Basic Numerical Optimization

Note: the slides are based on EE263 at Stanford. Reorganized, revised, and typed by Hao Su

Outline

- Least-squares
  - least-squares (approximate) solution of overdetermined equations
  - least-norm solution of underdetermined equations
  - unified solution form by SVD
- Low-rank Approximation
  - eigenface problem
  - principal component analysis

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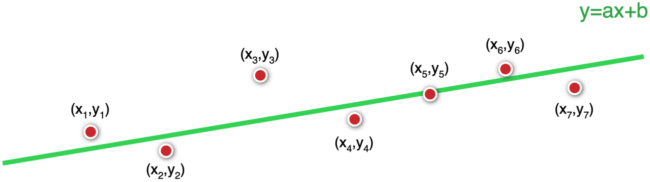
Example Application: Line Fitting



- Given $\{(x_i, y_i)\}$, find line through them.
  i.e., find a and b in $y = ax + b$
- Using matrix and vectors, we look for a and b such that

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \approx \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

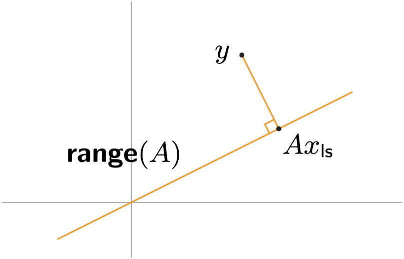
Overdetermined Linear Equations

- consider $y = Ax$ where $A \in \mathbb{R}^{m \times n}$ is (strictly) skinny, i.e., $m > n$
  - called *overdetermined* set of linear equations (more equations than unknowns)
  - for most y, cannot solve for x
- one approach to *approximately* solve $y = Ax$:
  - define *residual* or error $r = Ax - y$
  - find $x = x_{ls}$ that minimize $\|r\|$
- x_{ls} called *least-squares* (approximate) solution of $y = Ax$

Geometric Interpretation

Given $y \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ to minimize $\|Ax - y\|$

Ax_{ls} is point in **range**(A) closest to y (Ax_{ls} is *projection* of y onto **range**(A))



Least-squares (approximate) Solution

- assume A is full rank, skinny
- to find x_{ls}, we'll minimize norm of residual squared,

$$\|r\|^2 = x^T A^T A x - 2y^T A x + y^T y$$

- set gradient w.r.t. x to zero:

$$\nabla_x \|r\|^2 = 2A^T A x - 2A^T y = 0$$

- yields the *normal equation*: $A^T A x = A^T y$
- assumptions imply $A^T A$ invertible, so we have

$$x_{ls} = (A^T A)^{-1} A^T y$$

...a very famous formula

Least-squares (approximate) Solution

- x_{ls} is linear function of y
- $x_{ls} = A^{-1}y$ if A is square
- x_{ls} solves $y = Ax_{ls}$ if $y \in \textbf{range}(A)$

Least-squares (approximate) Solution

for A skinny and full rank, the *pseudo-inverse* of A is

$$A^\dagger = (A^T A)^{-1} A^T$$

- for A skinny and full rank, $A^\dagger$ is a *left inverse* of A

$$A^\dagger A = (A^T A)^{-1} A^T A = I$$

- if A is not skinny and full rank then $A^\dagger$ has a different definition

Underdetermined Linear Equations

- consider $y = Ax$ where $A \in \mathbb{R}^{m \times n}$ is (strictly) fat, i.e., $m < n$
  - called *underdetermined* set of linear equations
    (more unknowns than equations)
  - the solution may not be unique
- we find a specific solution to $y = Ax$ and the null space of A:

$$\begin{array}{rl} \underset{x}{\text{minimize}} & \frac{1}{2}\|x\|^2 \\ \text{s.t.} & y = Ax \end{array}$$

- this is called the least-norm solution

Least-norm Solution

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \frac{1}{2}\|x\|^2 \\ \text{s.t.} \quad & y = Ax \end{aligned}$$

- assume A is full (row-)rank, fat
- we use Lagrangian multiplier method to solve x:

$$\begin{aligned} L(x, \lambda) &= \frac{1}{2}\|x\|^2 - \lambda^T(y - Ax) \\ \nabla_x L(x, \lambda) &= x - A^T\lambda \end{aligned}$$

Set $\nabla_x L(x, \lambda) = 0$, we have $x = A^T\lambda$, so $y = Ax = AA^T\lambda$
Note that A is fat and full rank, so AA^T invertible
So, $\lambda = (AA^T)^{-1}y$ By $x = A^T\lambda$, we have

$$x = A^T(AA^T)^{-1}y$$

Least-norm Solution

for A fat and full rank, the *pseudo-inverse* of A is

$$A^{\dagger} = A^T(AA^T)^{-1}$$

- for A fat and full rank, $A^{\dagger}$ is a *right inverse* of A

$$AA^{\dagger} = AA^T(AA^T)^{-1} = I$$

Unifying least-square and least-norm solutions by SVD

Let the SVD decomposition of A be $A = U\Sigma V^T$ (the economic form of Σ that all the diagonals are non-zero).

