DS 503: Advanced Data Analytics

Week 2: Projection Techniques

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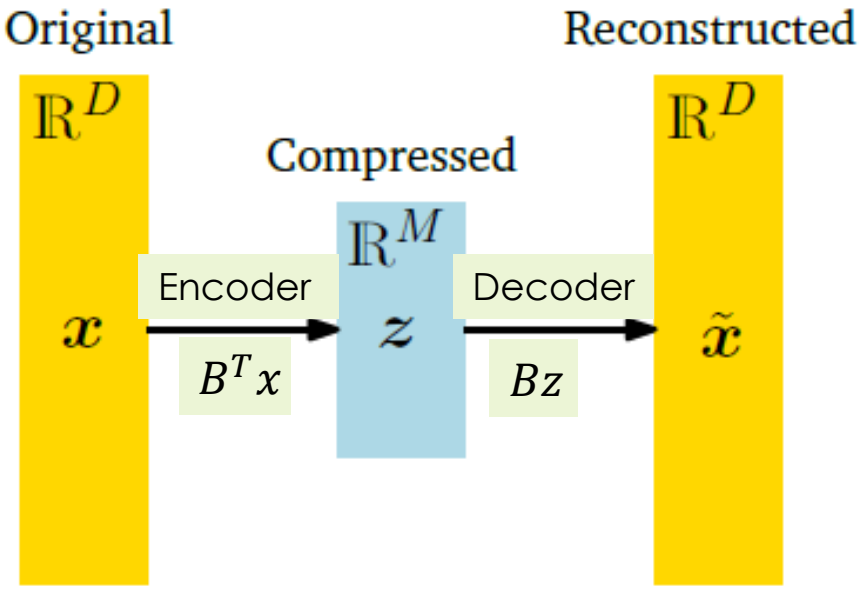
How to deal with high-dimensions?

- Project data to a low-dimensional space
- Fidelity: While doing so, don’t disturb the relative distances
- Where is this used?
  - Principal component analysis
  - Nearest Neighbor Search
  - Clustering
  - Text Embeddings
  - Graph Embeddings
  - Image manifolds

Problem statement

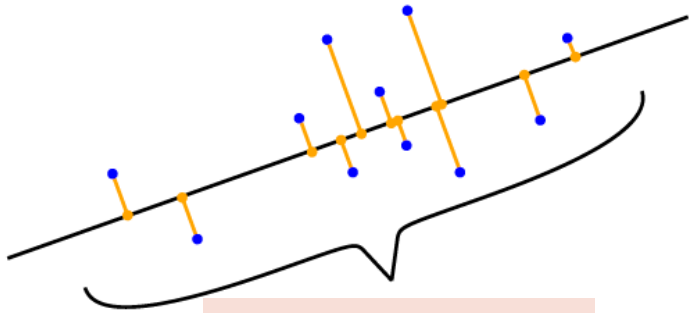
- $\boldsymbol{D}$ **x** $\boldsymbol{n}$ data matrix A (D rows and $\boldsymbol{n}$ columns)
  - Each column is a D-dimensional vector
  - Rows are normalized (mean = 0)
- Assume there is a projection matrix B, such that
  - $z = B^T x \in R^M$
  - $B = [b_1, b_2, \ldots, b_M]$ has orthogonal columns
- B is the best-fit M-dim. subspace S_M for columns of A
  - Minimize reconstruction error
  - Minimize sum of squared distances from A_i to S_M



Minimize:

$$||x - \tilde{x}||^2$$

Best fit subspaces and Maximizing Information



Best Line (1-d)

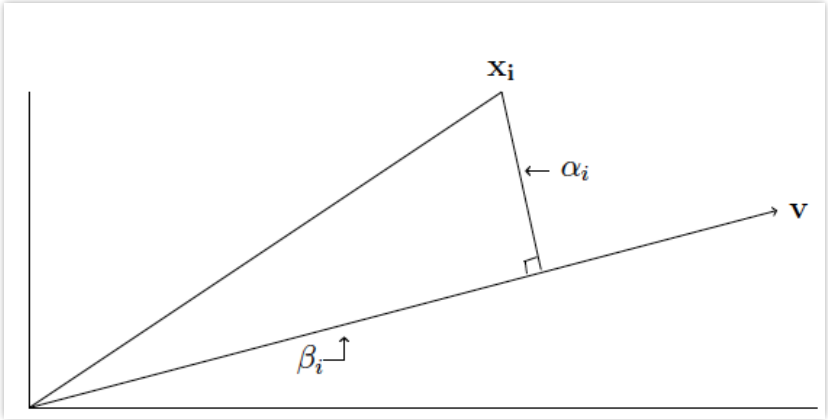
- Let's begin with the following question.
  - Find a direction in which the data ($\boldsymbol{D}$ **x** $\boldsymbol{n}$ matrix) has maximum information
  - Maximize $|Av_1|$, such that $|v_1| = 1$
  - This is also equivalent to Minimizing the sum of squared distances to the point nearest to the line.
- By successively solving the above problem, we can find the best-fit k-dimensional subspaces
  - Which preserve the maximum possible information (by maximizing projections)
  - Or equivalently, minimize the sum of squared distances of the vectors to the subspace
- When k=r, the rank of A, we get SVD

Projections, Distances and Data Variance

- Minimizing distance = maximizing projection
  - $\left|\left|\boldsymbol{x}\right|\right|_2^2 = (projection)^2 + (distance\ to\ line)^2$
- SVD: Find best fit 1-dimensional line
  - u_1 = unit vector along the best fit line
  - x_i= i-th column of A, length of its projection: $|\langle \boldsymbol{x}_i, u\rangle|$
- Sum of squared projection lengths: $\left|\left|A^T u\right|\right|_2^2$
- **First singular vector**:

$$\boldsymbol{u}_1 = \arg\max_{||u||_2=1} \left|\left|A^T u\right|\right|_2$$

- If there are ties, break arbitrarily
  - $\sigma_1(A) = \left|\left|A^T \boldsymbol{u}_1\right|\right|_2$ is the **first singular value**



