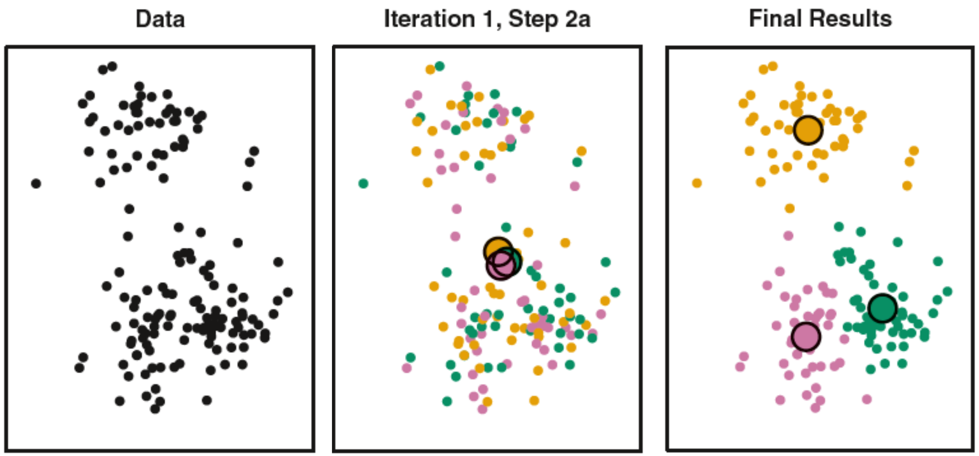
# Topics on Machine Learning

ECE 301 Linear Systems

# Machine Learning: An Overview

(James, Witten, Hastie, & Tibshirani, 2013)




- Unsupervised learning:
  - Learns from a set of unlabeled data to discover patterns, without human supervision.
  - We'll cover principal component analysis (PCA).
- Supervised learning:
  - Learns an input–output mapping based on labeled data.
  - We'll cover linear regression and neural networks.


(Li and Russakovsky, 2013)

# Machine Learning Topics and Learning Objectives

- Topic 1: Linear algebra
  - Explain linear algebra concepts such as linear independence, vector space, and orthogonal basis
  - Conduct eigendecomposition for symmetric matrices using Matlab
- Topic 2: Principal component analysis (unsupervised learning)
  - Explain the two equivalent goals of PCA
  - Implement the PCA algorithm and visualize the results
- Topic 3: Linear regression and prediction (supervised learning)
  - Interpret regression problem mathematically and geometrically
  - Apply linear regression to learning problems without overfit
- Topic 4: Convolutional neural network (CNN)
  - Describe the structure of CNN
  - Build and train simple CNNs using a deep learning package

# Linear Algebra

## Learning objectives

- Explain linear algebra concepts such as linear independence, vector space, and orthogonal basis
- Conduct eigendecomposition for symmetric matrices using Matlab

(Refer to ECE 220's textbook for a review on vector and matrix. A comprehensive treatment of linear algebra can be found in Scheffe's appendices, available on the library's course reserves.)

# Linear Algebra Review: Vector

- Vector: an <u>ordered</u> $n$-tuple.

  Row vector: $\mathbf{x} = \begin{bmatrix} x_1, & x_2, & \ldots, & x_n \end{bmatrix}$

  Column vector: $\mathbf{x} = \begin{bmatrix} x_1, & x_2, & \ldots, & x_n \end{bmatrix}^T$

  (Assume all vectors are column from now on.)

- Vector properties:

  $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$ (commutative)

  $\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z}$ (associative)

  $c\begin{bmatrix} x_1, \ldots, x_n \end{bmatrix} = \begin{bmatrix} cx_1, \ldots, cx_n \end{bmatrix}$ (scaling)

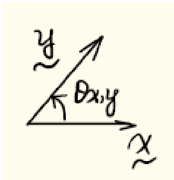
- Norm/length: $\|\mathbf{x}\| = (\mathbf{x}^T\mathbf{x})^{\frac{1}{2}}$, e.g., $\mathbf{x} = \begin{bmatrix} 3, 4 \end{bmatrix}^T$, $\|\mathbf{x}\| = 5$.

# Linear Algebra Review: Vector (cont'd)

- Inner product of $\mathbf{x}$ and $\mathbf{y}$:

$$\mathbf{x}^T\mathbf{y} = [x_1, \cdots, x_n]\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^n x_i y_i = \mathbf{y}^T\mathbf{x}.$$

- $\mathbf{x}^T\mathbf{y} = \|\mathbf{x}\| \cdot \|\mathbf{y}\| \cos\theta_{\mathbf{x},\mathbf{y}}$




Ex: $\mathbf{x} = [1, 0]$, $\mathbf{y} = [1, 1]$

$\cos\theta_{\mathbf{x},\mathbf{y}} = \frac{\mathbf{x}^T\mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|} = \frac{1\cdot 1 + 0\cdot 1}{\sqrt{1^2+0^2}\cdot\sqrt{1^2+1^2}} = \frac{\sqrt{2}}{2}$

$\Rightarrow \theta_{\mathbf{x},\mathbf{y}} = 45^\circ$

- Def: $\mathbf{x}$ and $\mathbf{y}$ are orthogonal if $\mathbf{x}^T\mathbf{y} = 0$.

- Remark: When $\mathbf{x}^T\mathbf{y} = 0$, $\cos^{-1}\left(\frac{0}{\|\mathbf{x}\|\|\mathbf{y}\|}\right) = \frac{\pi}{2}(2k+1)$.

# Linear Algebra Review: Matrix

- Matrix: $\mathbf{A} = [a_{kl}] = \begin{bmatrix} a_{11} & \cdots & a_{1N} \\ a_{21} & \cdots & a_{2N} \\ \vdots & \ddots & \vdots \\ a_{M1} & \cdots & a_{MN} \end{bmatrix} \in \mathbb{R}^{M \times N}$, $M$ rows, $N$ columns.

- Addition: $\mathbf{A} + \mathbf{B} = [a_{kl} + b_{kl}] = \mathbf{B} + \mathbf{A}$

- Scaling: $c\mathbf{A} = [ca_{kl}]$ Ex: $2\begin{bmatrix} 0 & 1 \\ 2 & 3 \end{bmatrix} - \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 1 & 2 \end{bmatrix}$

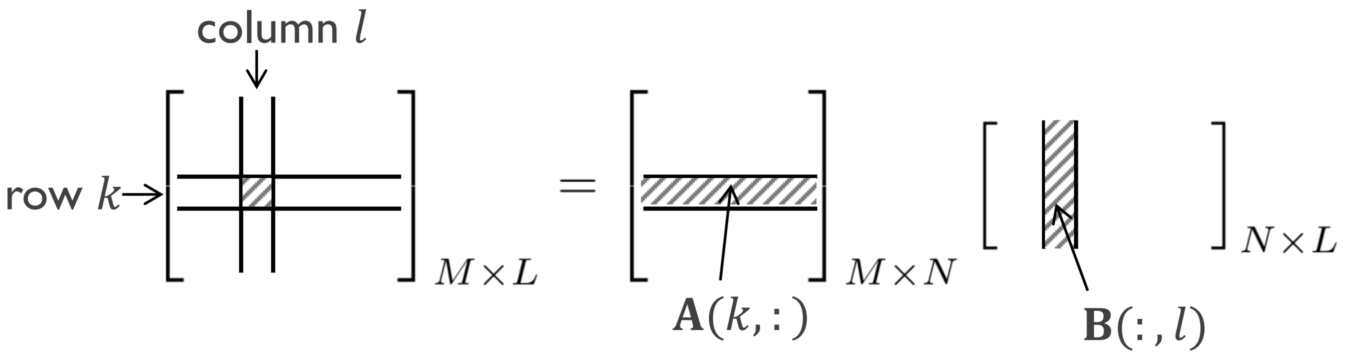
- Transpose "T": $\mathbf{A}^T = [a_{kl}]^T = [a_{lk}]$ Ex: $\begin{bmatrix} 1 & -1 & 1 \\ 2 & 4 & 6 \end{bmatrix}^T = \begin{bmatrix} 1 & 2 \\ -1 & 4 \\ 1 & 6 \end{bmatrix}$

- Special matrices: $\mathbf{0}_{M \times N} = [0]_{M \times N}$, $\mathbb{1}_{M \times N} = [1]_{M \times N}$,

Identity matrix $\mathbf{I}_M = \begin{bmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1 \end{bmatrix} = \text{diag}(\text{ones}(M, 1))$.

# Linear Algebra Review: Matrix (cont'd)

- Matrix Multiplication: $\mathbf{C} = \mathbf{AB}$, where $c_{kl} = \sum_{q=1}^{N} a_{kq} b_{ql} = \mathbf{A}(k,:)\mathbf{B}(:,l)$




Note: In general, $\mathbf{AB} \neq \mathbf{BA}$. Why?

Ex: $\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 3 & 4 \\ 5 & 6 \end{bmatrix} = \begin{bmatrix} 3+5 & 4+6 \\ -3+5 & -4+6 \end{bmatrix} = \begin{bmatrix} 8 & 10 \\ 2 & 2 \end{bmatrix}$

- Def: $\mathbf{A}^{-1} = \mathbf{B}$ if ① $\mathbf{A}$ is square, and ② $\mathbf{AB} = \mathbf{I} = \mathbf{BA}$.

# Linear Algebra Review: Matrix (cont'd)

- For 2-by-2 matrices: $\mathbf{A}^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \frac{1}{\det \mathbf{A}} \begin{bmatrix} a & -c \\ -b & d \end{bmatrix}^T = \frac{1}{ad-bc} \begin{bmatrix} a & -b \\ -c & d \end{bmatrix}$

Ex: $\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$

$$\mathbf{A}^{-1}(\mathbf{A}\mathbf{x}) = \mathbf{A}^{-1}\mathbf{b} \Longrightarrow \mathbf{x} = \mathbf{A}^{-1}\mathbf{b} = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$$

# Motivation: Linear Algebra for Discrete Convolution

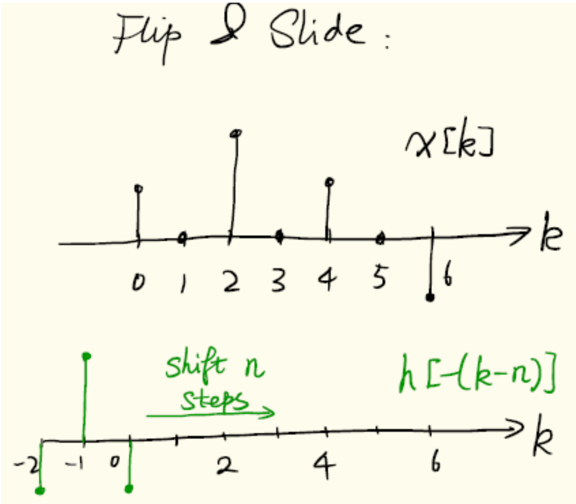
Ex: $x[n] = \{\underset{\uparrow}{1}, 0, 2, 0, 1, 0, -1\}$, $h[n] = \{\underset{\uparrow}{-1}, 2, -1\}$. $y[n] = x[n] * h[n] = ?$

$x[0]$ length = 7 $h[0]$ length = 3 length = ?

Matrix-vector form:

$$\begin{bmatrix} -1 \\ 2 \\ -3 \\ 4 \\ -3 \\ 2 \\ 0 \\ -2 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 & & & \cdots & & & 0 \\ 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ \vdots & & -1 & 2 & -1 & & \vdots \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \\ 0 & & & \cdots & & & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 2 \\ 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}$$

$\mathbf{y} \in \mathbb{R}^9$ $\mathbf{H} \in \mathbb{R}^{9\times 7}$ $\mathbf{x} \in \mathbb{R}^7$



# Linear Independence of a Set of Vectors

- Given $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$. Defs:

$$\alpha_1 \mathbf{v}_1 + \cdots + \alpha_n \mathbf{v}_n = \mathbf{0} \Rightarrow \alpha_i = 0, \forall i$$ (linearly independent)

$$\alpha_1 \mathbf{v}_1 + \cdots + \alpha_n \mathbf{v}_n = \mathbf{0} \Rightarrow \text{not all } \alpha_i = 0$$ (linearly dependent)

- For "linearly dependent" case (when $\alpha_1 \neq 0$ ) , we may write:

$$\mathbf{v}_1 = \beta_2 \mathbf{v}_2 + \cdots + \beta_n \mathbf{v}_n$$

Why?

