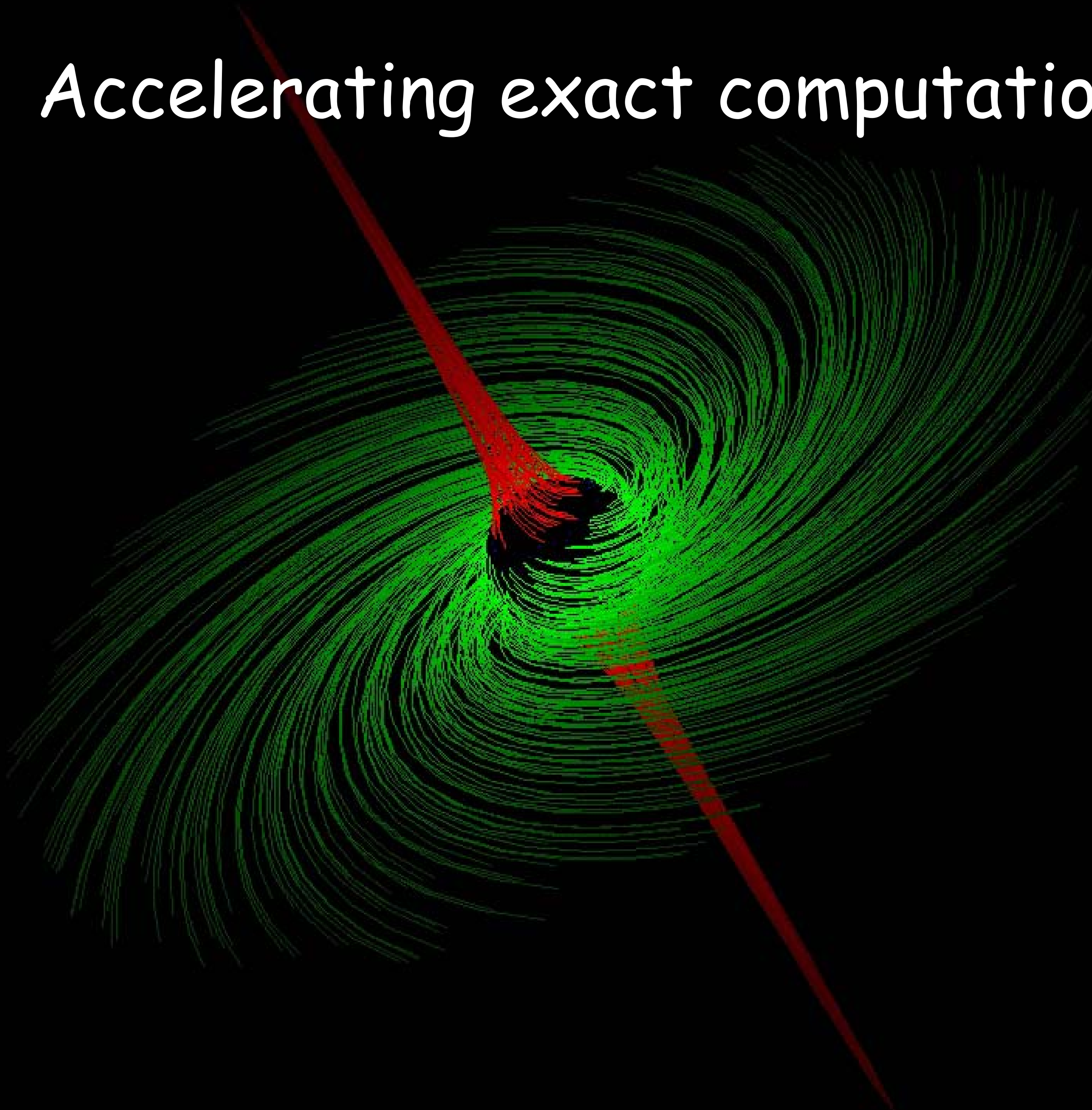
- Useful even for exact computations

Accelerating exact computations