Variance of z_1 of $z \in R^M$

$$V_1 := V[z_1] = \frac{1}{N}\sum_{n=1}^{N} z_{1n}^2$$

$$z_{1n} = b_1^T x_n$$

$$V_1 = b_1^T\, S\, b_1$$

Where S is the data-covariance matrix

$$\boldsymbol{S} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^\top .$$

Maximizing Variance using PCA

Optimization Problem

$$\max_{\boldsymbol{b}_1} \boldsymbol{b}_1^\top \boldsymbol{S} \boldsymbol{b}_1$$

$$\text{subject to } \|\boldsymbol{b}_1\|^2 = 1\,.$$

Encoder

$$z_{n1} = b_1^T x_n \in R$$

Decoder

$$\tilde{x}_n = b_1 z_{n1} = b_1 b_1^T x_n \in R^D$$

Lagrangian

$$\mathfrak{L}(\boldsymbol{b}_1, \lambda) = \boldsymbol{b}_1^\top \boldsymbol{S} \boldsymbol{b}_1 + \lambda_1 (1 - \boldsymbol{b}_1^\top \boldsymbol{b}_1)$$

Differentiating

$$\frac{\partial \mathfrak{L}}{\partial \boldsymbol{b}_1} = 2\boldsymbol{b}_1^\top \boldsymbol{S} - 2\lambda_1 \boldsymbol{b}_1^\top\,, \qquad \frac{\partial \mathfrak{L}}{\partial \lambda_1} = 1 - \boldsymbol{b}_1^\top \boldsymbol{b}_1\,,$$

$$\boldsymbol{S}\boldsymbol{b}_1 = \lambda_1 \boldsymbol{b}_1\,,$$

$$\boldsymbol{b}_1^\top \boldsymbol{b}_1 = 1\,.$$

b_1 is an eigenvector of S
λ_1 is the eigenvalue

$$V_1 = \boldsymbol{b}_1^\top \boldsymbol{S} \boldsymbol{b}_1 = \lambda_1 \boldsymbol{b}_1^\top \boldsymbol{b}_1 = \lambda_1\,,$$

- Variance of the data projected onto a one-dimensional subspace equals the **eigenvalue** that is associated with the **basis vector b1** that spans this subspace.
- To maximize the variance of the low-dimensional code, we choose the basis vector associated with the **largest eigenvalue** principal component of the **data covariance matrix**.
- This eigenvector is called the first *principal component*

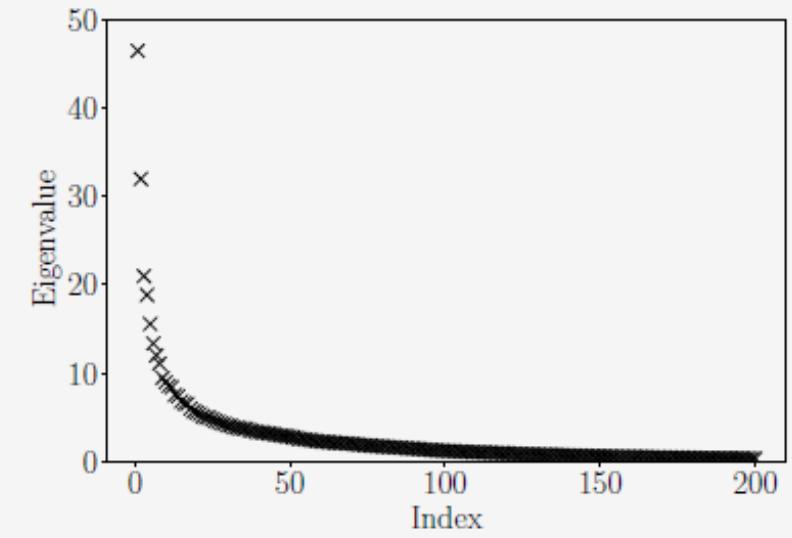
General Algorithm

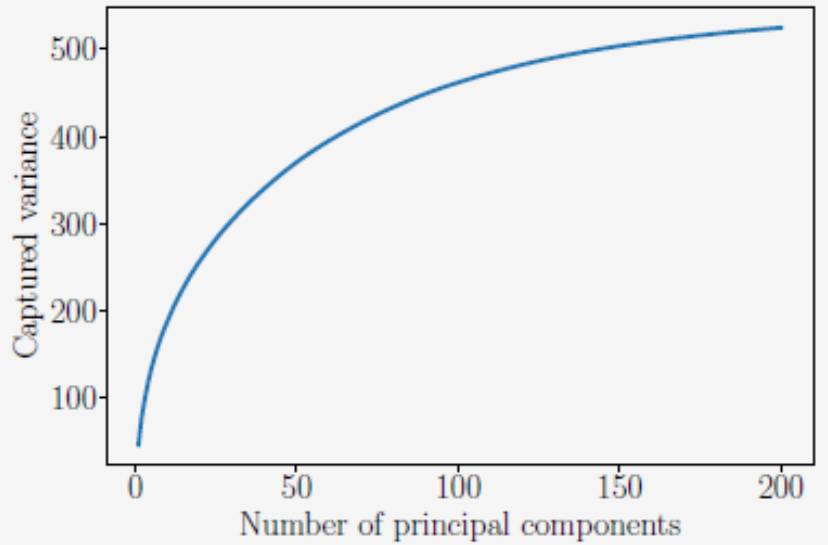
- In general, the largest M (orthonormal) eigenvectors of the data-covariance matrix span the best M dimensional subspace for A
- They also capture the variance equal to the sum of largest M eigenvalues
- We can iteratively compute the largest eigenvalue/eigenvector of the covariance matrix ‘S’ and continue till the sum of M eigenvalues captures a large fraction of the trace of S

$$V_M = \sum_{m=1}^{M} \lambda_m$$

$$1 - \frac{V_M}{V_D}.$$

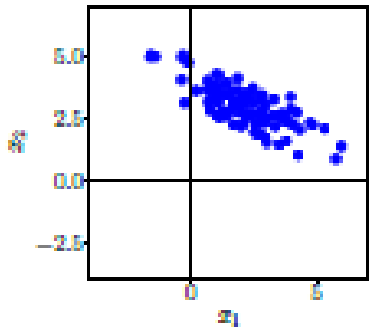
Stop when this become small



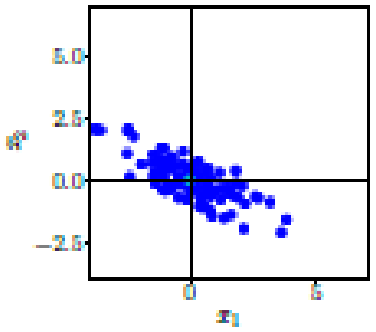


Key Steps of PCA in Practice

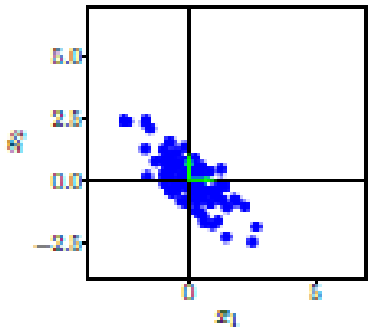
- Centering of the data
- Normalization
- Eigen decomposition of the Covariance Matrix
- Projection
- Mapping back to the original data space



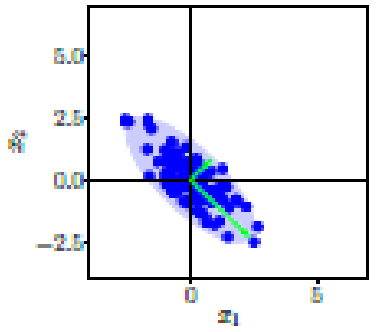
(a) Original dataset.