- Ex: $\mathbf{v}_1 = \begin{bmatrix} 1 & 2 & 1 \end{bmatrix}^T, \; \mathbf{v}_2 = \begin{bmatrix} 1 & 0 & 1 \end{bmatrix}^T.$

$$\alpha_1 \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} + \alpha_2 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \mathbf{0} \quad \Rightarrow \begin{cases} \alpha_1 + \alpha_2 = 0 \\ 2\alpha_1 + 0 = 0 \\ \alpha_1 + \alpha_2 = 0 \end{cases} \Rightarrow \begin{cases} \alpha_1 = 0 \\ \alpha_2 = 0 \end{cases} \Rightarrow \text{linearly independent}$$

# Linear Independence of a Set of Vectors (cont'd)

- Ex: $\mathbf{v}_1 = \begin{bmatrix}1 & 2 & 1\end{bmatrix}^T$, $\mathbf{v}_4 = \begin{bmatrix}-2 & -4 & -2\end{bmatrix}^T$.

$$\mathbf{v}_4 = -2\mathbf{v}_1 \Rightarrow \text{linearly dependent}$$

- Ex: $\mathbf{v}_1 = \begin{bmatrix}1 & 2 & 1\end{bmatrix}^T$, $\mathbf{v}_2 = \begin{bmatrix}1 & 0 & 1\end{bmatrix}^T$, $\mathbf{v}_3 = \begin{bmatrix}0 & 1 & 0\end{bmatrix}^T$.

$$\mathbf{v}_1 = \mathbf{v}_2 + 2\mathbf{v}_3 \Rightarrow \text{linearly dependent}$$

# Vector Space

- Def: Vector space: A set, $V$ of all vectors that are linear combination of $\{\mathbf{v}_i\}_{i=1}^n$ , i.e.,

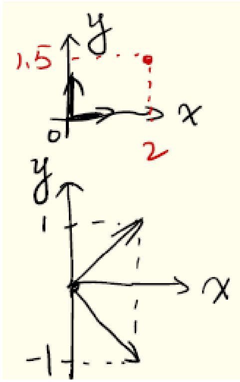
$$\boxed{V = \left\{\mathbf{v} = \sum_{i=1}^{n} \alpha_i \mathbf{v}_i,\ \alpha_i \in \mathbb{R}\right\}.}$$

  $\mathbf{v}_i$'s are said to span the vector space, i.e., $V = \text{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$.

- Ex:

$$V^{(1)} = \left\{\alpha_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \alpha_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix},\ \alpha_i \in \mathbb{R}\right\} = \mathbb{R}^2$$

$$V^{(2)} = \left\{r_1 \begin{bmatrix} 1 \\ 1 \end{bmatrix} + r_2 \begin{bmatrix} 1 \\ -1 \end{bmatrix},\ r_i \in \mathbb{R}\right\} = \mathbb{R}^2$$



# Basis for Vector Space

- Def: A basis for $V$ is a set of linearly independent vectors that span $V$.

- Ex: Q1. What is $V$? Q2. Are vectors linearly independent?

$$\left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right\}$$

$$\left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$$

$$\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$$

$$\left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\}$$

# Basis for Vector Space

- Def: A basis for $V$ is a set of linearly independent vectors that span $V$.
- Ex: Q1. What is $V$? Q2. Are vectors linearly independent?

$$\left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right\}$$ yes

$$\left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$$ yes

$$\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$$ yes

$$\left\{ \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \end{bmatrix} \right\}$$ no

# Dimension of Vector Space

- Def: The dimension of vector space $V$ is the number of vectors in any/a basis for $V$ (or the # of independent vectors in $V$).
- Column/row rank: The dimension of column/row vector space, respectively.
- Ex: What's the column rank of matrix

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 0 \\ 2 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}?$$

It's just another way to ask: what's the dimension of vector space

$$V = \left\{ \mathbf{v} = \alpha_1 \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} + \alpha_2 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \ \alpha_i \in \mathbb{R} \right\}?$$

# Dimension of Vector Space (cont'd)

- Approach 1: By observation, we notice that any (and only) two pairs of vectors spanned $V$ are linearly independent. Hence, we can immediately write out at least three bases:

$$\left\{ \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \right\} \quad \text{or} \quad \left\{ \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\} \quad \text{or} \quad \left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$$

  Hence, the column rank of $\mathbf{X}$ or dimension of vector space $V$ is 2.

- Approach 2: Define the three vectors to be $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, respectively.

$$\begin{aligned} V &= \left\{ \mathbf{v} = \alpha_1(\mathbf{v}_2 + 2\mathbf{v}_3) + \alpha_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 \right\} \\ &= \left\{ \mathbf{v} = (\alpha_1 + \alpha_2)\mathbf{v}_2 + (2\alpha_1 + \alpha_3)\mathbf{v}_3 \right\}. \end{aligned}$$

$\mathbf{v}_2 \perp \mathbf{v}_3 \Rightarrow$ they are linearly independent. So the dim/rank is 2.

# Projection of a Vector on a Unit Vector

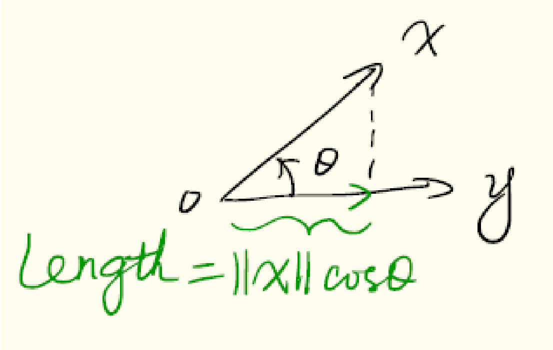
- Project a vector $\mathbf{x}$ on a unit vector $\mathbf{u}$:
  - Projection length is $\mathbf{u}^T\mathbf{x}$. (a number, with sign)
  - Projected vector is $(\mathbf{u}^T\mathbf{x})\mathbf{u}$. (a scaled vector along $\mathbf{u}$)

- Proof (projection length):

$$\mathbf{x}^T\mathbf{y} = \|\mathbf{x}\|\,\|\mathbf{y}\|\cos\theta$$

Divide both sides by $\|\mathbf{y}\|$ and let $\mathbf{u} = \mathbf{y}/\|\mathbf{y}\|$ :

$$\mathbf{x}^T\left(\frac{\mathbf{y}}{\|\mathbf{y}\|}\right) = \|\mathbf{x}\|\cos\theta = \mathbf{u}^T\mathbf{x}.$$



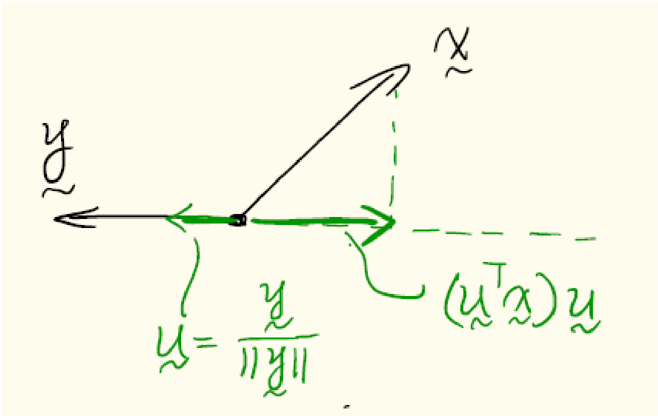
# Projection One Vector on Another

- Project a vector $\mathbf{x}$ on a vector $\mathbf{y}$:
  - Projection length is $\boldsymbol{y}^T\mathbf{x}/||\boldsymbol{y}||$. (a number, with sign)
  - Projected vector is $(\boldsymbol{y}^T\mathbf{x})\boldsymbol{y}/||\boldsymbol{y}||^2$. (a scaled vector along $\mathbf{y}$)

- Proof (projected vector):

$$\text{Projection of } \mathbf{x} \text{ onto } \mathbf{y} = \left(\mathbf{u}^T\mathbf{x}\right)\mathbf{u}$$

Placing $\mathbf{u}$ by $\mathbf{y}/\left\|\mathbf{y}\right\|$, we obtain :



# Projection One Vector on Another

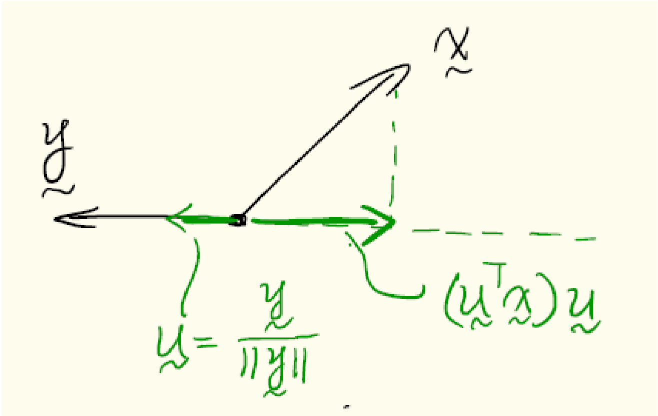
- Project a vector $\mathbf{x}$ on a vector $\mathbf{y}$:
  - Projection length is $\boldsymbol{y}^T\mathbf{x}/||\boldsymbol{y}||$. (a number, with sign)
  - Projected vector is $(\boldsymbol{y}^T\mathbf{x})\boldsymbol{y}/||\boldsymbol{y}||^2$. (a scaled vector along $\mathbf{y}$)

- Proof (projected vector):

$$\text{Projection of } \mathbf{x} \text{ onto } \mathbf{y} = \left(\mathbf{u}^T\mathbf{x}\right)\mathbf{u}$$

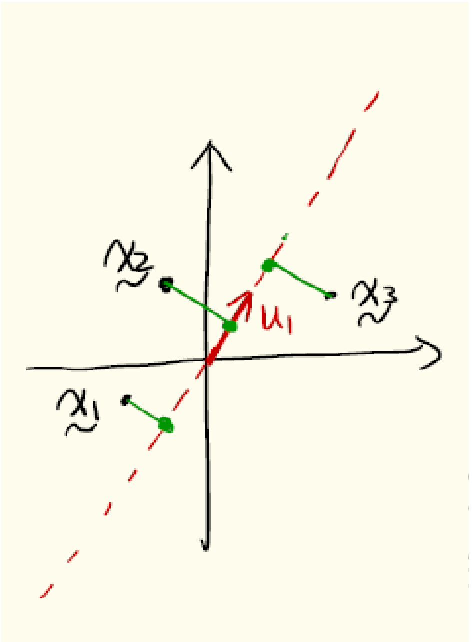
$$\text{Placing } \mathbf{u} \text{ by } \mathbf{y}/\left\|\mathbf{y}\right\|, \text{ we obtain :}$$

$$= \left[\left(\frac{\mathbf{y}}{\|\mathbf{y}\|}\right)^T \mathbf{x}\right]\frac{\mathbf{y}}{\|\mathbf{y}\|} = \left(\mathbf{y}^T\mathbf{x}\right)\mathbf{y}\Big/\left\|\mathbf{y}\right\|^2.$$



# Projection of a Vector on a Unit Vector

- Example:




$$\mathbf{u}_1 = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]^T$$
$$\mathbf{x}_1 = \left[-1, -\tfrac{1}{2}\right]^T$$
$$\mathbf{x}_2 = \left[-\tfrac{1}{2}, 1\right]^T$$
$$\mathbf{x}_3 = [2, 1]^T$$

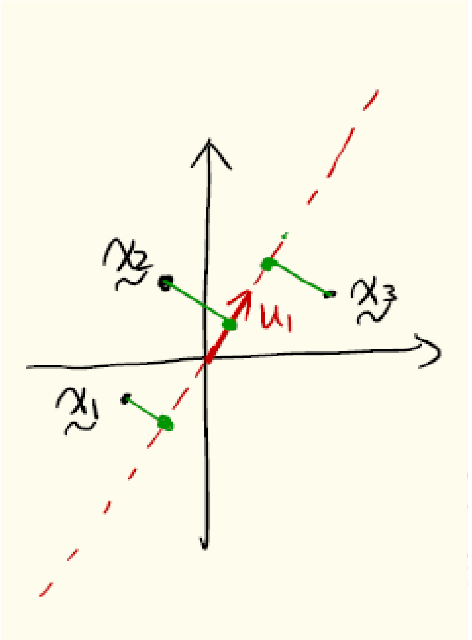
$$z_{11} = \mathbf{x}_1^T \mathbf{u}_1 =$$

$$z_{21} = \mathbf{x}_2^T \mathbf{u}_1 =$$

$$z_{31} = \mathbf{x}_3^T \mathbf{u}_1 =$$

# Projection of a Vector on a Unit Vector

- Example:




$$\mathbf{u}_1 = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]^T$$
$$\mathbf{x}_1 = \left[-1, -\frac{1}{2}\right]^T$$
$$\mathbf{x}_2 = \left[-\frac{1}{2}, 1\right]^T$$
$$\mathbf{x}_3 = [2, 1]^T$$

$$z_{11} = \mathbf{x}_1^T \mathbf{u}_1 = (-1) \cdot \frac{\sqrt{2}}{2} + \left(-\frac{1}{2}\right) \cdot \frac{\sqrt{2}}{2}$$

$$z_{21} = \mathbf{x}_2^T \mathbf{u}_1 = \frac{\sqrt{2}}{4}$$

$$z_{31} = \mathbf{x}_3^T \mathbf{u}_1 = \frac{3}{2}\sqrt{2}$$

# Orthonormal Basis

- Def: A basis $\{\mathbf{a}_1, \dots, \mathbf{a}_r\}$ for $V$ is called orthonormal if $r$ vectors are (i) pairwise orthogonal and (ii) have unit norms.
- Ex: Given a vector space

$$V = \left\{ \mathbf{v} = \alpha_1 \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} + \alpha_2 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \ \alpha_i \in \mathbb{R} \right\}$$

$$\left\{ \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \right\} \qquad \left\{ \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\} \qquad \left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\} \qquad \left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \right\}$$

# Orthonormal Basis

- Def: A basis $\{\mathbf{a}_1, \ldots, \mathbf{a}_r\}$ for $V$ is called orthonormal if $r$ vectors are (i) pairwise orthogonal and (ii) have unit norms.
- Ex: Given a vector space

$$V = \left\{ \mathbf{v} = \alpha_1 \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} + \alpha_2 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + \alpha_3 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \ \alpha_i \in \mathbb{R} \right\}$$

$$\left\{ \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \right\}$$

Basis
Not orthogonal
Not unit vectors

$$\left\{ \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$$

Basis
Not orthogonal
Not unit vectors

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$$

Basis w/ orthogonal vectors.
Can normalize $[1 \ 0 \ 1]^T$ to obtain an orthonormal basis.