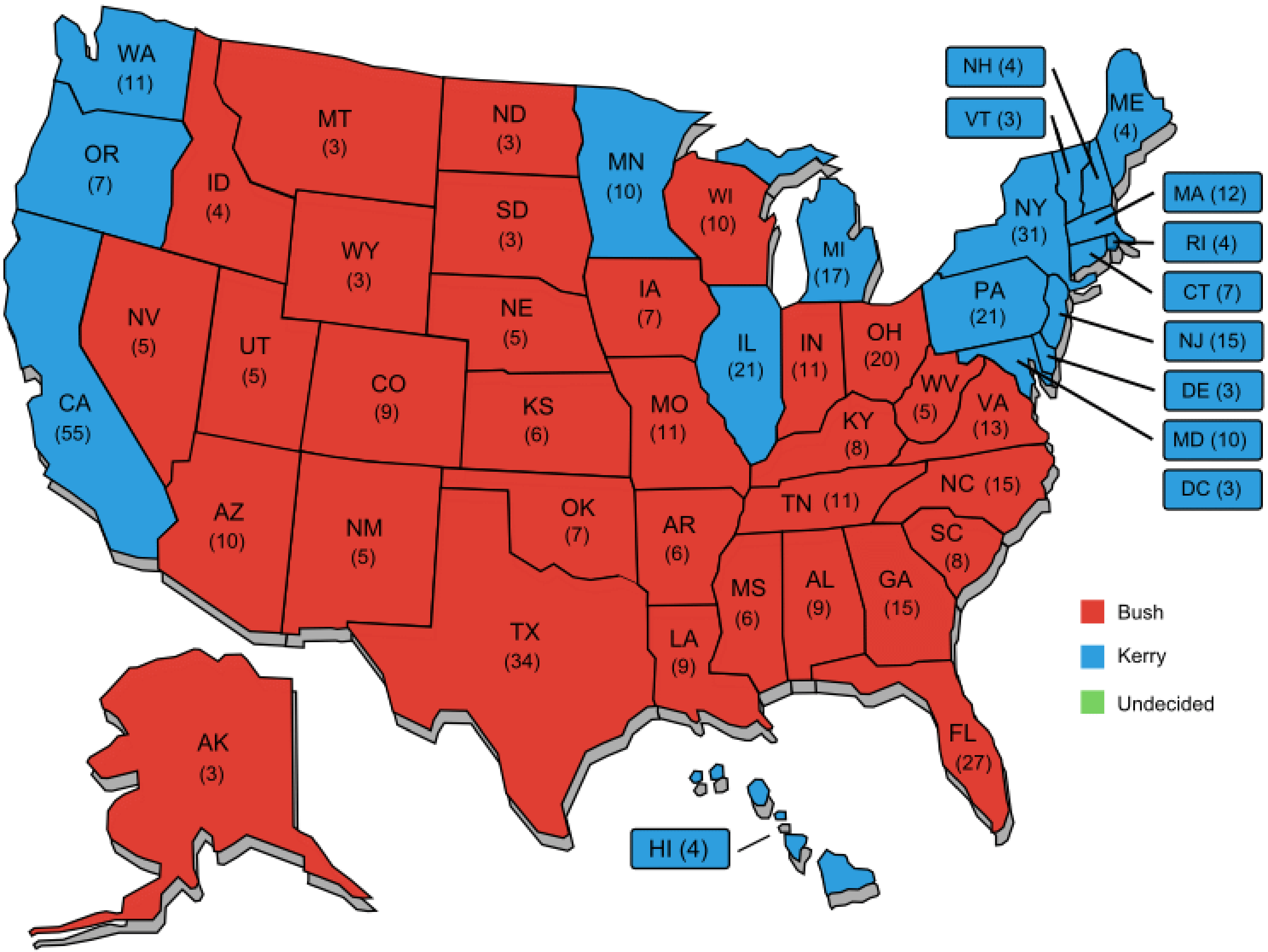


Kernels

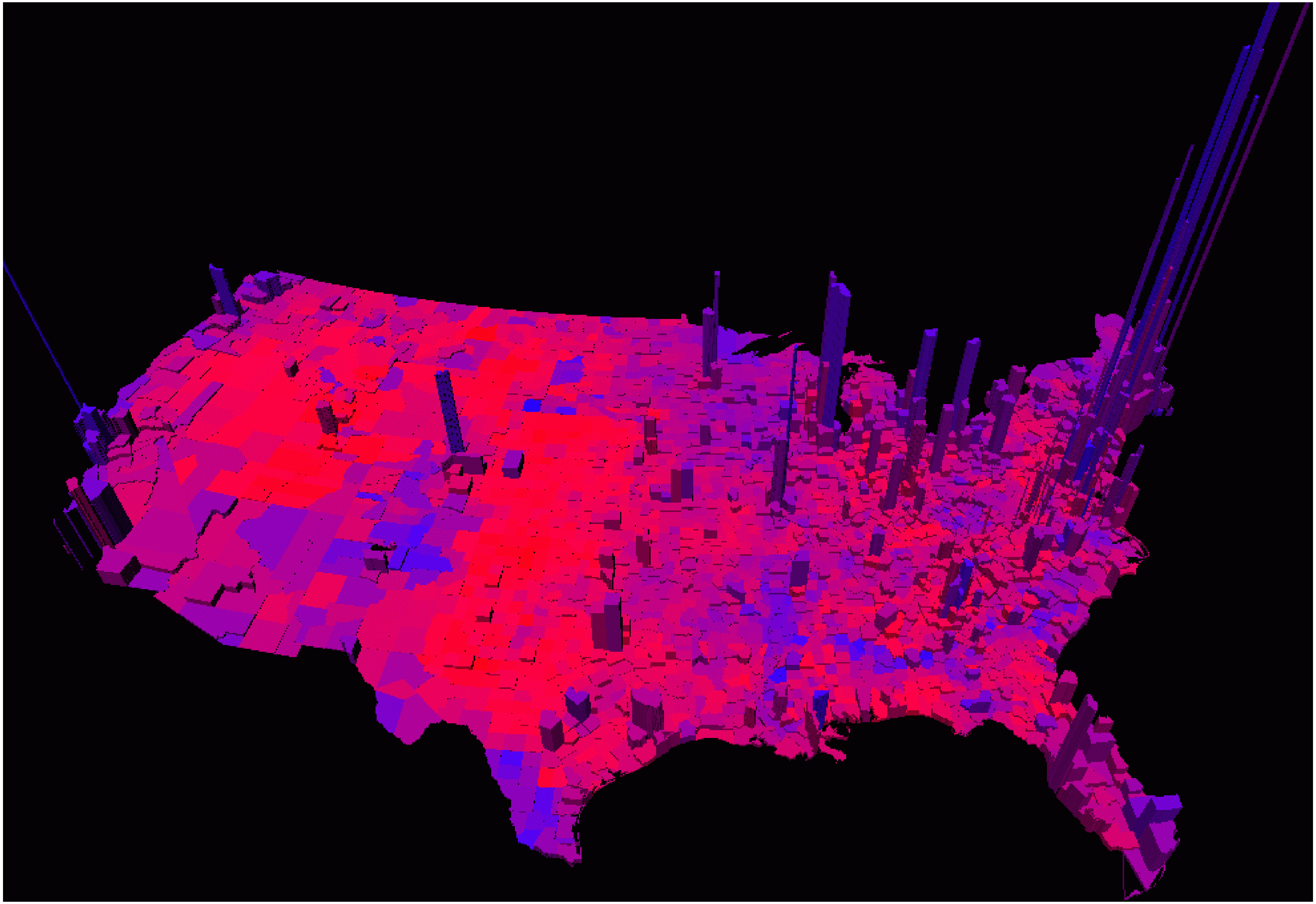
Kernels & Support Vector Machines

- Red and Blue pointclouds
- Which linear separator (hyperplane)?
- Maximum margin
- Optimal can be expressed by inner products with (a few) data points