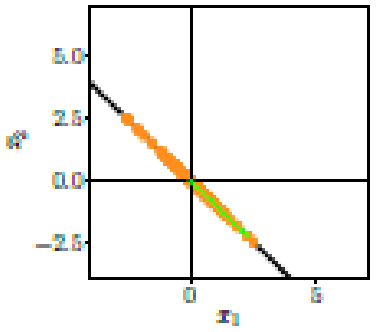
(b) Step 1: Centering by subtracting the mean from each data point.



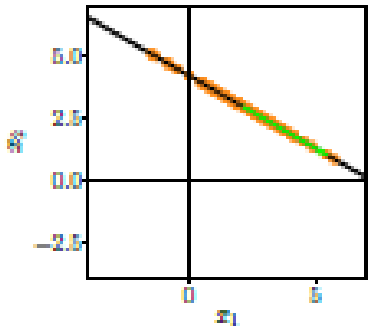
(c) Step 2: Dividing by the standard deviation to make the data unit free. Data has variance 1 along each axis.



(d) Step 3: Compute eigenvalues and eigenvectors (arrows) of the data covariance matrix (ellipse).



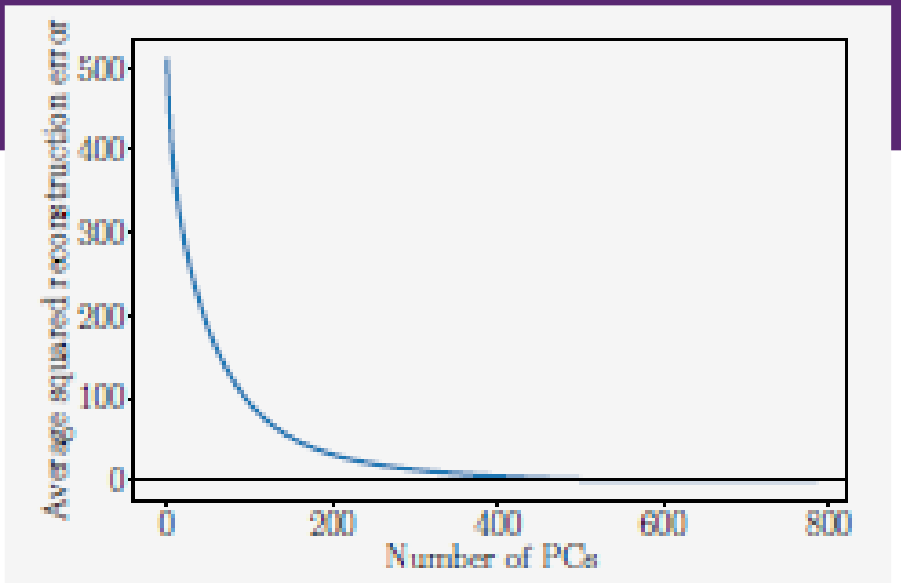
(e) Step 4: Project data onto the principal subspace.

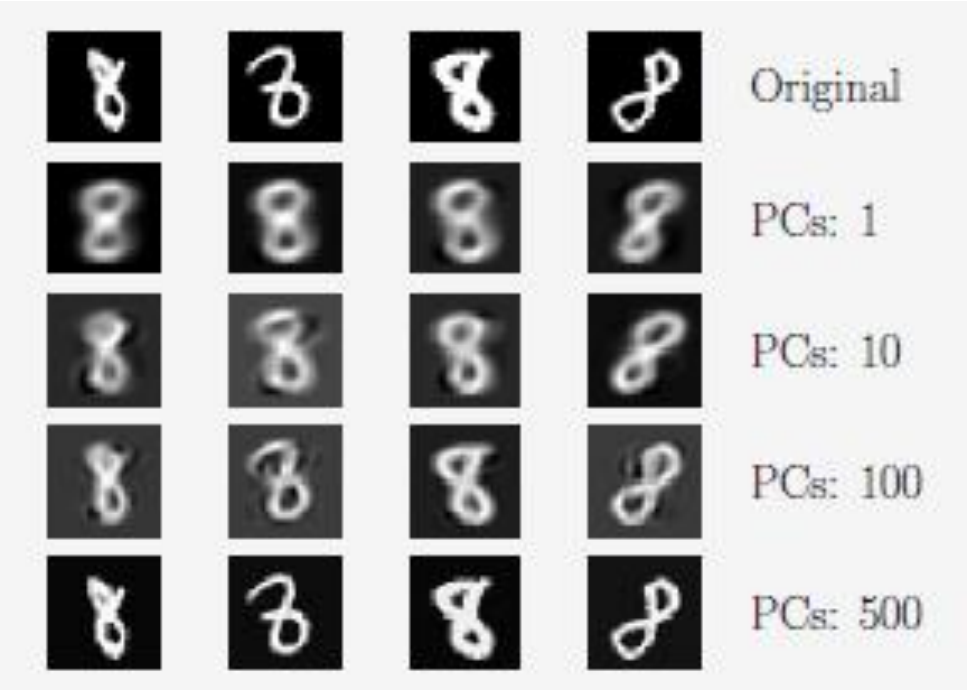


(f) Undo the standardization and move projected data back into the original data space from (a).