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \right\}$$

Not even a basis.
Why???

# Orthogonal Matrix (or Orthonormal Matrix)

- Def: A square matrix $\mathbf{P}$ is orthogonal if and only if its columns (or rows) constitute an orthonormal basis.
- Properties:
  - $\mathbf{P}^{\mathrm{T}}\mathbf{P} = \mathbf{P}\mathbf{P}^{\mathrm{T}} = \mathbf{I}$
  - $\mathbf{P}^{-1} = \mathbf{P}^{\mathrm{T}}$
- Ex:

$$\mathbf{P} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \end{bmatrix} = \begin{bmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} \quad \mathbf{P}^{\mathbf{T}} = \begin{bmatrix} \mathbf{v}_1^T \\ \mathbf{v}_2^T \\ \mathbf{v}_3^T \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{bmatrix}$$

$$\mathbf{P}\mathbf{P}^T = \begin{bmatrix} 0 + \left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}}\right)^2 & 0 & \frac{1}{2} - \frac{1}{2} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mathbf{I}$$

(Direct evaluation)

$$\mathbf{P}^T\mathbf{P} = \begin{bmatrix} \mathbf{v}_1^T \\ \hline \mathbf{v}_2^T \\ \hline \mathbf{v}_3^T \end{bmatrix} \left[\begin{array}{c|c|c} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 \end{array}\right] = \begin{bmatrix} \mathbf{v}_1^T\mathbf{v}_1 & 0 & 0 \\ 0 & \mathbf{v}_2^T\mathbf{v}_2 & 0 \\ 0 & 0 & \mathbf{v}_3^T\mathbf{v}_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mathbf{I}$$

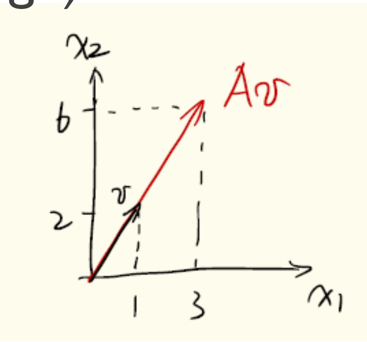
(Block trick)

# Eigenvector and Eigenvalue

- Def: Let $\mathbf{A}$ be an $n$-by-$n$ matrix. A nonzero vector $\mathbf{v}$ is called an eigenvector of $\mathbf{A}$ if $\mathbf{Av} = \lambda\mathbf{v}$. Here, $\lambda$ is called an eigenvalue of $\mathbf{A}$, and $\mathbf{v}$ is eigenvector corresponding to eigenvalue $\lambda$.
- Prefix "eigen" means "characteristic."
- The characteristic is of $\mathbf{A}$, not of $\mathbf{v}$.
- Physical interpretation: $\mathbf{v}$ is invariant to operator $\mathbf{A}$, which means that $\mathbf{A}$ acts on $\mathbf{v}$ can only change its length (and sign) but not orientation.
- Ex: Let $\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 8 & -1 \end{bmatrix}$, $\mathbf{v} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

  Since $\mathbf{Av} = \begin{bmatrix} 3 \cdot 1 + 0 \cdot 2 \\ 8 \cdot 1 - 1 \cdot 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \end{bmatrix} = 3\mathbf{v}$,

  the eigenvalue $\lambda = 3$.



# Eigendecomposition for Symmetric Matrices

- Def: A square matrix $\mathbf{A}$ is symmetric if $\mathbf{A} = \mathbf{A}^T$.
- Thm: A $p$-by-$p$ symmetric matrix $\mathbf{R}$ can be diagonalized by an orthogonal matrix $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_p]$. The following statements are equivalent:

**1.** $\mathbf{R} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$

$$= \left[\begin{array}{c:c:c} \mathbf{v}_1 & \cdots & \mathbf{v}_p \end{array}\right] \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_p \end{bmatrix} \left[\begin{array}{c} \mathbf{v}_1^T \\ \hdashline \vdots \\ \hdashline \mathbf{v}_p^T \end{array}\right]$$

$$= [\lambda_1 \mathbf{v}_1 \cdots \lambda_p \mathbf{v}_p] \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_p^T \end{bmatrix}$$

$$= \sum_{i=1}^{p} \lambda_i \mathbf{v}_i \mathbf{v}_i^T$$

**2.** $\mathbf{R}\mathbf{V} = \mathbf{V}\mathbf{\Lambda} = [\mathbf{v}_1 \cdots \mathbf{v}_p] \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_p \end{bmatrix}$

**3.** $\mathbf{R}\mathbf{v}_i = \lambda_i \mathbf{v}_i, \quad i = 1, \dots, p.$

# Eigendecomposition Using Matlab

- Ex: Use Matlab to decompose matrix $\mathbf{R} = \begin{bmatrix} 1 & 4 & 5 \\ 4 & -3 & 0 \\ 5 & 0 & 7 \end{bmatrix}$
- Source code:

```
R = [1 4 5; 4 -3 0; 5 0 7];
[V, Lambda] = eig(R);  % use built-in function for eigendecomposition

for j = 1 : size(Lambda, 1)
  if norm(R * V(:, j) - Lambda(j, j) * V(:, j)) < 1e-5  % verify result
    disp(['Eigenvector-value pair ' int2str(j) ' verified.'])
  end
end
```

Can you numerically verify the 3 equivalent expressions on the previous slide?

- Output:

```
V =
    0.5952    0.6072    0.5263
   -0.7707    0.6167    0.1601
   -0.2274   -0.5009    0.8351
```

```
Lambda =
   -6.0892         0         0
         0    0.9383         0
         0         0   10.1509
```

# Eigendecomposition by Hand (optional)

- Thm: Eigenvalues are roots of the *characteristic polynomial* $\det(\mathbf{A} - \lambda\mathbf{I})$.
- Ex: $\mathbf{A} = \begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix}$

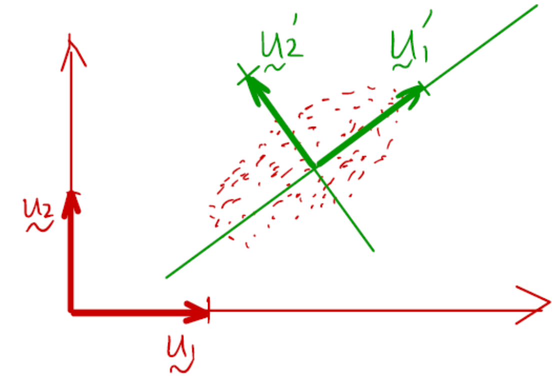
$$0 = \det\left(\begin{bmatrix} 5 & 4 \\ 1 & 2 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) = \det\left(\begin{bmatrix} 5-\lambda & 4 \\ 1 & 2-\lambda \end{bmatrix}\right)$$
$$= \lambda^2 - 7\lambda + 6 \Rightarrow \lambda_1 = 6,\ \lambda_2 = 1.$$

$$\text{For } \lambda_1 = 6, \quad (\mathbf{A} - \lambda_1\mathbf{I})\,\mathbf{v} = 0 \Leftrightarrow \begin{cases} -v_1 + 4v_2 = 0 \\ v_1 - 4v_2 = 0 \end{cases} \Rightarrow \mathbf{v} = \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

Nonunique solutions for underdetermined systems

$$\text{For } \lambda_2 = 1, \quad (\mathbf{A} - \lambda_2\mathbf{I})\,\mathbf{v} = 0 \Leftrightarrow \begin{cases} 4v_1 + 4v_2 = 0 \\ v_1 + v_2 = 0 \end{cases} \Rightarrow \mathbf{v} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

# Principal Component Analysis (Unsupervised Learning)



## Learning objectives

- Explain the two equivalent goals of PCA
- Implement the PCA algorithm and visualize the results

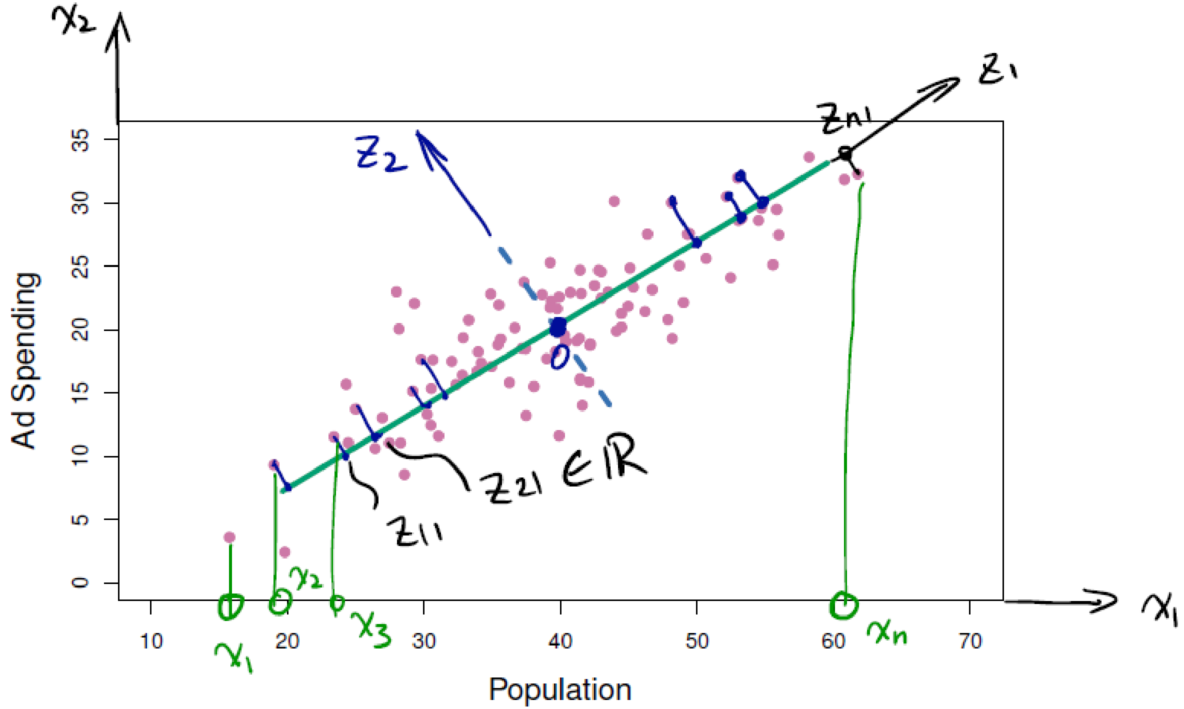
(Ref: 10.2 of James et al. 2013, 12.2 of Murphy 2012. Extra ref: 12.1 of Bishop 2006.)

# Unsupervised Learning

- Def: Learns from a set of unlabeled data to discover interesting patterns.
  - Visualize the data in an informative way.
  - Discover subgroups among observations/variables.
- Examples:
  - Movies grouped by ratings and behavioral data from viewers.
  - Groups of shoppers characterized by browsing & purchasing histories.
  - Subgroups of breast cancer patients grouped by gene expressions.
  - Tweets grouped by latent topics inferred from the use of words.

# PCA: Two Equivalent Goals

- Goals, i.e., cost/loss/objective functions, of PCA: (1) maximize variance, and (2) minimize error.




(James, Witten, Hastie, & Tibshirani, 2013)

# PCA Objective 1: Maximizing Variance

- Maximize variance: Project data onto a lower-dimensional subspace while maximizing the variance of the projected data.

- Details:

| | |
|---|---|
| $\{\mathbf{x}_i\}_{i=1}^n, \quad \mathbf{x}_i \in \mathbb{R}^p$ | A dataset of $n$ data points |
| $\mathbf{u}_1 \;:\; \|\mathbf{u}_1\|^2 = 1$ | Unit vector / direction $\mathbf{u}_1$ (to figure out!) |
| $z_{i1} = \mathbf{u}_1^T \mathbf{x}_i$ | Projection of $\mathbf{x}_i$ along $\mathbf{u}_1$ |

- Naming:
  - $z_{i1}$—score, coefficient, transformed coefficient, weight, projected values, …
  - $\mathbf{u}_1$—loading, (1st) principal component vector, …

$$\text{Spread} = \frac{1}{n-1}\sum_{i=1}^{n}\left(z_{i1} - \overline{z_1}\right)^2 \quad :$$

where $\overline{z_1} \stackrel{\text{def}}{=} \frac{1}{n}\sum_{i=1}^{n} z_{i1}$ is the *sample mean*.