- For skinny matrix, the least-square solution: $x = (A^T A)^{-1} A^T y = V\Sigma^{-1} U^T y$
- For fat matrix, the least-norm solution: $x = A^T (AA^T)^{-1} y = V\Sigma^{-1} U^T y$

Solution to linear equation system $y = Ax$

$$x = V\Sigma^{-1} U^T y$$

Note:

- For least-norm solution, $x = V\Sigma^{-1} U^T y$ is a special solution
- Ex: how to obtain all the solutions? (Hint: the null space of U^T)

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Example Application: Face Retrieval

Suppose you have *10 million* face images,
Question:

- How can you find the 5 faces closest to a query (maybe yours!) in just 0.1 sec?
- How can you show all of them in a single picture?

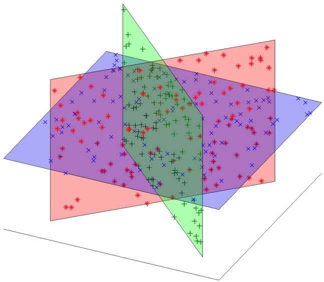
Example Application: Face Retrieval

Suppose you have *10 million* face images,
Question:

- How can you find the 5 faces closest to a query (maybe yours!) in just 0.1 sec?
- How can you show all of them in a single picture?
- *SVD can help you do it!*

Data as Points in a Euclidean Space

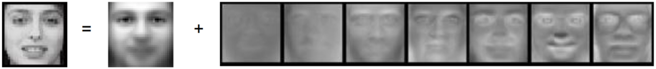
- While data can be represented as high-dimensional vectors
- *Lower-dimensional structure* is often present in data



The Space of All Face Images

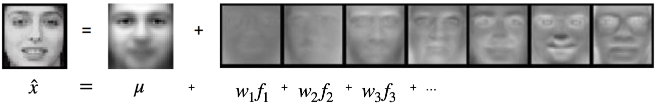
- When viewed as vectors of pixel values, face images are extremely high-dimensional
  - 100×100 image$=10,000$ dims
  - Slow and lots of storage is needed
- But very few $10,000$-dimensional vectors are valid face images
- We want to *effectively* model the subspace of face images

Low-Dimensional Face Space



$$\hat{x} = \mu + w_1 f_1 + w_2 f_2 + w_3 f_3 + \cdots$$

Reconstruction Formulation



- Data matrix of face images: $X = \begin{bmatrix} x_1^T \\ x_2^T \\ \dots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times m}$, each row is a face image
- Orthonormal basis of the face subspace: $F = \begin{bmatrix} f_1^T \\ f_2^T \\ \dots \\ f_r^T \end{bmatrix} \in \mathbb{R}^{r \times m}, r << m$
- Face coordinates: $W = \begin{bmatrix} w_1^T \\ w_2^T \\ \dots \\ w_n^T \end{bmatrix} \in \mathbb{R}^{n \times r}$
- Reconstruction: $\hat{X} = WF + \mu$, where $\mu \in \mathbb{R}^{n \times m}$ replicates the mean face vector at each row.

Optimization Formulation of Face Subspace Learning

- Frobenius norm of a matrix: $\|X\|_F = \sqrt{\sum_{ij} x_{ij}^2}$
- We use $\|\cdot\|_F$ to measure $X \approx \hat{X}$:

$$\|X - \hat{X}\|_F^2 = \|X - (WF + \mu)\|_F^2 = \|(X - \mu) - WF\|_F^2$$

- Let $D = X - \mu$, we have an optimization problem:

$$\underset{W\in\mathbb{R}^{n\times r}, F\in\mathbb{R}^{r\times m}}{\text{minimize}} \quad \|D - WF\|_F^2$$