MNIST Digits: reconstruction

- MNIST dataset contains of handwritten digits 0 to 9
- Each digit is an image of 28x28 pixels, that is equivalent to a vector of dimension 784
- The picture on the right is performing PCA on the 5389 samples of “8” from the dataset
- We check the reconstruction error curve to decide how many components to keep





Variants of PCA

- **Sparse PCA** : Add a L1 regularization term to remove features with small coefficients. Find sparse low rank matrices B and C so that $A \approx BC$
- **Non-negative Matrix Factorization:** Find non-negative matrices U and V so that $A \approx UV$
- **Kernel PCA** : Account for a non-linear relationship among features by using the "kernel trick"
- **Probabilistic PCA (PPCA):** Formulates PCA as a generative process which allows us to simulate new data

Application Areas:

- **Facial Feature Extraction**

Find a few basic faces so that every face can be expressed as a combination

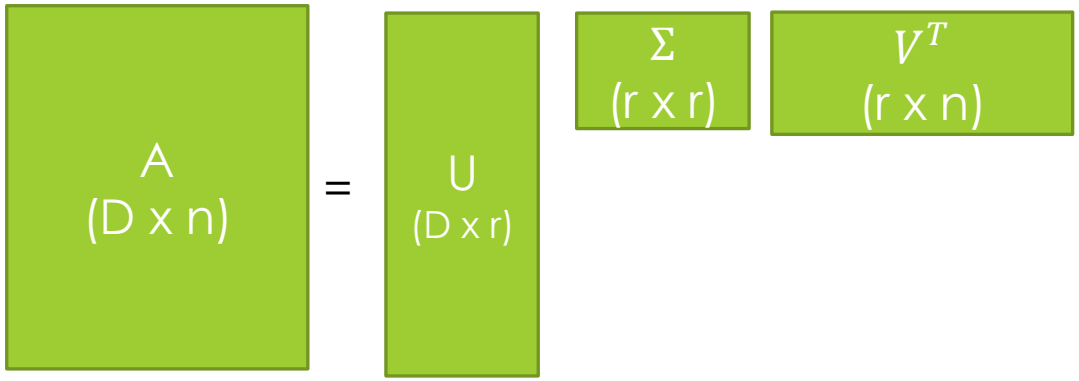
- **Gene Expressions**

Find out which genes are playing a role in a particular phenomenon

- **Text Mining and Document Classification**

Combine the various topics in a document

Properties of SVD



- SVD: $A = U\Sigma V^T$
- Σ = Diagonal matrix (positive real entries σ_{ii})
- U, V: orthonormal columns:
  - $\boldsymbol{u}_1, \dots, \boldsymbol{u}_r \in \mathbb{R}^D$ (directions that maximize projections of x_i)
  - $\boldsymbol{v}_1, \dots, \boldsymbol{v}_r \in \mathbb{R}^n$ (projections of x_i on u_i)
  - $\langle \boldsymbol{u}_i, \boldsymbol{u}_j \rangle = \delta_{ij}, \langle \boldsymbol{v}_i, \boldsymbol{v}_j \rangle = \delta_{ij}$
- $A = \sum_i \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$
- Thus, any matrix can be represented as sum of “r” rank-1 matrices

Singular Values vs. Eigenvalues

- If A is a square matrix:
  - Vector $\boldsymbol{v}$ such that $A\boldsymbol{v} = \lambda\boldsymbol{v}$; is an eigenvector with eigenvalue = λ
  - For symmetric real matrices, A, $\boldsymbol{v}$'s are orthonormal
    - A can be expressed as: $A = V\Sigma V^T = U\Sigma U^T$
    - $V's$ columns are eigenvectors of A
  - Diagonal entries of Σ are eigenvalues $\lambda_1, \ldots, \lambda_n$
- SVD is defined for all matrices (not just square)
  - Orthogonality of singular vectors is automatic

$$A\boldsymbol{v}_i = \sigma_i\boldsymbol{u}_i \text{ and } A^T\boldsymbol{u}_i = \sigma_i\boldsymbol{v}_i \text{ (will show)}$$

$AA^T u_i = \sigma_i^2\boldsymbol{u}_i \Rightarrow u_i's$ are eigenvectors of AA^T ((N-1) times sample covariance matrix)

SVD: Greedy Construction

- Find best fit 1-dimensional line, repeat r times (until projection is 0)
- **Second singular vector and value:**

$$\boldsymbol{u}_2 = \arg \max_{u \perp u_1, ||u||_2 = 1} ||A^T u||_2$$

$$\sigma_2(A) = ||A\boldsymbol{u}_2||_2$$

- **k-th singular vector and value:**

$$\boldsymbol{u}_k = \arg \max_{u \perp \boldsymbol{u}_1, \ldots \boldsymbol{u}_{k-1}, ||u||_2 = 1} ||A^T u||_2$$

$$\sigma_k(A) = ||A^T \boldsymbol{u}_k||_2$$

- We can show that: $(\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k)$ is best-fit subspace

Best low rank approximations of a Matrix

- Suppose I have to find the best "k" rank approximation A_k matrix.

  Let $A_k = \sigma_1 u_1 v_1^T + \ldots + \sigma_k u_k v_k^T$
  Eckart-Young: If B has rank k then $||A - B|| \geq ||A - A_k||$

- This result has been proven for multiple norms
- Spectral: $||A||_2 = \max \frac{||Ax||}{||x||} = \sigma_1$
- Frobenius: $||A||_F^2 = \sigma_1^2 + \cdots + \sigma_r^2 = \sum_{i,j} |a_{i,j}|^2 = trace\ of\ AA^T$
- Nuclear: $||A_N|| = \sigma_1 + \ldots + \sigma_r$ (the trace norm)

Applications of low rank approximations

- Principal component analysis (fitting a hyperplane to data and more!)
- Model reduction in analyzing physical systems
- Fast algorithms in scientific computing
- PageRank and other spectral methods in data analysis
- Diffusion geometry and manifold learning
- Many, many more …

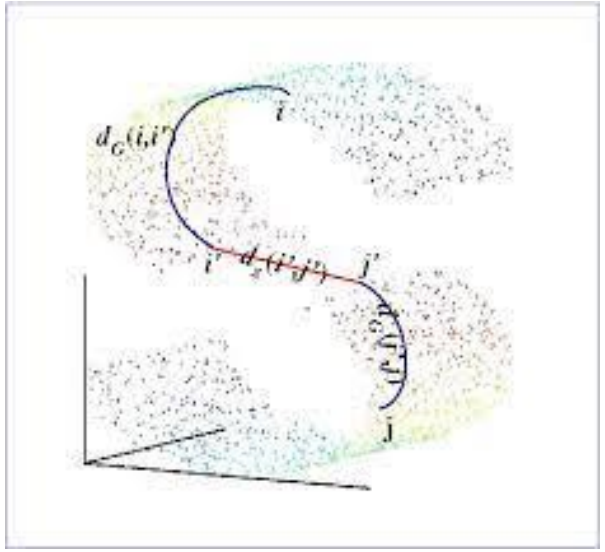
Computing the SVD: Power iteration method