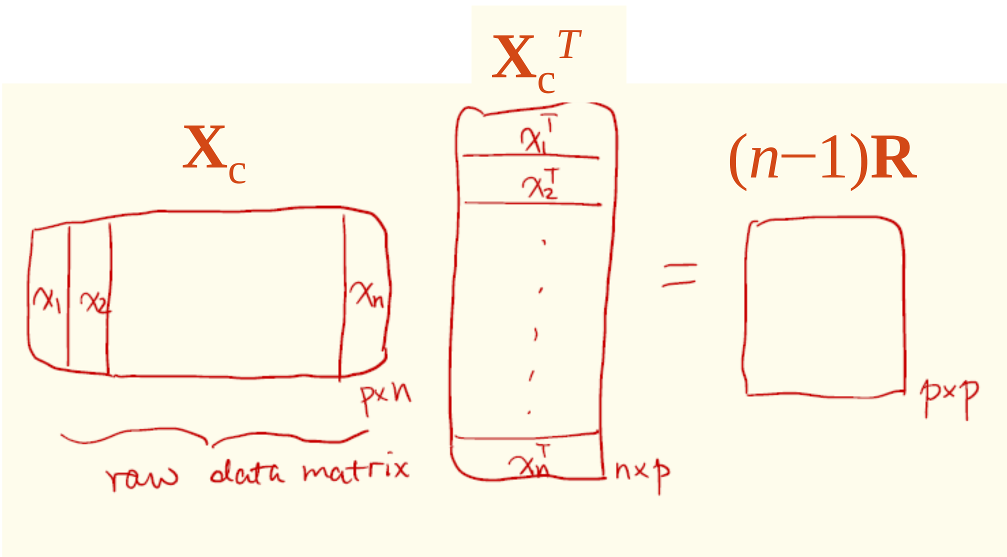
*Sample variance* measures spread of the projected data along $\mathbf{u}_1$.

$$= \frac{1}{n-1}\sum_{i=1}^{n}\left(\mathbf{u}_1^T\mathbf{x}_i - \mathbf{u}_1^T\bar{\mathbf{x}}\right)^2$$

$$= \frac{1}{n-1}\sum_{i=1}^{n}\mathbf{u}_1^T\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)^T\mathbf{u}_1$$

$$= \mathbf{u}_1^T \underbrace{\left[\frac{1}{n-1}\sum_{i=1}^{n}\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)^T\right]}_{\mathbf{R},\ \text{sample covariance}}\mathbf{u}_1$$

Matrix form for calculating $\mathbf{R}$:

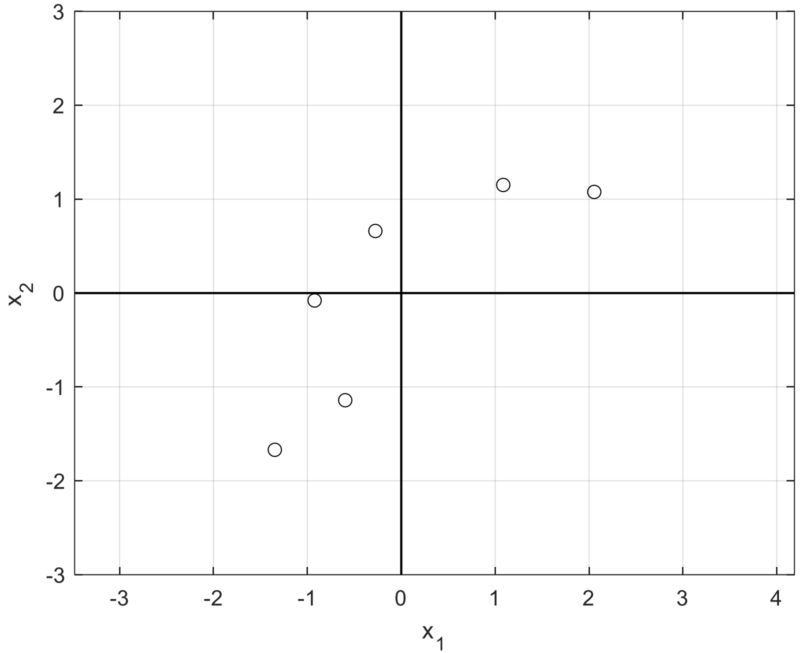



(Assuming all $\mathbf{x}_i$ are already "centered," i.e., $\mathbf{x}_i \leftarrow \mathbf{x}_i - \bar{\mathbf{x}},\ \forall i$.)

# Source code:

```
plot(X_c(1, :), X_c(2, :), 'ko');
xlabel('x_1'); ylabel('x_2');
axis([-3 3 -3 3]); axis equal;
hold on;

R = (X_c * X_c') / (n-1);
```




# Output:

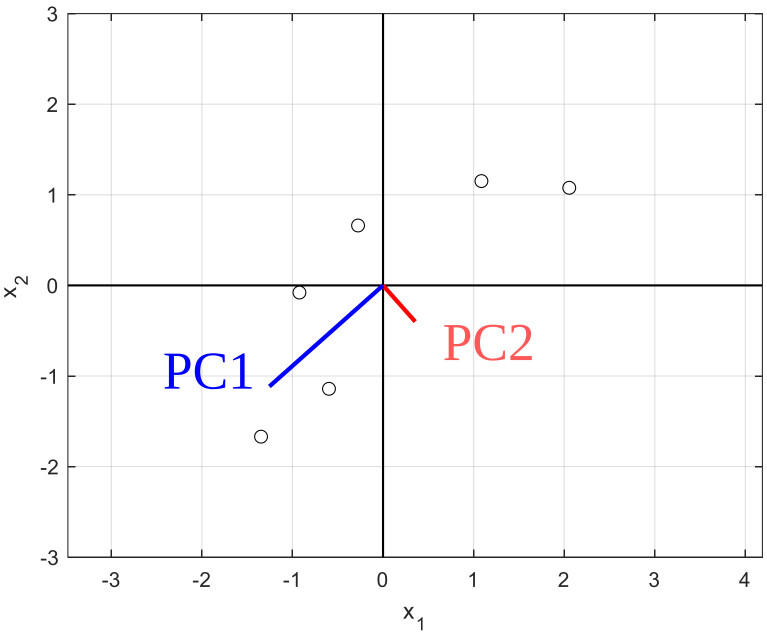
```
X_c =
   -0.9229    1.0864   -1.3466    2.0556   -0.5967   -0.2758
   -0.0789    1.1515   -1.6695    1.0773   -1.1415    0.6611

R =
    1.7006    1.2570
    1.2570    1.4040
```

## Source code:

```
[U, Lambda] = eig(R);
eigenvalues = diag(Lambda);

for k = 1 : size(U, 2)
  u = U(:, k);
  len = sqrt(eigenvalues(k));
  plot([0 len*u(1)], [0 len*u(2)],
'LineWidth', 2, 'color', color_arr(k));
end
```




## Output:

```
U =
     0.6644   -0.7474
    -0.7474   -0.6644
```

PC2 PC1

```
Lambda =
     0.2865        0
          0   2.8181
```

$\lambda_2$ $\lambda_1$

(Optional)

$$\text{maximize}_{\mathbf{u}} \quad \mathbf{u}^T\mathbf{R}\mathbf{u} \qquad \text{subject to } \|\mathbf{u}\| = 1$$

Use Lagrange, we have $J(\mathbf{u}) = \mathbf{u}^T\mathbf{R}\mathbf{u} + \lambda\left(1 - \mathbf{u}^T\mathbf{u}\right)$. Taking the gradient $\nabla_{\mathbf{u}}$ (i.e., a vector of partial derivatives, $[\frac{\partial}{\partial u_1}, \dots, \frac{\partial}{\partial u_p}]^T$) for $J(\mathbf{u})$ and set it to the $\mathbf{0}$ vector

$$\nabla_{\mathbf{u}} J(\mathbf{u}) = 2\mathbf{R}^T\mathbf{u} + \lambda(-2\mathbf{u}) = \Big|_{\mathbf{u}=\hat{\mathbf{u}}} \quad \mathbf{0},$$

we obtain $\mathbf{R}\hat{\mathbf{u}} = \lambda\hat{\mathbf{u}}$. Left multiply $\hat{\mathbf{u}}^T$ to both sides, we have

$$\hat{\mathbf{u}}^T\mathbf{R}\hat{\mathbf{u}} = \hat{\mathbf{u}}^T\lambda\hat{\mathbf{u}} = \lambda\|\hat{\mathbf{u}}\|^2 = \lambda.$$

The cost function is then simplified to finding the largest $\lambda$, or largest eigenvalue of $\mathbf{R}$. $\hat{\mathbf{u}}$ is the eigenvector that corresponds to the largest eigenvalue.

Vector calculus cheat sheet (p. 521–527): https://www.cs.cmu.edu/~epxing/Class/10701-08s/recitation/mc.pdf

# PCA: Forward Transform and Reconstruction

## i) Analysis/Forward Transform:

Also known as Karhunen–Loeve Transform (KLT)

$$\begin{bmatrix} z_{i1} \\ z_{i2} \\ \vdots \\ z_{in} \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1^T \\ \hline \mathbf{u}_2^T \\ \hline \vdots \\ \hline \mathbf{u}_n^T \end{bmatrix} \begin{bmatrix} \\ \mathbf{x}_i \\ \\ \end{bmatrix}$$

$$\mathbf{z}_i = \mathbf{U}^T \mathbf{x}_i$$

## ii) Synthesis/Reconstruction:

$$\mathbf{x}_i = \mathbf{U}\mathbf{z}_i = \begin{bmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_n \end{bmatrix} \begin{bmatrix} z_{i1} \\ \vdots \\ z_{in} \end{bmatrix} = \sum_{k=1}^{n} z_{ik}\mathbf{u}_k$$

## Analysis example:

$$\underbrace{\begin{bmatrix} -1.58 \\ -0.14 \end{bmatrix}}_{\mathbf{z}_i} = \underbrace{\begin{bmatrix} -0.75 & 0.66 \\ -0.66 & -0.75 \end{bmatrix}^T}_{\mathbf{U}^\mathbf{T}} \underbrace{\begin{bmatrix} 1.09 \\ 1.15 \end{bmatrix}}_{\mathbf{x}_i}$$

## Synthesis example:

$$\underbrace{\begin{bmatrix} 1.09 \\ 1.15 \end{bmatrix}}_{\mathbf{x}_i} = \underbrace{\begin{bmatrix} -0.75 & 0.66 \\ -0.66 & -0.75 \end{bmatrix}}_{\mathbf{U}} \underbrace{\begin{bmatrix} -1.58 \\ -0.14 \end{bmatrix}}_{\mathbf{z}_i}$$

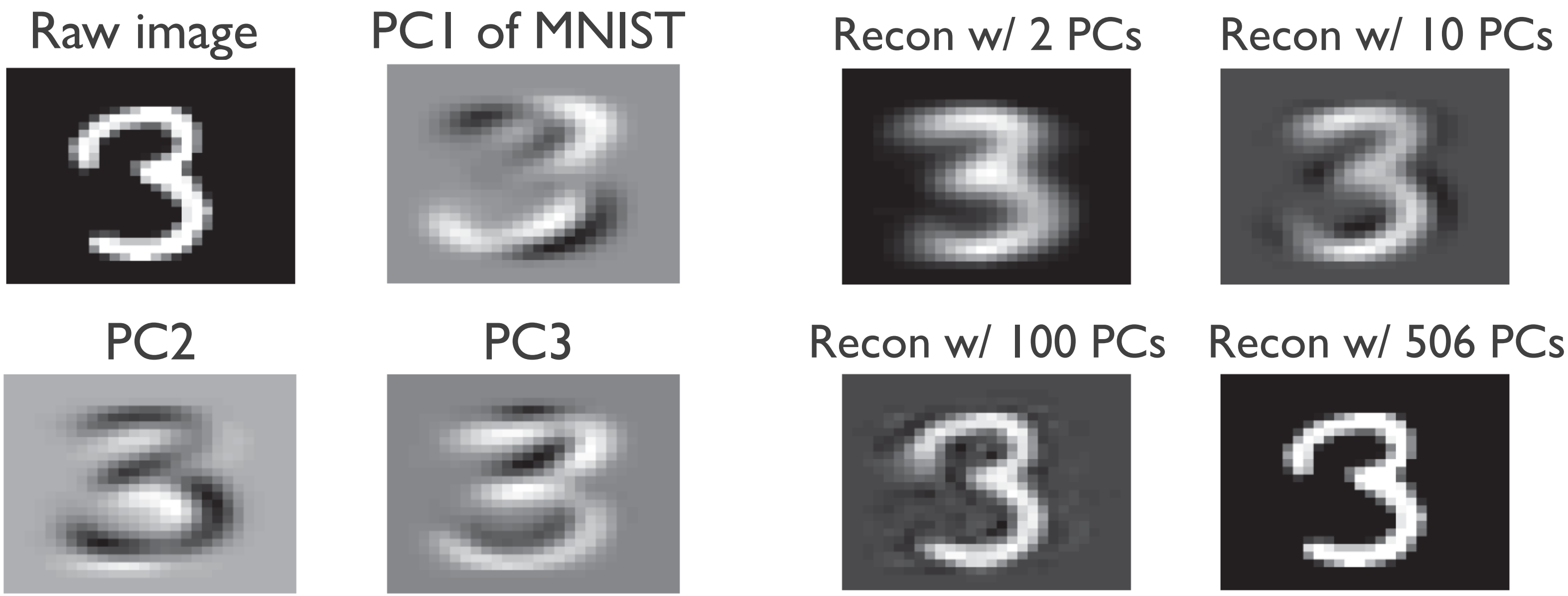
$$= -1.58 \begin{bmatrix} -0.75 \\ -0.66 \end{bmatrix} - 0.14 \begin{bmatrix} 0.66 \\ -0.75 \end{bmatrix}$$

$$= \begin{bmatrix} 1.19 \\ 1.04 \end{bmatrix} + \begin{bmatrix} -0.09 \\ 0.11 \end{bmatrix}$$

