Basic Numerical Optimization

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

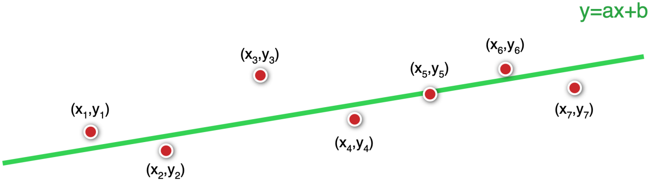
Outline

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

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

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

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

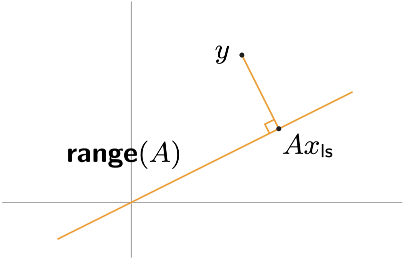
Overdetermined Linear Equations

- 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 $\mathbf{range}(A)$ closest to y (Ax_{ls} is *projection* of y onto $\mathbf{range}(A)$)



Least-squares (approximate) Solution

- assume A is full rank, skinny

llrll^2=llAx-yll^2=(Ax-y)^T(Ax-y)

- 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:

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

- this is called the least-norm solution

Least-norm Solution

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

||x||^2=x^T x=x^T I x
g=2x

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

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

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

A=US(V^T)
U: m x m
S: m x m
V^T: m x n

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

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

0=Az
x is a solution to y=Ax
x+z is also a solution

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

Solution to linear equation system $y = Ax$

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

Note:

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

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

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?

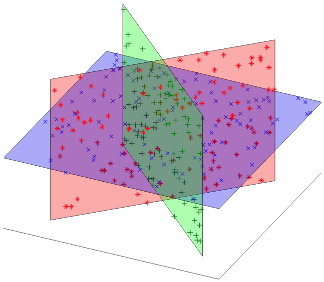
Example Application: Face Retrieval

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

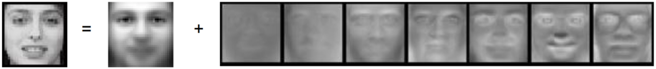
- While data can be represented as high-dimensional vectors
- *Lower-dimensional structure* is often present in data



The Space of All Face Images

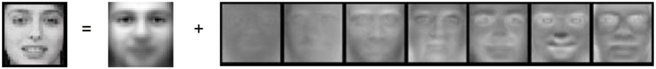
- When viewed as vectors of pixel values, face images are extremely high-dimensional
  - 100×100 image$=10,000$ dims
  - Slow and lots of storage is needed
- But very few $10,000$-dimensional vectors are valid face images
- We want to *effectively* model the subspace of face images

Low-Dimensional Face Space



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

Reconstruction Formulation



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

nimg x 10000

- 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: $F = \begin{bmatrix} f_1^T \\ f_2^T \\ \dots \\ f_r^T \end{bmatrix} \in \mathbb{R}^{r \times m}, r << m$

7 x 10000

- Face coordinates: $W = \begin{bmatrix} w_1^T \\ w_2^T \\ \dots \\ w_n^T \end{bmatrix} \in \mathbb{R}^{n \times r}$

nimg x 7

- 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

D=USV^T=[u_1, u_2, ..., u_n] S [v_1\\ v_2\\... v_n]
=\sum_{i=1}^n (sigma_i) (u_i) (v_i^T)
~\sum_{i=1}^r (sigma_i) (u_i) (v_i^T)

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

- 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

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

Principal Component Analysis

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

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

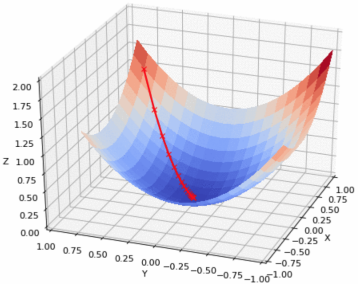
Least-square (overdetermined)

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

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!