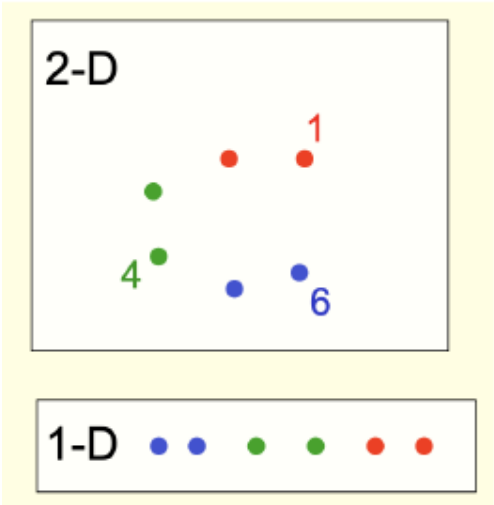
- Begin with a random vector x_0 that is not in the null space of S = AA^T
- Follow the iteration $\mathrm{x_{k+1}} = \frac{S\,x_k}{||S\,x_k||}$
- This converges to the eigenvector associated with the largest eigenvalue of S
- Also used in the page-rank algorithm for ranking web-pages based on their hyperlinks
- Issues: S can be very large
- Alternative 1: If N << D, then we can instead work with the matrix $A^T A$ which also has the same eigenvalues (square of singular values).
- This can happen, for example, when we are dealing with large size images with millions of pixels.

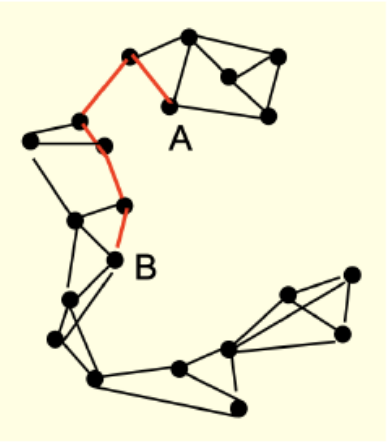
SVD works well for small matrices (m, n< 5000) or sparse matrices. The function for computing SVD is not so easy to write.

Multi-dimensional Scaling and Isomap

- PCA had the goal of minimizing the reconstruction error/preserving variance of the data when projecting to lower dimensions
- MDS has the goal of preserving inter-point distances; i.e. $|z_i - z_j| \approx |x_i - x_j|$
  - This is also modeled as a related objective of preserving the inner-products
    - Minimize Error = $\sum(< x_i, x_j > - < z_i, z_j >)$
  - Turns out that it is also very similar to PCA and can be solved using SVD
- One generalization of MDS to non-linear dimensionality reduction is called Isomap
  - Here a graph is constructed among the points in the dataset
  - Shortest path distance is computed along the graph
  - This is used to model the distance along the manifold



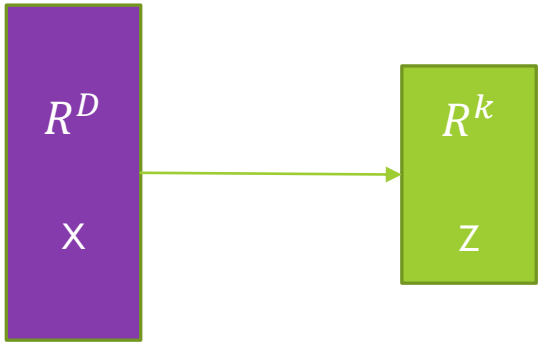




JL Lemma and Random Projections (FoDS section 2.7)

- Suppose $x_1, x_2, \dots, x_n$ are any n points in R^D and $k \geq \frac{8 \ln n}{\epsilon^2}$.
- ∃ a distance preserving projection J from R^D to R^k which works ∀ pairwise distances:
  - $$\boxed{(1-\epsilon)\left|\left|x_i - x_j\right|\right|^2 \leq \left|\left|Jx_i - Jx_j\right|\right|^2 \leq (1+\epsilon)\left|\left|x_i - x_j\right|\right|^2}$$
- There are multiple proofs and one of the proof shows that w.h.p. a random projection (kxD) is very likely to keep the n points apart.
- Project each $\boldsymbol{x} \in \boldsymbol{A}$ onto $f(\boldsymbol{x})$, where $f: \mathbb{R}^{\boldsymbol{D}} \rightarrow \mathbb{R}^{\boldsymbol{k}}$
- Pick $\boldsymbol{k}$ Gaussian vectors with unit variance; $\boldsymbol{u}_1, \dots, \boldsymbol{u}_{\boldsymbol{k}}$ i.i.d: $\boldsymbol{u}_i \sim N_D(0^D, I)$

$$f(\boldsymbol{v}) = (\langle \boldsymbol{u}_1, \boldsymbol{v} \rangle, \dots, \langle \boldsymbol{u}_{\boldsymbol{k}}, \boldsymbol{v} \rangle)$$



  - Since the k vectors were Gaussian, the projections are also Gaussian
    - W.h.p. $|f(v)| \approx \sqrt{k}|v|$ and thus $|f(v_1) - f(v_2)| \approx \sqrt{k}|v_1 - v_2|$
    - Distances increase because u_i are not unit vectors
  - Application of Gaussian Annulus theorem allows to bound the deviation in the distances (Thm 2.10)

Applications

- Suppose $x_1, x_2, \ldots, x_n$ are any n points in R^D, where D is very large. Tasks:
- Suppose the points almost live on a linear subspace of (small) dimension *k*.
  - Find a basis for the "best" subspace. (Principal component analysis.)
- Given *k*, find the subset of *k* vectors with maximal spanning volume.
- Suppose the points almost live on a low-dimensional nonlinear manifold.

  Find a parameterization of the manifold.
- Given *k*, find for each vector $\boldsymbol{x_i}$, its *k* closest neighbors.
- Partition the points into clusters.

Note: Some of these don't have well-defined solutions and some are combinatorially hard. If we can embed the points in a low-dimensional subspace, while preserving distance approximately, then a variety of algorithms for solving these problems become possible.

Application: Nearest Neighbors Search

Goal: Given a database of n points in R^D where n and D are usually large. Query points in R^D. Queries should be fast.