Contribution from PC2 is **small**

# Reconstruction Using Dominant PCs

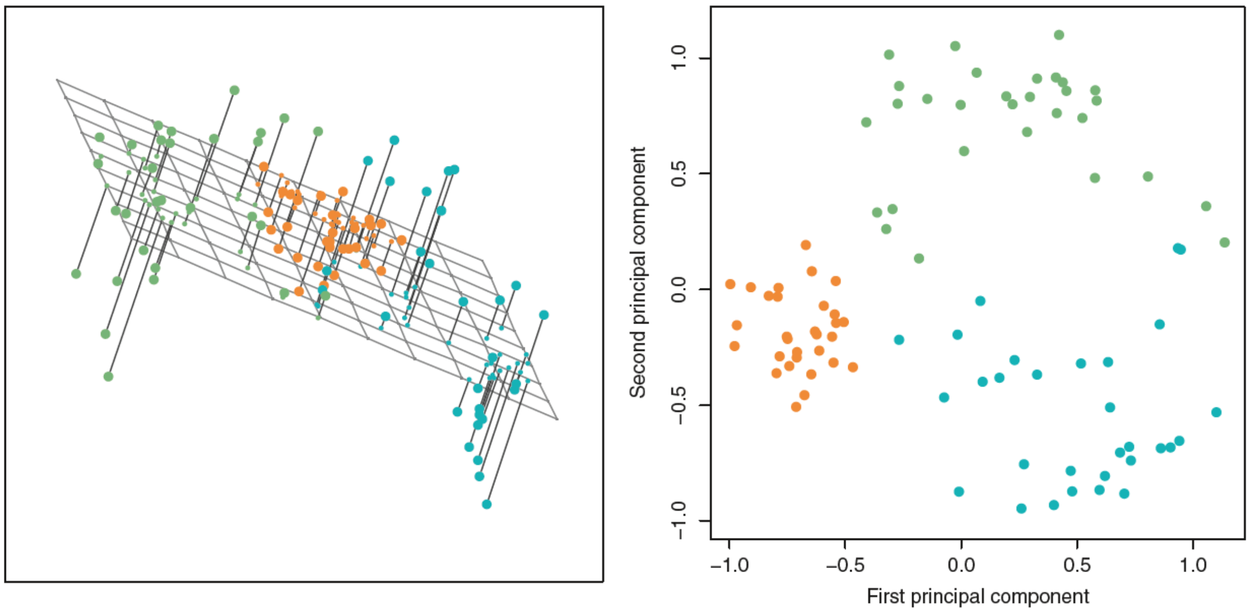
(Murphy 2012)




- Each image of 50x50 is stacked into a column vector of length 2,500.
- Sample covariance matrix will be of size 2,500x2,500.
- Eigenvectors/principal components (PCs) of length 2,500 are **reshaped** to 50x50 for display. May call them "eigen-images."

# PCA Objective 2: Minimizing Error

- Approximate the data points using a presentation in a lower-dimensional subspace.




(James, Witten, Hastie, & Tibshirani, 2013)

Assume $\mathbf{x}_i$'s are centered, i.e., $\mathbf{x}_i \leftarrow \mathbf{x}_i - \bar{\mathbf{x}}$ , $\forall i$.

(Optional)

$$J(\mathbf{u}_1, z_{i1}) = \frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - z_{i1}\mathbf{u}_1\|^2 = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - z_{i1}\mathbf{u}_1)^T(\mathbf{x}_i - z_{i1}\mathbf{u}_1)$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^T\mathbf{x}_i - 2z_{i1}\mathbf{x}_i^T\mathbf{u}_1 + z_{i1}^2\mathbf{u}_1^T\mathbf{u}_1)$$

$$\frac{\partial}{\partial z_{j1}}J = \frac{1}{n}(-2\mathbf{x}_j^T\mathbf{u}_1 + 2z_{j1}\underbrace{\mathbf{u}_1^T\mathbf{u}_1}_{=1}) = \Big|_{z_{j1}=\hat{z}_{j1}} 0 \Rightarrow \hat{z}_{j1} = \mathbf{u}_1^T\mathbf{x}_j$$

(Does this result look familiar?)

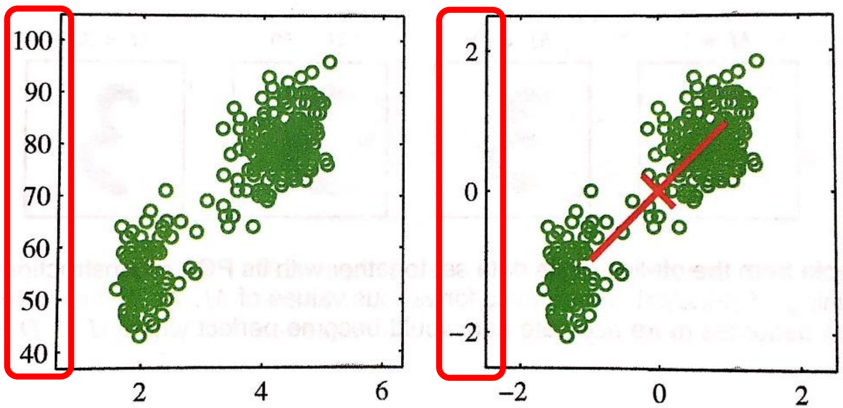
$$J = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i^T\mathbf{x}_i - 2z_{i1}^2 + z_{i1}^2) \quad \text{(skip the hat of } z_{i1} \text{ for simplicity)}$$

$$\min_{\mathbf{u}_1} J = \max_{\mathbf{u}_1}\sum_{i=1}^{n} z_{i1}^2 = \underline{\text{maximize the spread!}}$$

Same as the Objective 1

# PCA's Caveat: Proper Standardization May be Needed

- If coordinates of $\mathbf{x}_j = \left[x_{1,j}, \ldots, x_{p,j}\right]^T$ have different **units**, maximal variance direction may be biased toward $x_{i,j}$ with largest magnitude.




(Bishop 2006)

- Why is standardization needed in this case?
- Do the hand-written digit and face recognition need standardization?

- When proper standardization of coordinate/variable/feature $i$ is needed:

$$\tilde{x}_{ij} = \frac{x_{ij} - \bar{x}_{i\cdot}}{\sqrt{\frac{1}{n}\sum_{j=1}^{n}(x_{ij} - \bar{x}_{i\cdot})^2}}, \quad i = 1, \ldots, p.$$

**Should standardize along the feature/horizontal direction** rather than within each data point.

# PCA: Applications and Beyond

- PCA is lightweight yet powerful. Should be tried before applying more sophisticated tools.
- Modern replacement of PCA:
  - Data visualization: t-SNE, UMAP.
  - Dimensionality reduction: Nonlinear dimensionality reduction algorithms.
  - Lossy data compression: Data-independent transforms tailored for data following certain statistical behaviors.
  - Feature extraction: Topic modeling (unsupervised), CNN self-learned feature extraction (supervised).

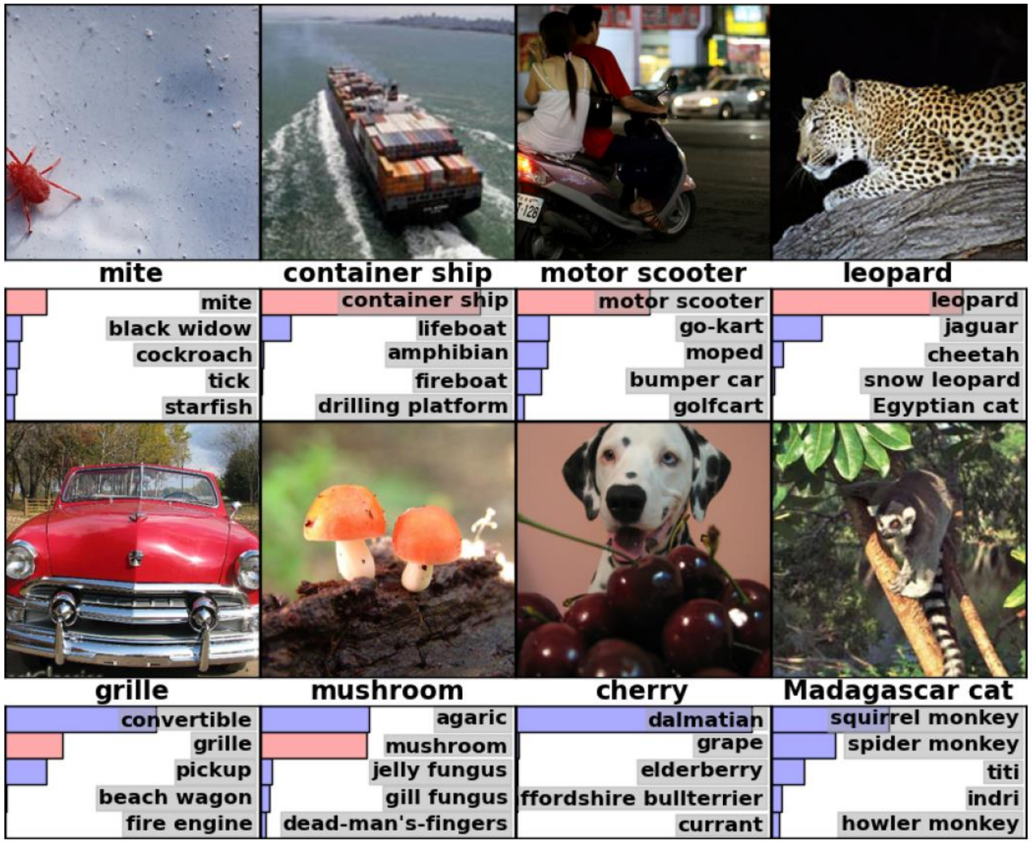
# Linear Regression and Prediction (Supervised Learning)

## Learning objectives

- Interpret regression problem mathematically and geometrically
- Apply linear regression to learning problems without overfit

(A comprehensive treatment of basic linear regression can be found in Scheffe Ch1, available on the library's course reserves.)

