# 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

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- Least-squares
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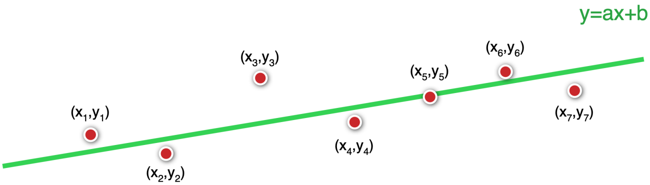
# Example Application: Line Fitting




- 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

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

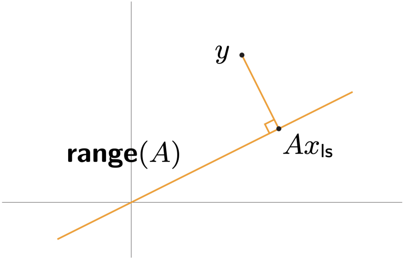
# Overdetermined Linear Equations

- 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 $\Sigma$ 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?

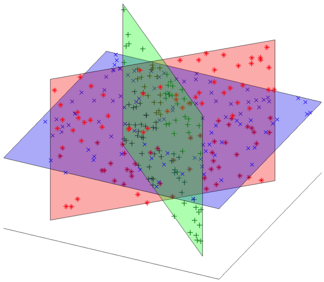
# Example Application: Face Retrieval

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

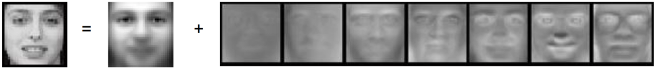
- While data can be represented as high-dimensional vectors
- *Lower-dimensional structure* is often present in data



# The Space of All Face Images

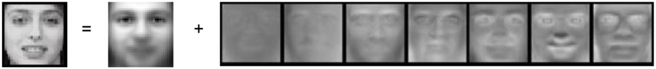
- When viewed as vectors of pixel values, face images are extremely high-dimensional
  - $100 \times 100$ image$=10,000$ dims
  - Slow and lots of storage is needed
- But very few $10,000$-dimensional vectors are valid face images
- We want to *effectively* model the subspace of face images

# Low-Dimensional Face Space



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

## Reconstruction Formulation



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

- 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:

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

# Low-rank Approximation Theorem

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

- Let $D = U \Sigma V^T \in \mathbb{R}^{n \times m}$, $n \geq m$ be the singular value decomposition of $D$ and partition $U$, $\Sigma$, 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 $\mu$
2. Subtract $\mu$ 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

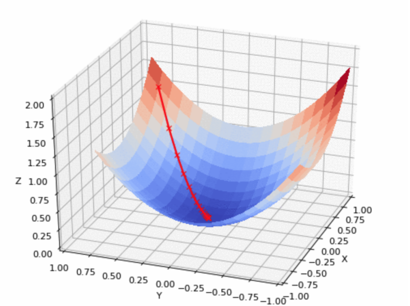
## Least-square (overdetermined)

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

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!