- If the database has n1 points and n2 queries are expected during the lifetime of the algorithm, take n = n1 + n2
- Project database (using random vectors) to a k-dimensional space
- Store projections in an efficient data structure (more in next lecture)
- On receiving a query, project the query to the same subspace and compute nearby database points.
- The JL Lemma says that with high probability this will yield the right answer whatever the query

Linear Regression (Problem setup)

- We are given observations **(x,** y)
  - Let us build a linear model to predict y from the observations **x** s. t. $w_0 + \sum_{i=1}^{d} w_i x_i = y$
- Compute the "best" solution to the model $Xw = y$ that minimizes SSE (sum of squared distances)
- This problem is very similar to solving $Ax = b$, a system of linear equations
- In most cases, there may be no exact solution to this problem
- But, there are many approaches we can take to get the "least squares" solution
  - This minimizes the sum of square errors $||b - A\hat{x}||^2$

Normal Equations

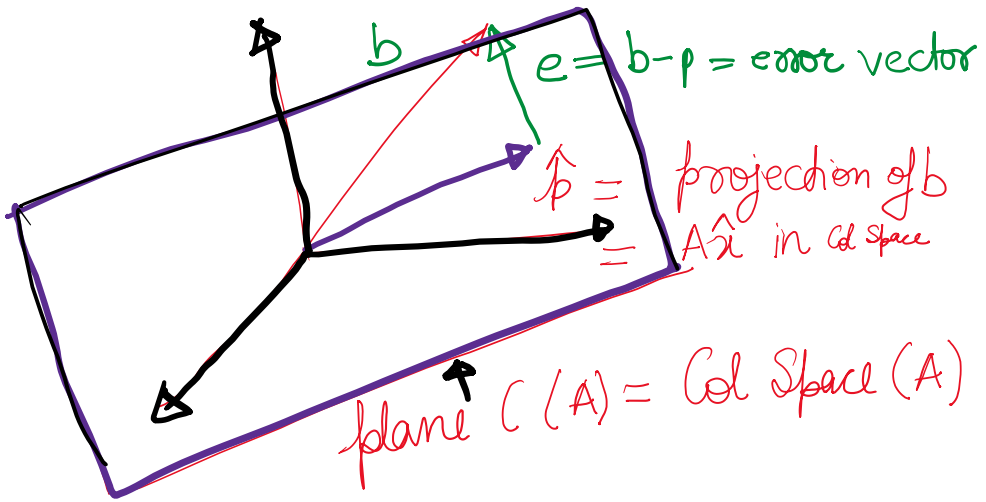
Since $(b - A\hat{x})$ is perpendicular to all vectors Ax in the column space, $(Ax)^T(b - A\hat{x}) = \mathrm{x^T A^T (b - A\hat{x})} = 0$

Normal Equation for solving $\hat{x}$ **:** $A^T A\hat{x} = A^T b$

Least squares sol to Ax=b: $\hat{x} = (A^T A)^{-1} A^T b$

Projection of b onto Col(A): $p = A\hat{x} = A(A^T A)^{-1} A^T b$

Projection matrix that multiplies b to give p: $P = A(A^T A)^{-1} A^T$

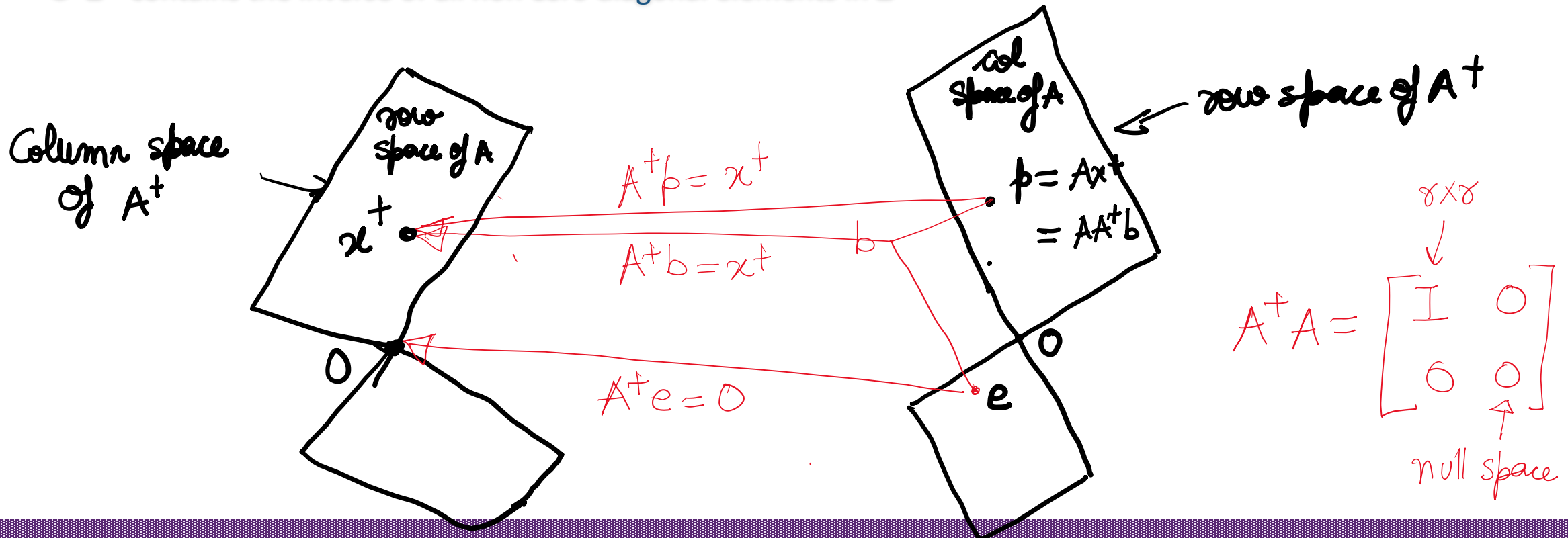


Pseudo Inverse Method

- Pseudo Inverse Method: $\hat{x} = A^{+}b$
  - If A has independent columns, $A^{+} = (A^{T}A)^{-1}A^{T}$
  - If A has independent rows, $A^{+} = A^{T}(AA^{T})^{-1}$
  - Pseudo inverse can be computed using SVD: $A^{+} = V\Sigma^{+}U^{T}$
  - Σ^{+} contains the inverse of all non-zero diagonal elements in Σ