# Supervised Learning: Classification




<u>Goal of classification:</u>

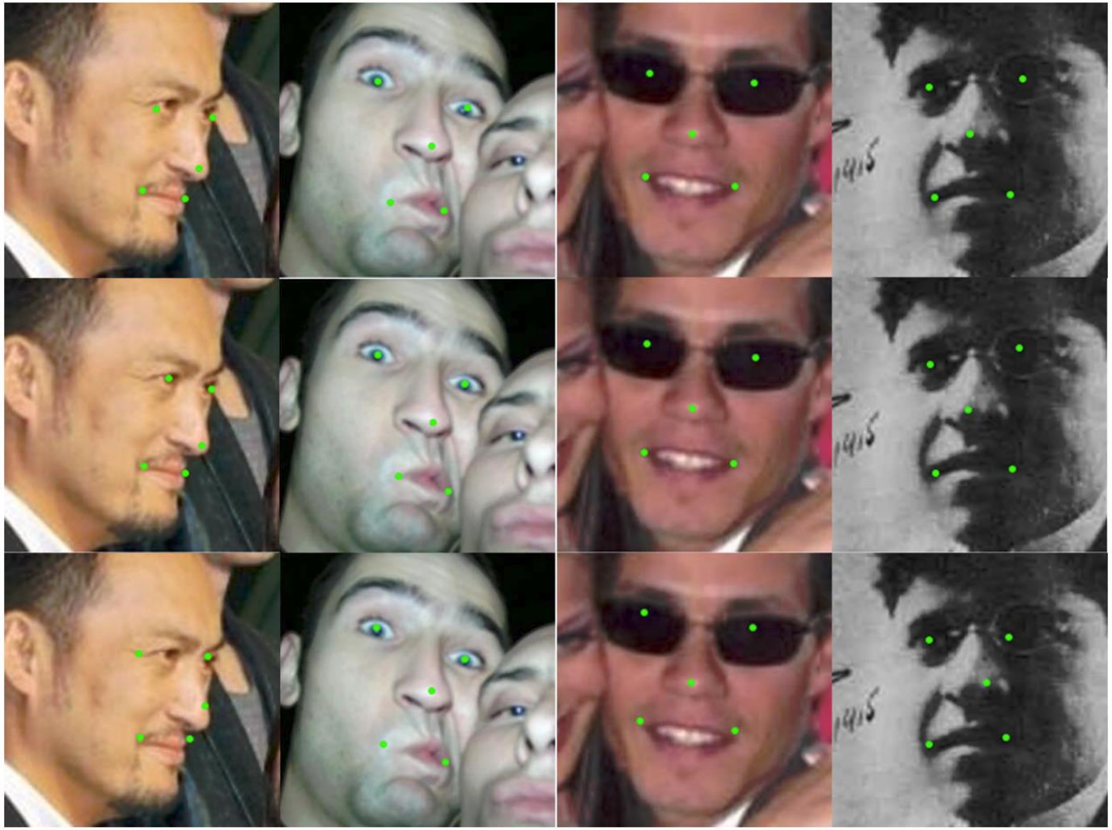
Assign a **categorical/ qualitative label**, or a class, to an given input.

← Given an image, it returns the class label.

Optionally, provide a “confidence score.”

Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, ImageNet Classification with Deep Convolutional Neural Networks, *NIPS*, 2012.

# Supervised Learning: Regression




Goal of regression:
Assign a number to each input.

Loosely, ML people also call it "label."

← Given a facial image, it returns the 2D location for each key point of the face.

Yi Sun, Xiaogang Wang, Xiaoou Tang, Deep Convolutional Network Cascade for Facial Point Detection, *CVPR*, 2013.

# Supervised Learning: Definition

- **Terminologies:**
  - Training data: $\mathcal{D}_{\text{tr}} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$
  - Test data: $\mathcal{D}_{\text{te}} = \{(\mathbf{x}_i, y_i)\}_{i=n+1}^{n+m}$
  - Learned model: $y = f(\mathbf{x})$

- **Goal**: Given a set of training data $\mathcal{D}_{\text{tr}}$ as the inputs, we would like to compute a learned model $y = f(\mathbf{x})$ such that it can generate accurate predicted outputs

$$\hat{y}_i = f(\mathbf{x}_i), \quad i = n+1, \ldots, n+m,$$

from a set of new inputs $\{\mathbf{x}_i\}_{i=n+1}^{n+m}$ of the test data $\mathcal{D}_{\text{te}}$ whose labels $\{y_i\}_{i=n+1}^{n+m}$ have never been taken into account when the model is computed.

# Quantifying the Accuracy of Prediction

- Quantify the accuracy of the learned model by a *loss function* (or cost/objective function), based on predicted output, $\hat{y}_i$, and the true output, $y_i$, namely, $L(\hat{\mathbf{y}}, \mathbf{y})$

- A typical choice for the loss function for a continuous-valued output is the *mean squared error*:

$$L(\hat{\mathbf{y}}, \mathbf{y}) = \frac{1}{m} \sum_{i=n+1}^{n+m} (\hat{y}_i - y_i)^2$$

- Key ML assumption: Test data shouldn't have been seen before (at the training stage), or there will be overfit.

# Simplest Example: Linear Model

Data: $(x_i, Y_i), \quad i = 1, \ldots, n$

Model: $Y_i = \beta_0 + \beta_1 x_i + e_i$

# Simplest Example: Linear Model

Data: $(x_i, Y_i), \quad i = 1, \ldots, n$

random $\mathbb{E}[e_i] = 0$

Model: $Y_i = \beta_0 + \beta_1 x_i + e_i$

intercept

noise: measurement noise, biological variation

dependent var.
/observation

independent var./predictor

$\boldsymbol{\theta} = [\beta_0, \beta_1]^T$ is the parameter vector/weights.

$\mathbb{E}[Y_i] = \beta_0 + \beta_1 x_i =$ linear combination of unknowns $\beta_0$ and $\beta_1$ with known coefficient 1 and $x_i$.

# Linear Model in Matrix-Vector Form

$$\boxed{\begin{aligned}&Y_i = \beta_0 + \beta_1 x_i + e_i,\\ &i = 1, \ldots, n.\end{aligned}}$$

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix}_{n\times 1}, \quad \mathbf{X} = \begin{bmatrix} \underbrace{\begin{matrix}1\\ \vdots \\ 1\end{matrix}}_{\mathbb{1}} & \underbrace{\begin{matrix}x_1\\ \vdots \\ x_n\end{matrix}}_{\mathbf{x}} \end{bmatrix}_{n\times 2}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}_{2\times 1}, \quad \mathbf{e} = \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix}_{n\times 1}$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$$ "Matrix–vector form"

data matrix

# Linear Model with Multiple Predictors / Features

- Multiple (Linear) Regression Model:

$$Y_i = \sum_{j=1}^{p} x_{ij}\beta_j + e_i, \quad i = 1, \ldots, n.$$

$$\mathbf{Y}_{n\times 1} = \mathbf{X}_{n\times p}\boldsymbol{\beta}_{p\times 1} + \mathbf{e}_{n\times 1}$$

vector of random elements

# Linear Regression Example

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + e_i, \quad i = 1, \ldots, 50.$$

$Y_i$ : grade

$x_{i1}$ : time spent on HW

$x_{i2}$ : time spent on review

$$\begin{bmatrix} Y_1 \\ \vdots \\ Y_{50} \end{bmatrix} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} \\ \vdots & \vdots & \vdots \\ 1 & x_{50,1} & x_{50,2} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} e_1 \\ \vdots \\ e_{50} \end{bmatrix}$$

How to estimate model parameters $\beta_0$, $\beta_1$, and $\beta_2$? Least-Squares!

# Linear Regression Example

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + e_i, \quad i = 1, \ldots, 50.$$

$Y_i$ : grade

$x_{i1}$ : time spent on HW

$x_{i2}$ : time spent on review

$$\begin{bmatrix} Y_1 \\ \vdots \\ Y_{50} \end{bmatrix} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} \\ \vdots & \vdots & \vdots \\ 1 & x_{50,1} & x_{50,2} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} e_1 \\ \vdots \\ e_{50} \end{bmatrix}$$

How to estimate model parameters $\beta_0$, $\beta_1$, and $\beta_2$? Least-Squares!

# Least-Squares for Parameter Estimation

Problem Setup: $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$, where $\mathbf{X} \triangleq [\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_p]$.

Estimate $\boldsymbol{\beta}$ such that $J(\boldsymbol{\beta}) = \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|^2$ is minimized.

$$\text{or } J(\boldsymbol{\beta}) = \sum_{i=1}^{n} (Y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

This is called the *least-squares* procedure.

# Least-Squares via Vector Calculus

$$\boxed{\text{Recall: } J(\boldsymbol{\beta}) = \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|^2}$$

$$\textbf{Method 1: } \nabla_{\boldsymbol{\beta}} J(\boldsymbol{\beta}) = \Big|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}} 0,$$

$$\nabla_{\boldsymbol{\beta}} J(\boldsymbol{\beta}) = 2\left[-\mathbf{X}^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})\right] = \Big|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}} \mathbf{0}$$

$$\boxed{\mathbf{X}^T\mathbf{Y} = \mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}}} \qquad \boxed{\mathbf{X}^T(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) = \mathbf{0}}$$

(Error orthogonal to data)

<u>Normal Equation (N.E.)</u>

Vector calculus cheat sheet (p. 521–527): https://www.cs.cmu.edu/~epxing/Class/10701-08s/recitation/mc.pdf

# Least-Squares via Partial Differentiation (optional)

If linear algebra is not used, the derivation can be much more involved:

**Method 2** :

$\boxed{\text{Recall: } J(\boldsymbol{\beta}) = \sum_{i=1}^{n}\left(Y_i - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2}$

$$\frac{\partial J}{\partial \beta_k} = \sum_{i=1}^{n} 2(Y_i - \sum_{j=1}^{p} x_{ij}\beta_j)\underbrace{\frac{\partial}{\partial \beta_k}\Big(-(\cdots + x_{ik}\beta_k + \cdots)\Big)}_{-x_{ik}}$$

$$=|_{\beta_j=\hat{\beta}_j} 0, \quad k = 1, \cdots, p$$

$$\Longleftrightarrow \sum_i Y_i x_{ik} = \sum_i \sum_j x_{ij}\hat{\beta}_j x_{ik} \Longleftrightarrow \boxed{\mathbf{X}^T\mathbf{Y} = \mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}}}$$

Normal Equation (N.E.)

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

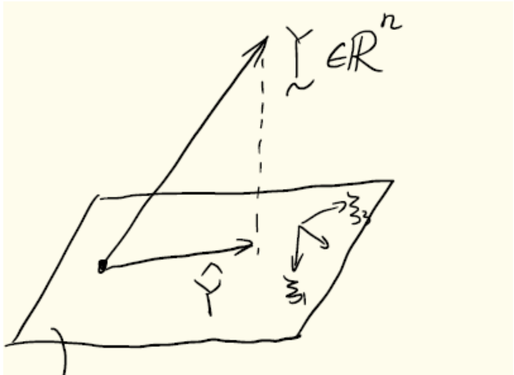
where $\mathbf{X}^T\mathbf{Y} = \left[\sum_{i=1}^{n} x_{ik}Y_i\right]_{p\times 1}$, $\mathbf{X}^T\mathbf{X} = \left[\sum_{i=1}^{n} x_{ij}x_{ik}\right]_{p\times p}$

$$\mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}} = \left[\sum_{j=1}^{p}\left(\sum_{i=1}^{n} x_{ij}x_{ik}\right)\hat{\beta}_j\right]_{p\times 1}$$

# Geometric Interpretation of Least-Squares (LS)

- Lemma: The LS procedure finds a vector $\widehat{\boldsymbol{\beta}}$ in the column (vector) space of $\mathbf{X}$, i.e., $\mathcal{C}(\mathbf{X}) = \{\mathbf{Xb}, \mathbf{b} \in \mathbb{R}^p\}$ such that
  - $\widehat{\mathbf{Y}} = \mathbf{X}\widehat{\boldsymbol{\beta}}$ is as close as possible to $\mathbf{y}$, or
  - $(\mathbf{Y} - \widehat{\mathbf{Y}}) \perp \mathcal{C}(\mathbf{X})$.

$$
\begin{aligned}
& (\mathbf{Y} - \hat{\mathbf{Y}}) \perp \mathcal{C}(\mathbf{X}) \\
\Longleftrightarrow\ & (\mathbf{Y} - \hat{\mathbf{Y}}) \perp \mathbf{Xb}, \quad \forall \mathbf{b} \in \mathbb{R}^p \\
\Longleftrightarrow\ & \boldsymbol{\xi}_j^T (\mathbf{Y} - \hat{\mathbf{Y}}) = 0, \quad j = 1, \cdots, p \\
\Longleftrightarrow\ & [\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_p]^T (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) = \mathbf{0} \\
\Longleftrightarrow\ & \mathbf{X}^T \mathbf{Y} = \mathbf{X}^T \mathbf{X} \hat{\boldsymbol{\beta}}
\end{aligned}
$$




$\mathcal{C}(X) = \{ X\underset{\sim}{b},\ \underset{\sim}{b} \in \mathbb{R}^p \}$

$X \overset{\text{def}}{=} [\underset{\sim}{\xi}_1, \underset{\sim}{\xi}_2, \cdots, \underset{\sim}{\xi}_p]$

$\dim(\mathcal{C}(X)) = r \le p$

# Properties of Least-Square Estimate

If $\text{rank}(\mathbf{X}) \triangleq r = p$ ① $\boxed{\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}}$ is unique soluntion.

$$\mathbb{E}[\hat{\boldsymbol{\beta}}] = \mathbb{E}[(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}] = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}\boldsymbol{\beta}) = \boldsymbol{\beta} \text{ (unbiased)}$$

② $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \underbrace{\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T}\mathbf{Y} = \mathbf{H}\mathbf{Y}$

$\mathbf{H}$ : "hat" matrix, or "orthogonal projector." $\mathbf{H}^n = \mathbf{H}$. Why?