Not always linearly separable



Population density



Kernel PCA

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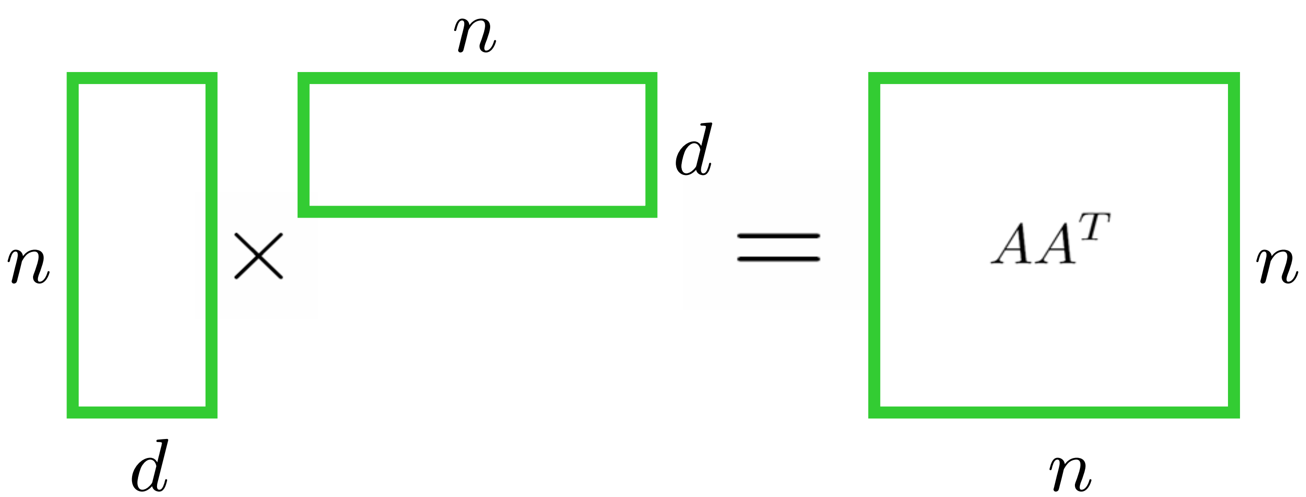

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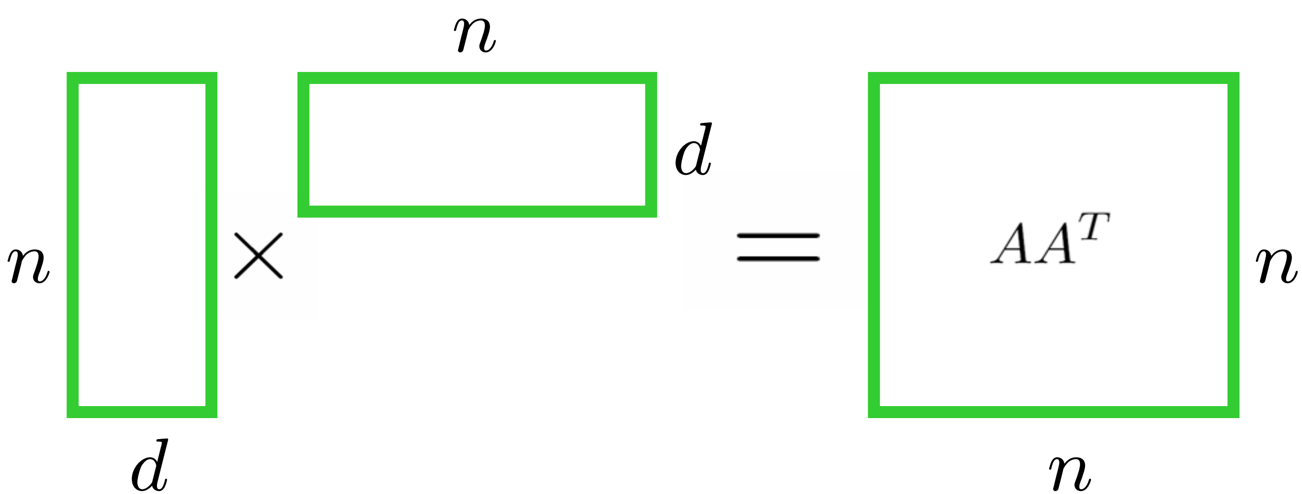