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\Sigma^{+} = \begin{bmatrix} 1/\sigma_1 & 0 & 0 \\ 0 & 1/\sigma_2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



$$A^{+}A = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}$$

$r \times r$

null space

QR (Gram-Schmidt) Method

- Decompose $A = QR$
  - Where Q is an orthogonal matrix, and R is a triangular matrix
- Then, $A^T A = R^T Q^T QR = R^T R$ and the normal equation $A^T A\hat{x} = \mathrm{A^T b}$, can be solved as
  - $\hat{\boldsymbol{x}} = (R^T R)^{-1} R^T Q^T \boldsymbol{b} = \boldsymbol{R^{-1} Q^T b}$
- This is computationally efficient to solve

$$q_1 = a_1 / \|a_1\| \quad ; \quad \|q_1\| = 1$$

Key step:

$$A_2 = a_2 - (a_2^T q_1) q_1$$

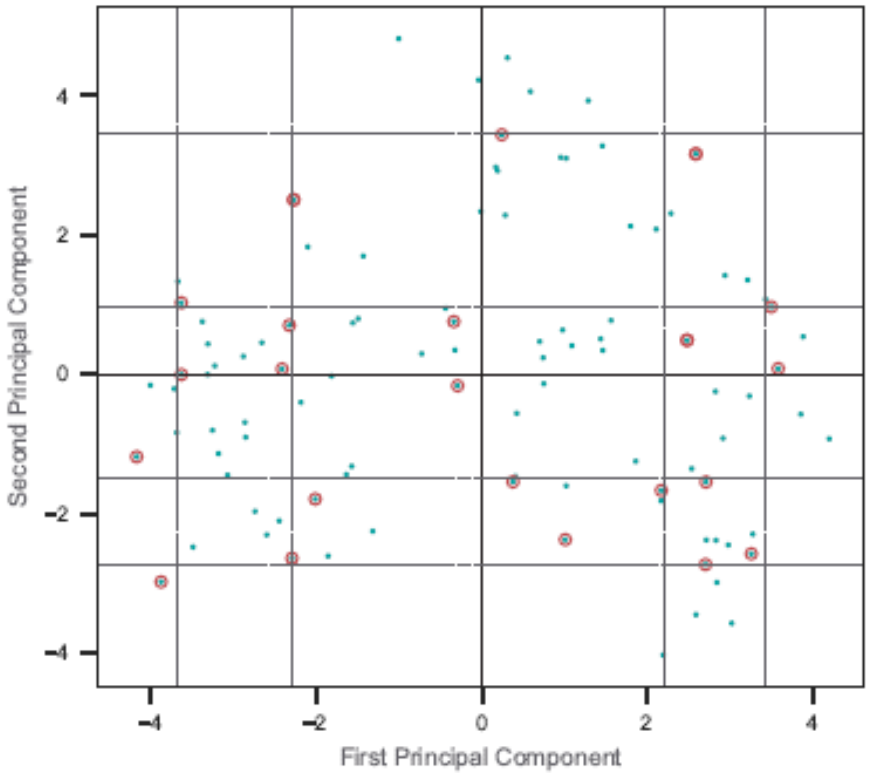
$$q_2 = A_2 / \|A_2\|$$

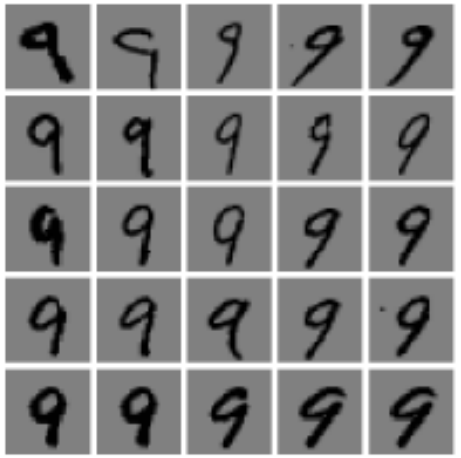
$$r_{ij} = q_i^T a_j$$

$$\begin{bmatrix} | & | & | \\ a_1 & a_2 & a_3 \\ | & | & | \end{bmatrix} = \begin{bmatrix} | & | & | \\ q_1 & q_2 & q_3 \\ | & | & | \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{bmatrix}$$

q_i^S are orthonormal

Interpreting the data (1)





The first principal component (horizontal direction) seems to capture the orientation of the digit,
Second component (vertical direction) seems to capture line thickness.

Interpreting the data (2)