# Ex: Linear Model for Learning and Prediction

- Training data (3 data points / a *random sample* of size 3):
  - *Feature*/*predictor* 1: (2, 1, 1). Feature/predictor 2: (1, 2, 1).
  - Labels: (1, 1, 1).
- Test data (2 data points / a random sample of size 2):
  - Feature 1: (1.2, 1.8). Feature 2: (0.9, 1.3).
  - Labels: (0.9, 0.8).
- Tasks:
  a) Learn a linear model without intercept.
  b) Using drawing to illustrate the data and learned model.
  c) Evaluate the mean squared errors (MSEs) of training and testing.

a) $\mathbf{X} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \\ 1 & 1 \end{bmatrix}$ $\mathbf{Y} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$ $(\mathbf{X}, \mathbf{Y})$ : training data

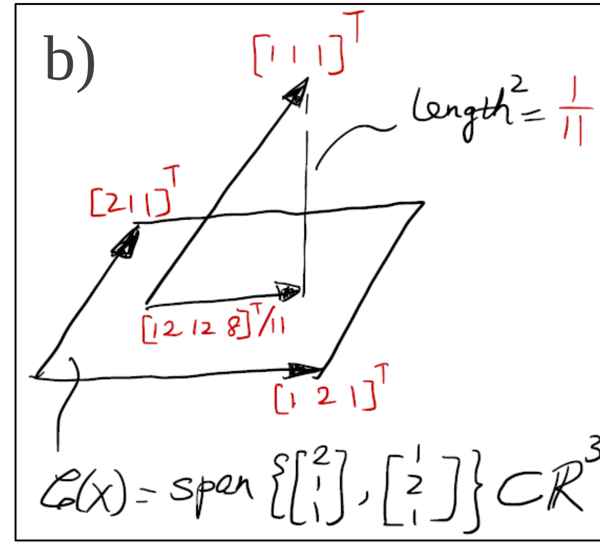
Estimated/ trained model parameters:

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{Y}$$

$$= \left(\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix}\begin{bmatrix} 2 & 1 \\ 1 & 2 \\ 1 & 1 \end{bmatrix}\right)^{-1}\left(\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}\right)$$

$$= \begin{bmatrix} 6 & 5 \\ 5 & 6 \end{bmatrix}^{-1}\begin{bmatrix} 4 \\ 4 \end{bmatrix} = \begin{bmatrix} 6 & -5 \\ -5 & 6 \end{bmatrix} \cdot \frac{1}{11} \cdot \begin{bmatrix} 4 \\ 4 \end{bmatrix}$$

$$= \frac{4}{11}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$




Predicted output based on training data:

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \\ 1 & 1 \end{bmatrix}\frac{4}{11}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{11}\begin{bmatrix} 12 \\ 12 \\ 8 \end{bmatrix} \neq \mathbf{Y}, \text{ or}$$

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T = \frac{1}{11}\begin{bmatrix} 2 & 1 \\ 1 & 2 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 6 & -5 \\ -5 & 6 \end{bmatrix}\begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix} = \frac{1}{11}\begin{bmatrix} 10 & -1 & 3 \\ -1 & 10 & 3 \\ 3 & 3 & 2 \end{bmatrix}$$

$$\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y} = \frac{1}{11}\begin{bmatrix} 12 \\ 12 \\ 8 \end{bmatrix}$$

c) Training error (in MSE):

$$\frac{1}{3}\sum_{i=1}^{3}\left(y_i - \mathbf{x}_i^T\hat{\boldsymbol{\beta}}\right)^2 = \frac{1}{3}\|\mathbf{Y} - \hat{\mathbf{Y}}\|^2 = \frac{1}{3}\|\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}\|^2$$

$$= \frac{1}{3}\cdot\frac{1}{11^2}\left\|\begin{bmatrix} 12-11 \\ 12-11 \\ 8-11 \end{bmatrix}\right\|^2 = \frac{1}{3}\cdot\frac{1}{11^2}(1+1+9) = \frac{1}{3}\cdot\frac{1}{11} = 0.03$$

Testing error (in MSE):

$$\mathbf{X}_{\text{test}} = \begin{bmatrix} 1.2 & 0.9 \\ 1.8 & 0.3 \end{bmatrix} \quad \mathbf{Y}_{\text{test}} = \begin{bmatrix} 0.9 \\ 0.8 \end{bmatrix} \quad (\mathbf{X}_{\text{test}}, \mathbf{Y}_{\text{test}}):$$ testing data

$$\frac{1}{2}\sum_{i=4}^{5}\left(y_i - \mathbf{x}_i^T\hat{\boldsymbol{\beta}}\right)^2 = \frac{1}{2}\|\mathbf{Y}_{\text{test}} - \hat{\mathbf{Y}}_{\text{test}}\|^2 = \frac{1}{2}\|\mathbf{Y}_{\text{test}} - \mathbf{X}_{\text{test}}\hat{\boldsymbol{\beta}}\|^2$$

$$= \frac{1}{2}\left\|\begin{bmatrix} 0.9 \\ 0.8 \end{bmatrix} - \begin{bmatrix} 1.2 & 0.9 \\ 1.8 & 0.3 \end{bmatrix}\left(\frac{4}{11}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\right)\right\|^2 = \frac{1}{2}\left\|\begin{bmatrix} 0.14 \\ 0.04 \end{bmatrix}\right\|^2 = 0.01$$

Testing error is usually larger than training error.

# Convolutional Neural Network (CNN)

## Learning objectives

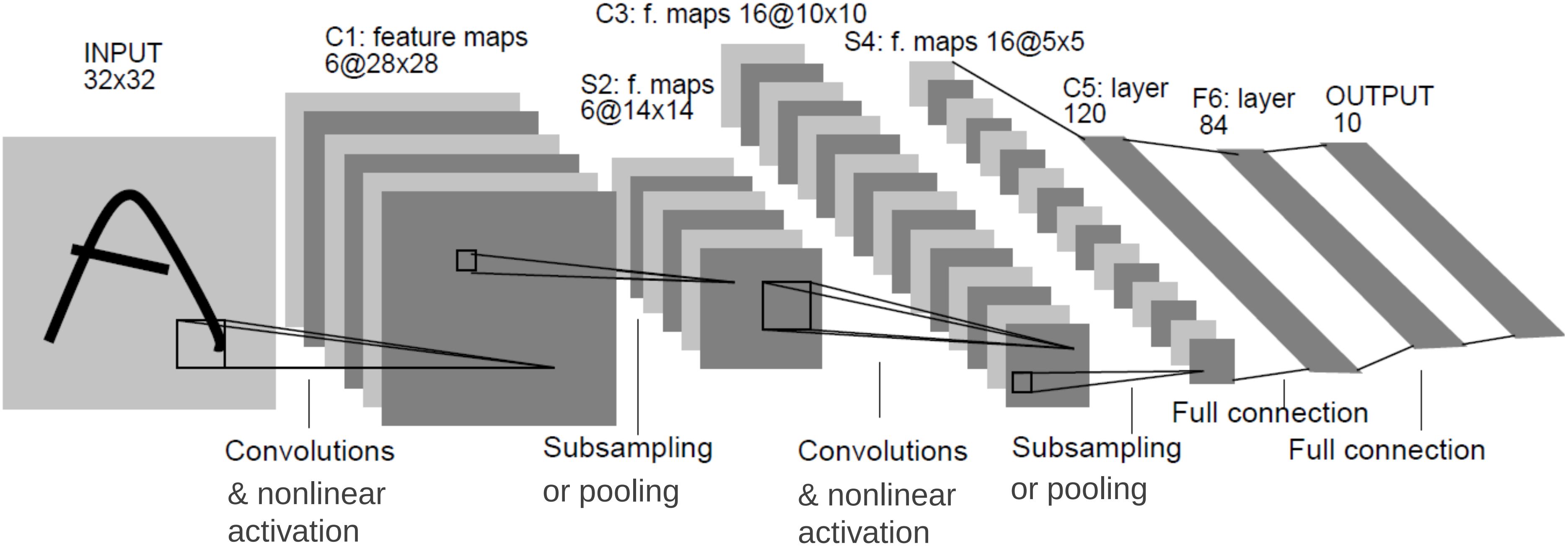
- Describe the structure of CNN
- Build and train simple CNNs using a deep learning package

(Ref: Ch 9 of Goodfellow et al. 2016)

Some slides were adapted from Stanford's CS231n by Fei-Fei Li et al.: http://cs231n.stanford.edu/

# Convolutional Neural Network (CNN)

The **single** most important technology that fueled the rapid development of ***deep learning*** and ***big data*** in the past decade.




LeCun, Bottou, Bengio, Haffner, "Gradient-Based Learning Applied to Document Recognition," *Proc. IEEE*, **1998**.

# Why is Deep Learning so Successful?

1. **Improved model:** convolutional layer, more layers ("deep"), simpler activation (i.e., ReLU), skip/residual connection (i.e., ResNet), attention (i.e., Transformer)
2. **Big data:** huge dataset, transfer learning
3. **Powerful computation:** graphical processing units (GPUs)

- Example of big data: ImageNet (22K categories, 15M images)

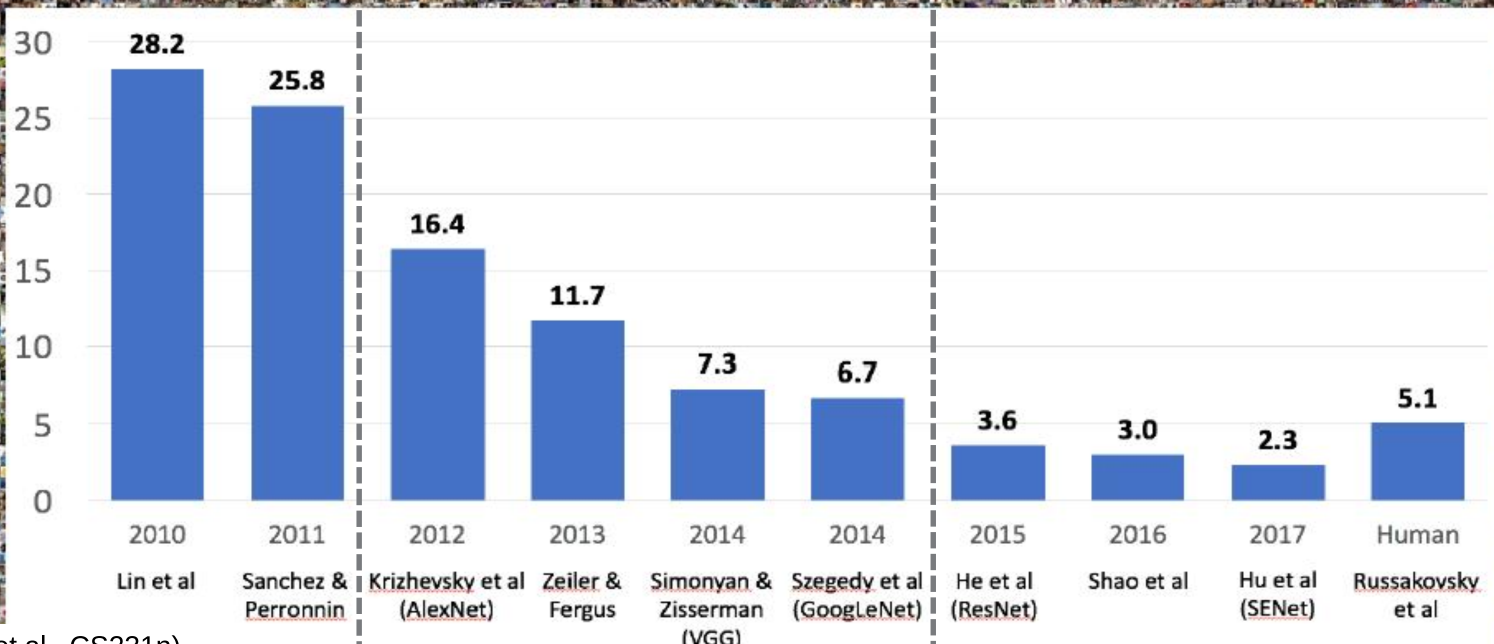

Deng, Dong, Socher, Li, Li & Fei-Fei, "ImageNet: A Large-Scale Hierarchical Image Database," *IEEE CVPR*, 2009.