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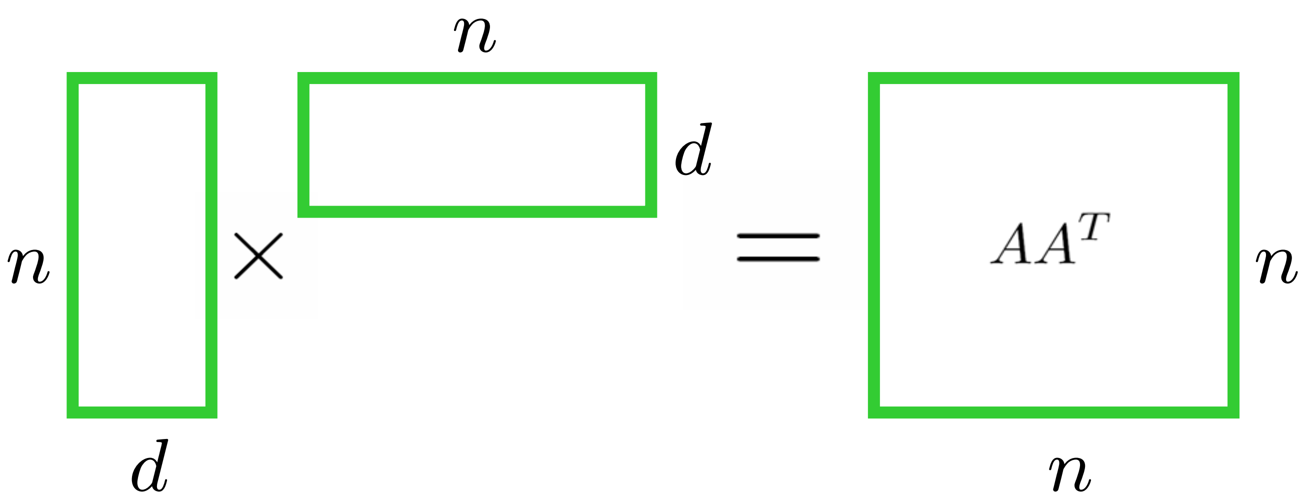

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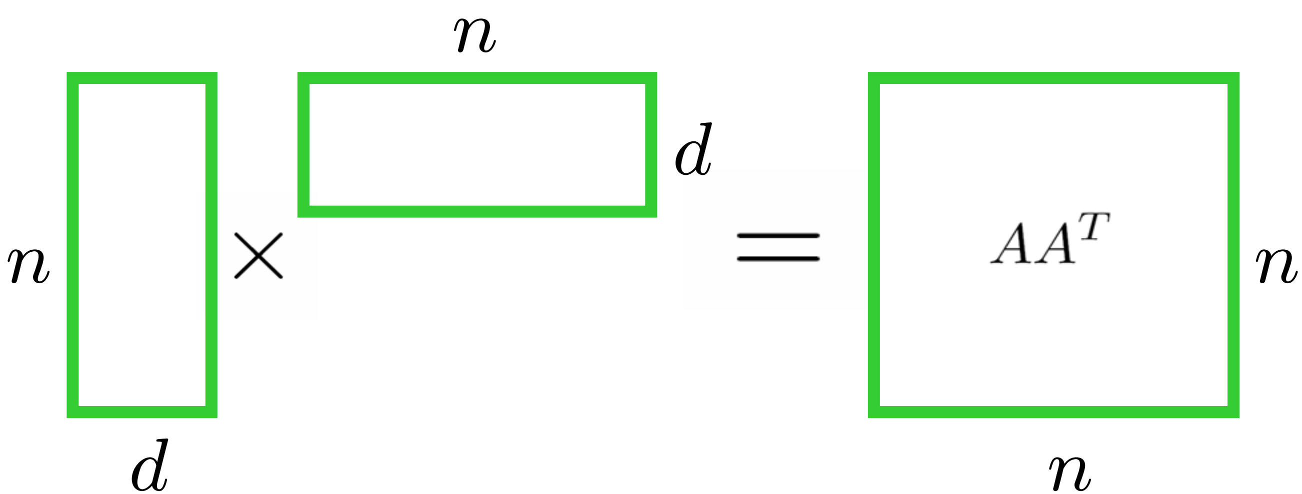