- We do not know how to obtain the global minimum of the above problem (non-convex); however, we can solve the following equivalent problem:

$$\begin{aligned} \underset{\hat{D}}{\text{minimize}} \quad & \|D - \hat{D}\|_F^2 \\ \text{s.t.} \quad & \text{rank}(\hat{D}) \leq r \end{aligned}$$

Low-rank Approximation Theorem

$$\begin{aligned} \underset{\hat{D}}{\text{minimize}} \quad & \|D - \hat{D}\|_F^2 \\ \text{s.t.} \quad & \text{rank}(\hat{D}) \leq r \end{aligned}$$

- Let $D = U\Sigma V^T \in \mathbb{R}^{n\times m}$, $n \geq m$ be the singular value decomposition of D and partition U, Σ, and V as follows:

$$U = [U_1 \;\; U_2], \Sigma = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix}, V = [V_1, V_2],$$

  where $U_1 \in \mathbb{R}^{m\times r}$, $\Sigma_1 \in \mathbb{R}^{r\times r}$, and $V_1 \in \mathbb{R}^{n\times r}$.
- Then the solution is

$$\hat{D} = U_1 \Sigma_1 V_1^T$$

SVD for the eigenface problem

Let $W = U_1 \Sigma_1$ and $F = V_1^T$

This is a general dimension reduction technique!

Principal Component Analysis (SVD version)

Goal: Find r-dim projection that best preserves data

1. Compute mean vector μ
2. Subtract μ from data matrix
3. SVD and select top r right-singular vectors
4. Project points onto the subspace spanned by them

Reconstruction Results for Faces

- after computing eigenfaces using 400 face images from ORL face database

Homework: PCA for 2D plane detection in 3D point cloud

Review: Three Optimization Problems We Learned Today

Least-square (overdetermined)

$$\underset{x}{\text{minimize}} \quad \|Ax - y\|^2 \tag{1}$$

Least-square (underdetermined)

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \|x\|^2 \\ \text{s.t.} \quad & Ax = y \end{aligned} \tag{2}$$

Low-rank Approximation (underdetermined)

$$\begin{aligned} \underset{\hat{D}}{\text{minimize}} \quad & \|D - \hat{D}\|_F^2 \\ \text{s.t.} \quad & \text{rank}(\hat{D}) \leq r \end{aligned} \tag{3}$$

Gradient Descent

Least-square (overdetermined)

$$\underset{x}{\text{minimize}} \quad \|Ax - y\|^2 \tag{4}$$

Closed form solution: $x = A^{\dagger} y$

We can also use *gradient descent* to optimize the problem:

$$x_n = x_{n-1} - \alpha \nabla f(x_{n-1})$$

Congrats!

You have done the warm-up job for analyzing pictures!

Appendix: Principal Component Analysis (Covariance Version)

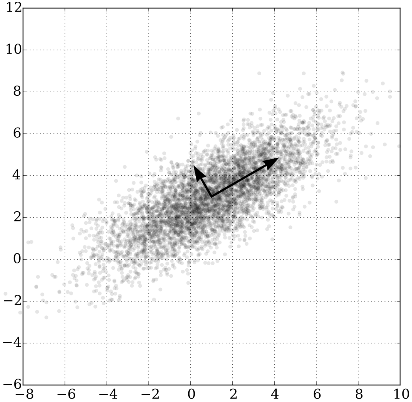
Goal: Find r-dim projection that best preserves data

1. Compute mean vector μ
2. Subtract μ from data matrix: $D = X - \begin{bmatrix} \mu^T \\ \vdots \\ \mu^T \end{bmatrix}$
3. Build co-variance matrix $C = \frac{1}{n-1} D^T D$
4. Eigen decompositon of C and select top r eigenvectors
5. Project points onto the subspace spanned by them.

Appendix: Statistical Interpretation of PCA

- Commonly used for dimension reduction
- Project each data point onto only the first few principal components to obtain lower-dimensional data while *preserving as much of the data's variation* as possible
- The first principal component can equivalently be defined as a direction that maximizes the variance of the projected data
- The i^{th} principal component can be taken as a direction orthogonal to the first $i - 1$ principal components that maximizes the variance of the projected data

Appendix: Visualization of PCA



PCA of a multivariate Gaussian distribution centered at $(1, 3)$ with a standard deviation of 3 in roughly the $(0.866, 0.5)$ direction and of 1 in the orthogonal direction. The vectors shown are the eigenvectors of the covariance matrix scaled by the square root of the corresponding eigenvalue, and shifted so their tails are at the mean.