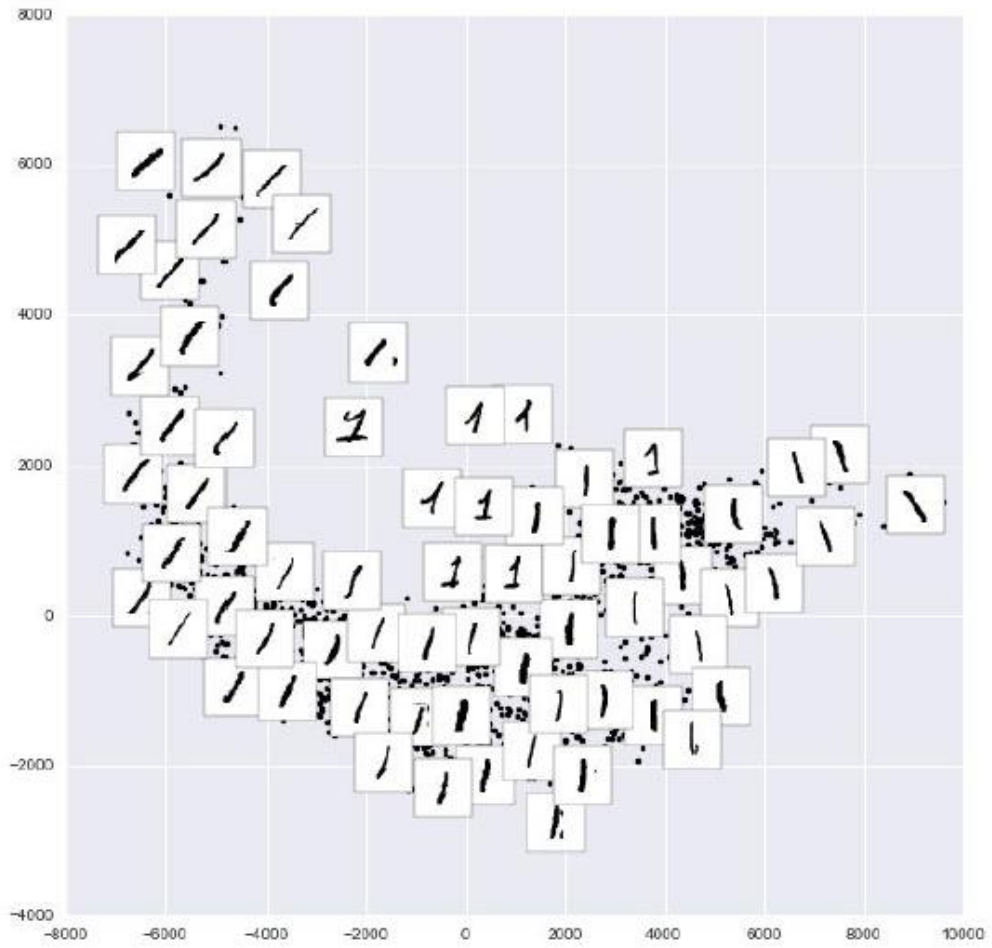


Figure 5-109. Isomap embedding of only the 1s within the digits data

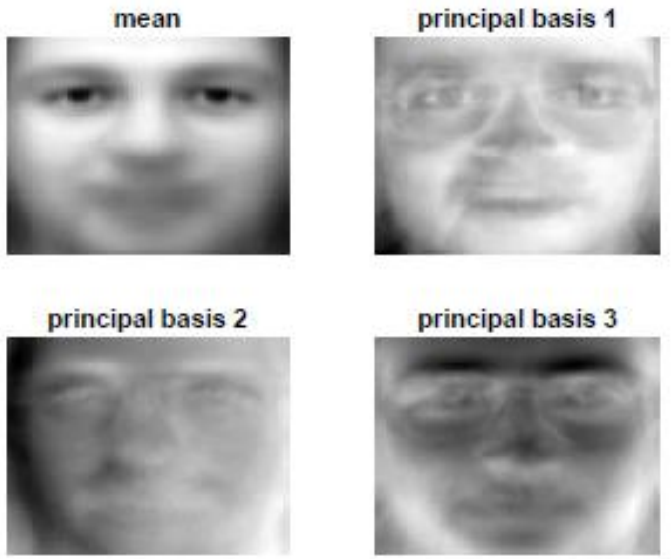
Data lies along a broad curve in the projected space, which appears to trace the orientation of the digit.

As we move up the plot, we find **ones** that have hats and/or bases, though these are very sparse within the dataset.

The projection lets us identify outliers that have data issues

Interpreting the data (3)

(a)



(b)

We see that the main modes of variation in the data are related to overall lighting, and then differences in the eyebrow region of the face.

Alternatives to compute Low Rank Approximations

- Let A be an mxn matrix of low numerical rank
- Suppose that you can't afford to compute the full SVD or you don't have a good implementation
- How can you compute a low-rank approximation to A?
  - Gram-Schmidt: Keep reducing a rank-1 component from A
    - Complexity: O(mnk)
  - Krylov Methods: Restrict the matrix A to the k-dimensional "Krylov subspace"
    - Span $(r, Ar, A^2r, \ldots, A^{k-1}r)$
    - Compute eigen-decomposition of resulting matrix

(1) **for** $k = 1, 2, 3, \ldots$

(2) Let i denote the index of the largest column of $\mathbf{A}$.

(3) Set $\mathbf{q}_k = \dfrac{\mathbf{A}(:,i)}{\|\mathbf{A}(:,i)\|}$.

(4) $\mathbf{A} = \mathbf{A} - \mathbf{q}_k(\mathbf{q}_k^* \mathbf{A})$ or $A = A - q_k(q_k^T A)$

(5) **if** $\|\mathbf{A}\| \leq \varepsilon$ **then break**

(6) **end while**

(7) $\mathbf{Q} = [\mathbf{q}_1\ \mathbf{q}_2\ \ldots \mathbf{q}_k]$.

Each of these approximations result in a factorization of the form

$$A \approx Q\ Q^T A$$

Where Q is an approximate orthonormal basis for the column space of A

Randomized Low Rank Approximations

Range Finding (Basis) Problem: Given an m x n matrix A and an integer k < min(m,n). Find an orthonormal m x k matrix Q such that $A \approx Q\,Q^T A$

Solving the primitive problem via randomized sampling — intuition:

1. Draw Gaussian random vectors $g_1, g_2, \ldots, g_k \in R^n$
2. Form "sample" vectors $y_1 = Ag_1, y_2 = Ag_2, \ldots, y_k = Ag_k \in R^m$
3. Form orthonormal vectors $q_1, q_2, \ldots, q_k \in R^m$ such that

   Span$(q_1, q_2, \ldots, q_k)$ = Span$(y_1, y_2, \ldots, y_k)$

   For instance, Gram-Schmidt can be used — pivoting is rarely required.

If A has exact rank k, then Span$\{q_j\}_{j=1}^{k}$ = Range(A) with probability 1.

Randomized SVD

- **Goal:** Given an *m x n* matrix **A**, compute an approximate rank-*k* SVD $\boxed{A \approx U\Sigma V^T}$
- **Algorithm:**
- 1. Draw an *n x k* Gaussian random matrix **G**. G = randn(n,k)
- 2. Form the *m x k* sample matrix **Y = AG** Y = A * G
- 3. Form an *m x k* orthonormal matrix **Q** such that **Y = QR** [Q, ~] = qr(Y)
- 4. Form the *k x n* matrix **B** = $Q^T A$ B = Q' * A
- 5. Compute the SVD of the small matrix **B**: **B** = $\widehat{U}\Sigma V^T$ [Uhat, Sigma, V] = svd(B,0)
- 6. Form the matrix **U** = $Q\widehat{U}$ U = Q * Uhat
- **Power iteration to improve the accuracy:** The computed factorization is close to optimally accurate when the singular values of **A** decay rapidly. When they do not, a small amount of power iteration should be incorporated, i.e. replace Step 2 by **Y =** $\left(AA^T\right)^t$**AG** for a small integer *t*, say *t* = 1 or *t* = 2.

Randomized Embeddings: "Fast" JL Transforms

- So far, the only randomized embedding we have described takes the form

$$\boxed{f: R^D \rightarrow R^k : x \rightarrow \frac{1}{\sqrt{k}} Gx}$$

where **G** is a matrix drawn from a Gaussian distribution. Evaluating $f(\mathbf{x})$ costs $O(nk)$.

- The cost can be reduced to $O(n \log k)$ or even less, by using *structured* random maps.
  - Subsampled Fourier transforms. (Or Hadamard transform / cosine transform / . . .)
  - Sparse random embeddings — pick matrix that consists mostly of zeros.
  - Chains of random Givens' rotations.