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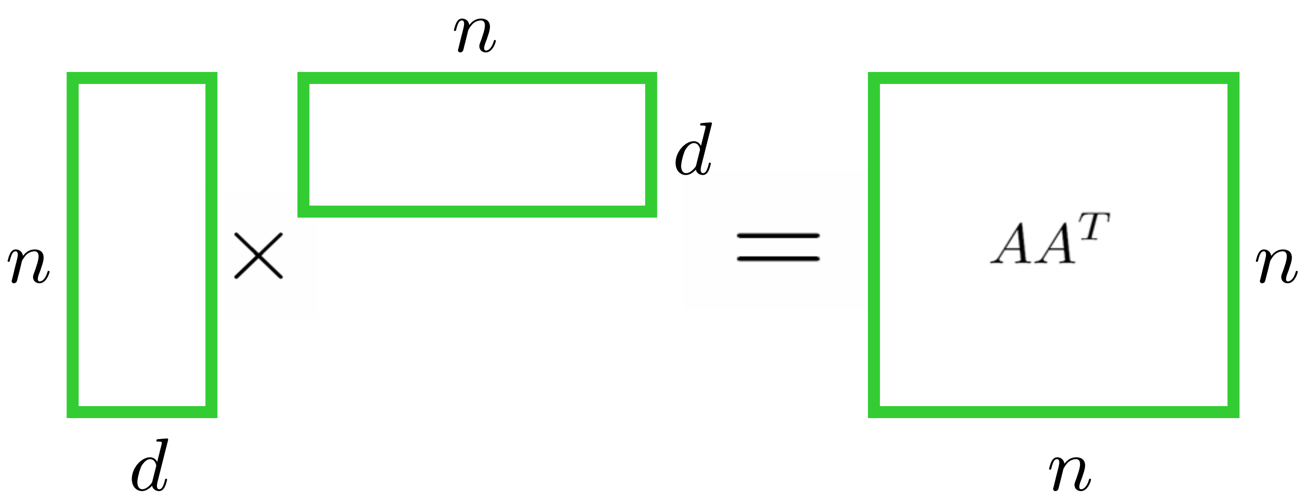

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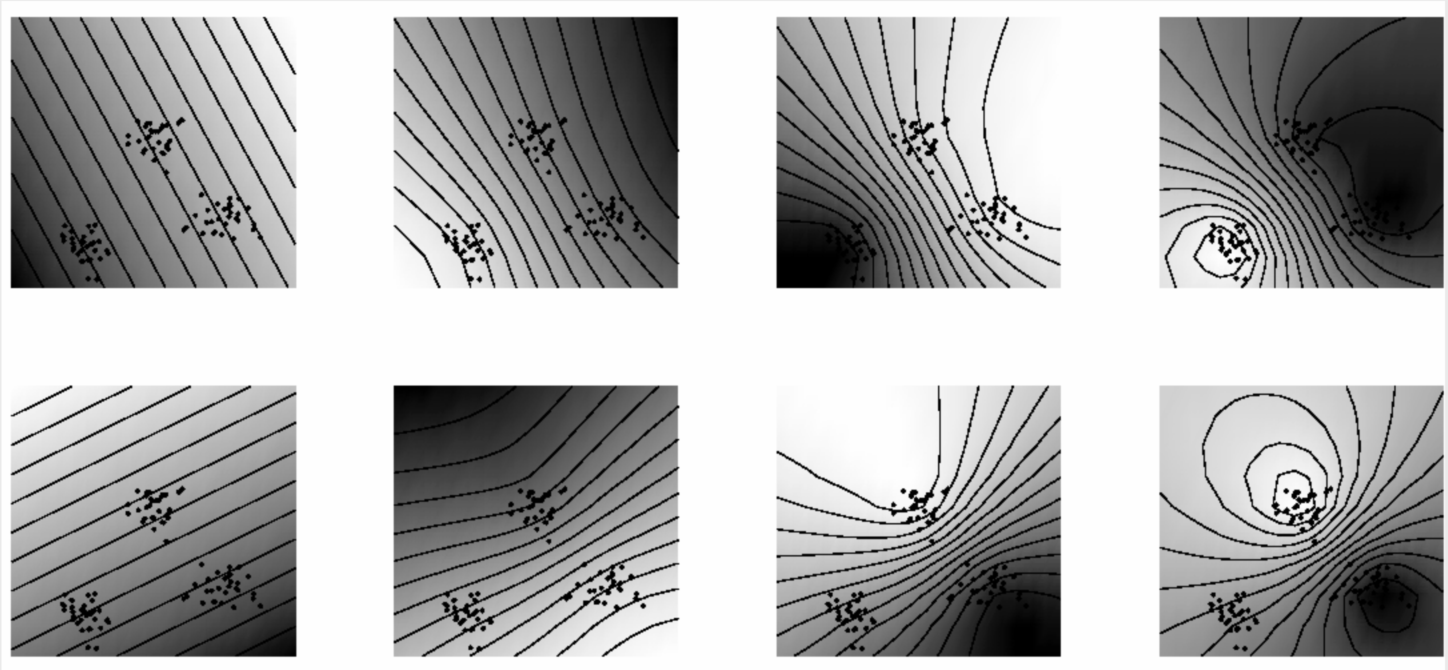
- Replace inner product with a kernel function
- Work implicitly in high-dimensional space
- Good linear separators in that space

From linear to non-linear PCA

$||X-Y||^p$ kernel illustrates how the contours of the first 2 components change from straight lines for p=2 to non-linea for p=1.5, 1 and 0.5.

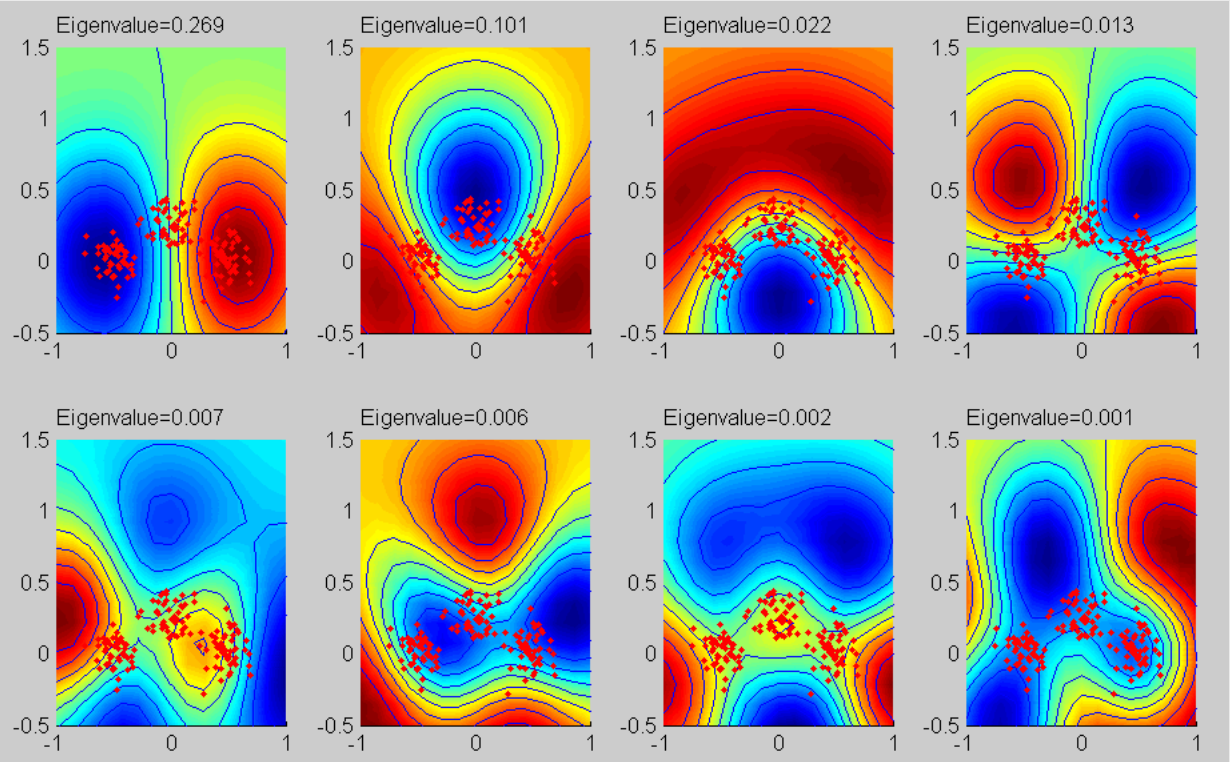


From Schölkopf and Smola, Learning with kernels, MIT 2002

Kernel PCA with Gaussian Kernel

KPCA with Gaussian kernels. The contours follow the cluster densities!

First two kernel PCs separate the data nicely.



Linear PCA has only 2 components, but kernel PCA has more, since the space dimension is usually large (in this case infinite)

KPCA in brief

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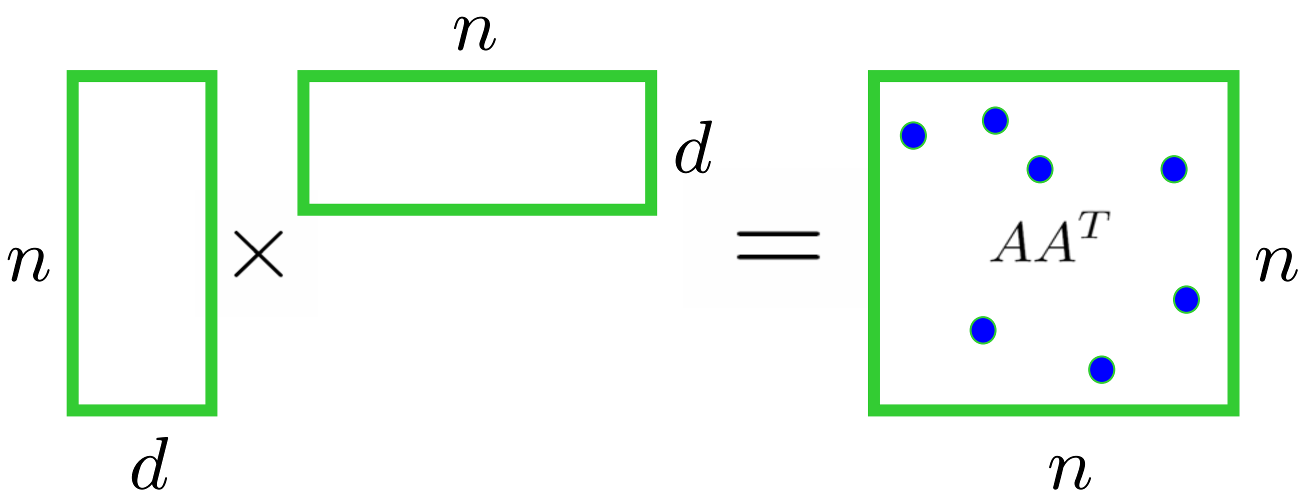
Good News:

[Shaw-Taylor et al. '03]

good generalization $\Longleftrightarrow$ rapid spectral decay

So, it's enough to sample...



- In practice, 1% of the data is more than enough
- In theory, we can go down to $n \times \mathrm{polylog}(n)$

Important Features are Preserved

Each feature/eigenvector of K has an associated eigenvalue.

Each eigenvalue measures the *importance* of the corresponding feature for reconstructing K.

- Let $B(t)$ be an orthonormal basis for those features which have eigenvalue at least t in K.

- Let $B_\perp(t)$ be an orthonormal basis for the complement of $B(t)$.

- Similarly for $\widehat{B}(t), \widehat{B}_\perp(t)$

Theorem 2 *For every* $\xi_1 > \xi_2$

$$\left| \widehat{B}^T(\xi_1) B_\perp(\xi_2) \right|_2 \leq \frac{|K - \widehat{K}|_2}{\xi_1 - \xi_2}$$

Open Problems

- How general is this “stability under noise”?
- For example, does it hold for

  Support Vector Machines?
- When can we prove such stability in a black-box fashion, i.e. as with matrices?
- Can we exploit if for data privacy?