# IMAGENET Large Scale Visual Recognition Challenge

## The Image Classification Challenge:

## 1,000 object classes

## 1,431,167 images




(Fei-Fei Li et al., CS231n)

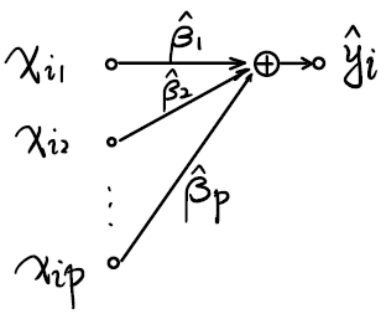
# Linear Model to Neural Network

Recall linear model w/ multiple predictors / features / inputs.

$$\underbrace{y_i}_{\text{true output}} = \sum_{j=1}^{p} x_{ij}\beta_j + e_i = \underbrace{[\beta_1, \dots, \beta_p]}_{\text{true weights}} \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix} + e_i \quad , i = 1, \dots, n.$$

$$\underbrace{\hat{y}_i}_{\text{predicted output}} = \sum_{j=1}^{p} x_{ij}\hat{\beta}_j = \underbrace{[\hat{\beta}_1, \dots, \hat{\beta}_p]}_{\text{estimated weights}} \begin{bmatrix} x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix} \quad , i = n+1, \dots, n+m.$$

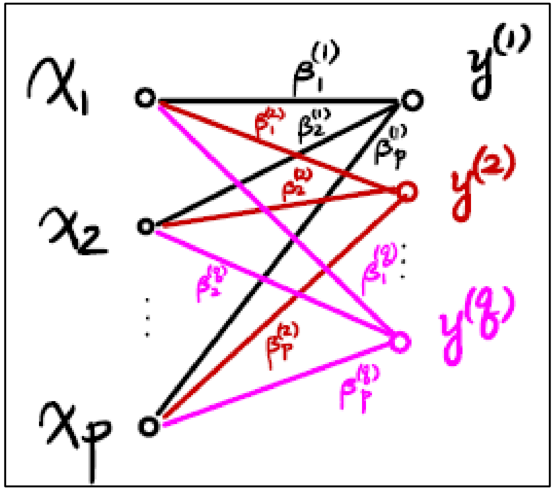
Graphically we have:




① Use multiple linear models

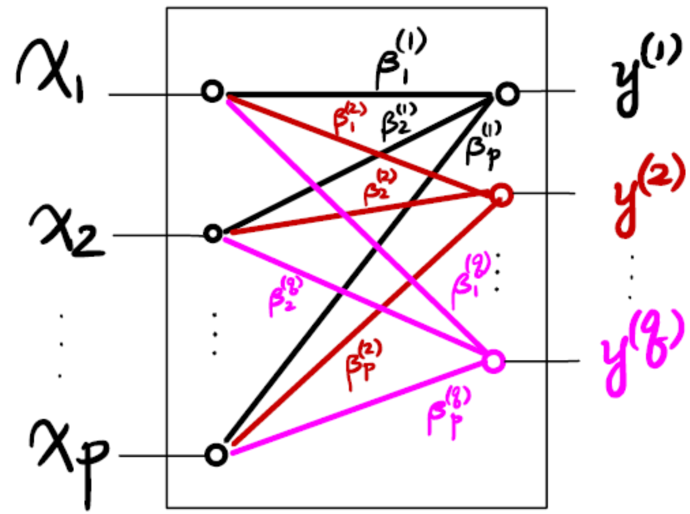
$\longrightarrow$

② Simplify the notations.



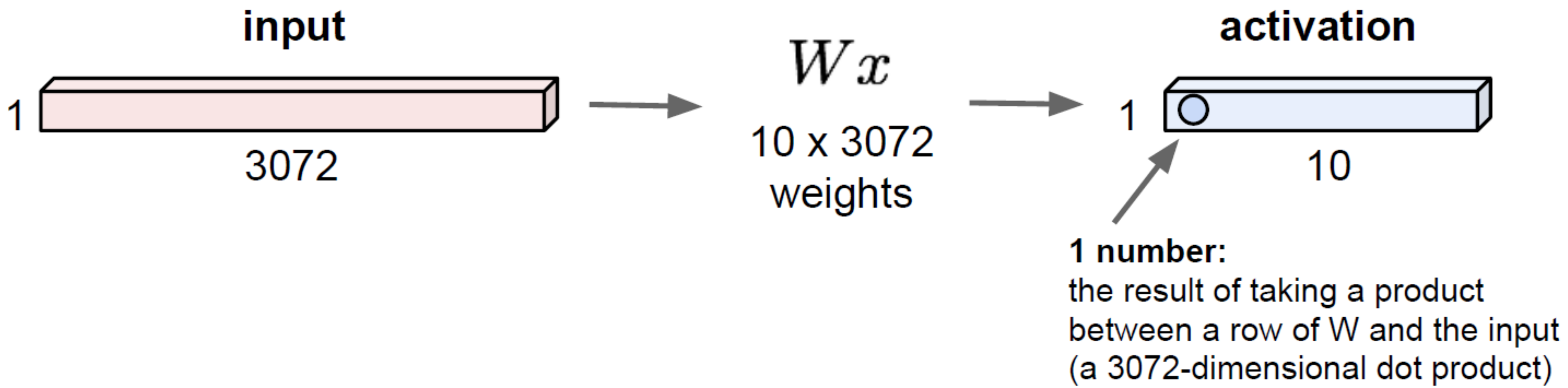
# Fully-Connected Layer for 1D Signal

$$
\underbrace{\begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(q)} \end{bmatrix}}_{\substack{\text{layer} \\ \text{output,} \\ \underset{\sim}{y} \in \mathbb{R}^{q}}}
=
\underbrace{\begin{bmatrix} \beta_1^{(1)} & \beta_2^{(1)} & \cdots & \beta_p^{(1)} \\ \beta_1^{(2)} & \beta_2^{(2)} & \cdots & \beta_p^{(2)} \\ \vdots & & & \vdots \\ \beta_1^{(q)} & \beta_2^{(q)} & \cdots & \beta_p^{(q)} \end{bmatrix}}_{\substack{\text{dense weight} \\ \text{matrix} \\ B \in \mathbb{R}^{q \times p}}}
\underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix}}_{\substack{\text{layer input,} \\ \underset{\sim}{x} \in \mathbb{R}^{p}}}
$$



# Fully-Connected Layer for RGB Image

32x32x3 image -> stretch to 3072 x 1

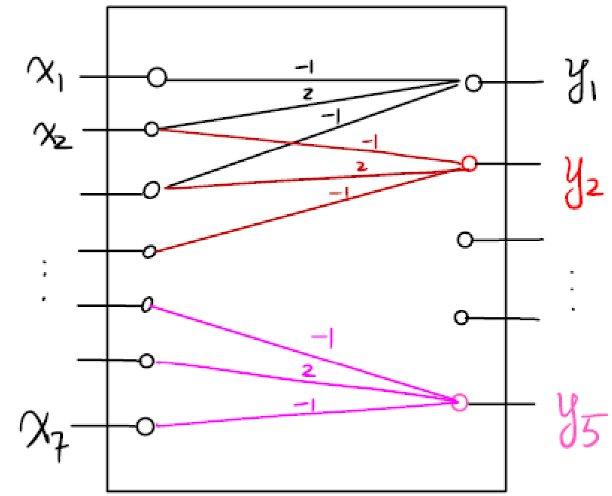



(Fei-Fei Li et al., CS231n)

# Convolutional Layer for 1D Signal

$$\begin{bmatrix} y_1 \\ \vdots \\ y_5 \end{bmatrix} = \begin{bmatrix} -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & -1 & 2 & -1 & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_7 \end{bmatrix}$$

Sparse weight matrix



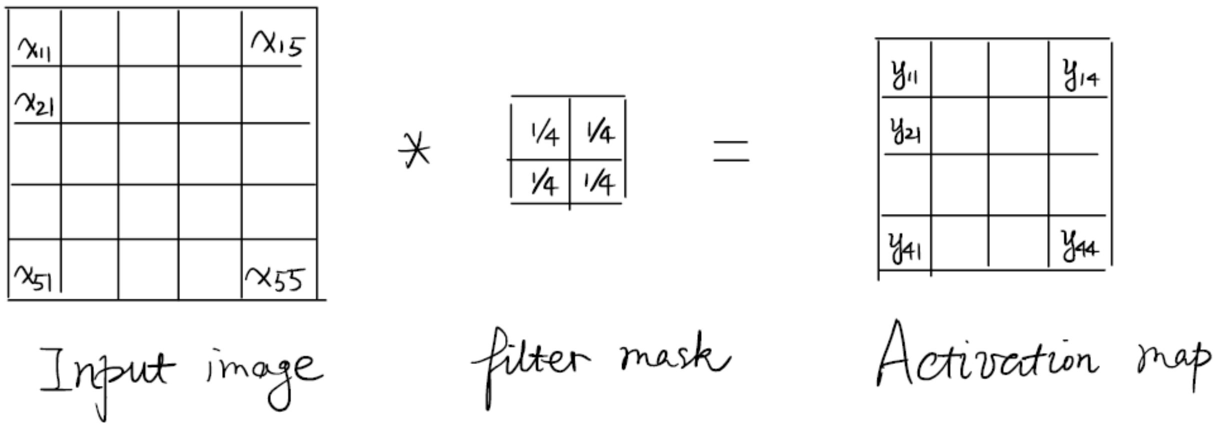

Input: | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | $x_7$ | — length 7

$*$

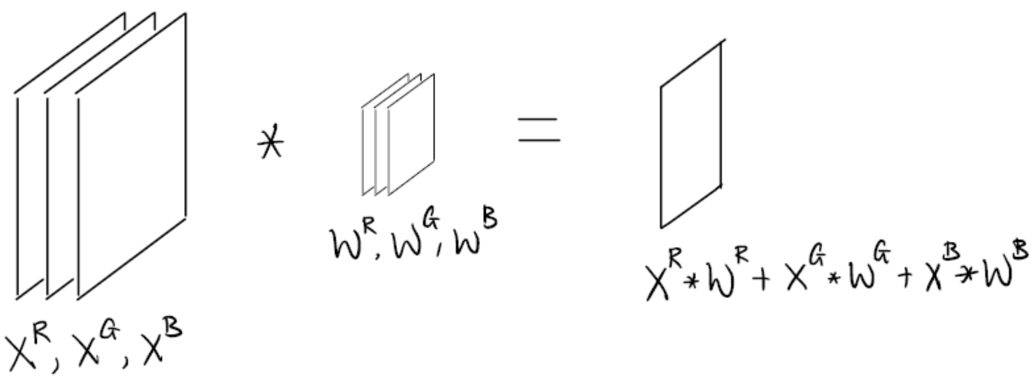
Convolution filter mask: | $-1$ | $2$ | $-1$ | — length 3

Output (w/o boundary elements): | $y_1$ | $y_2$ | $y_3$ | $y_4$ | $y_5$ | — length $7-(3-1)=5$

# Convolutional Layer for 2D Matrix/Image



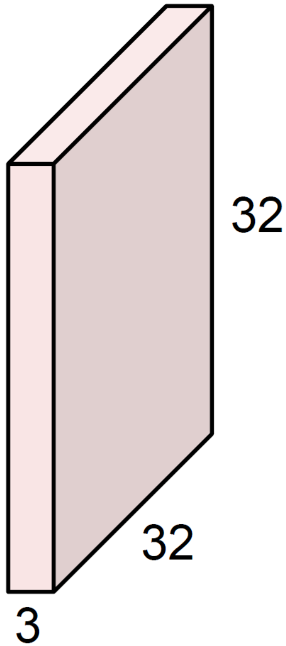

2D Convolution



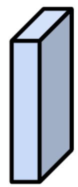

Multiple color channels need multiple filter masks

# Convolutional Layer for RGB Image

32x32x3 image

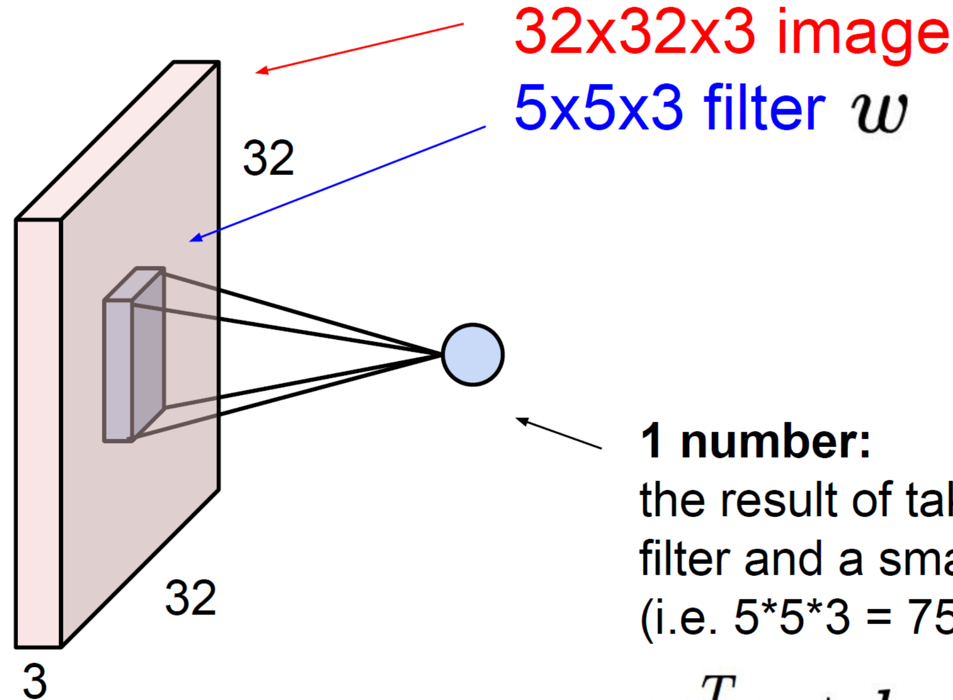



5x5x3 filter



**Convolve** the filter with the image
i.e. “slide over the image spatially, computing dot products”

(Fei-Fei Li et al., CS231n)

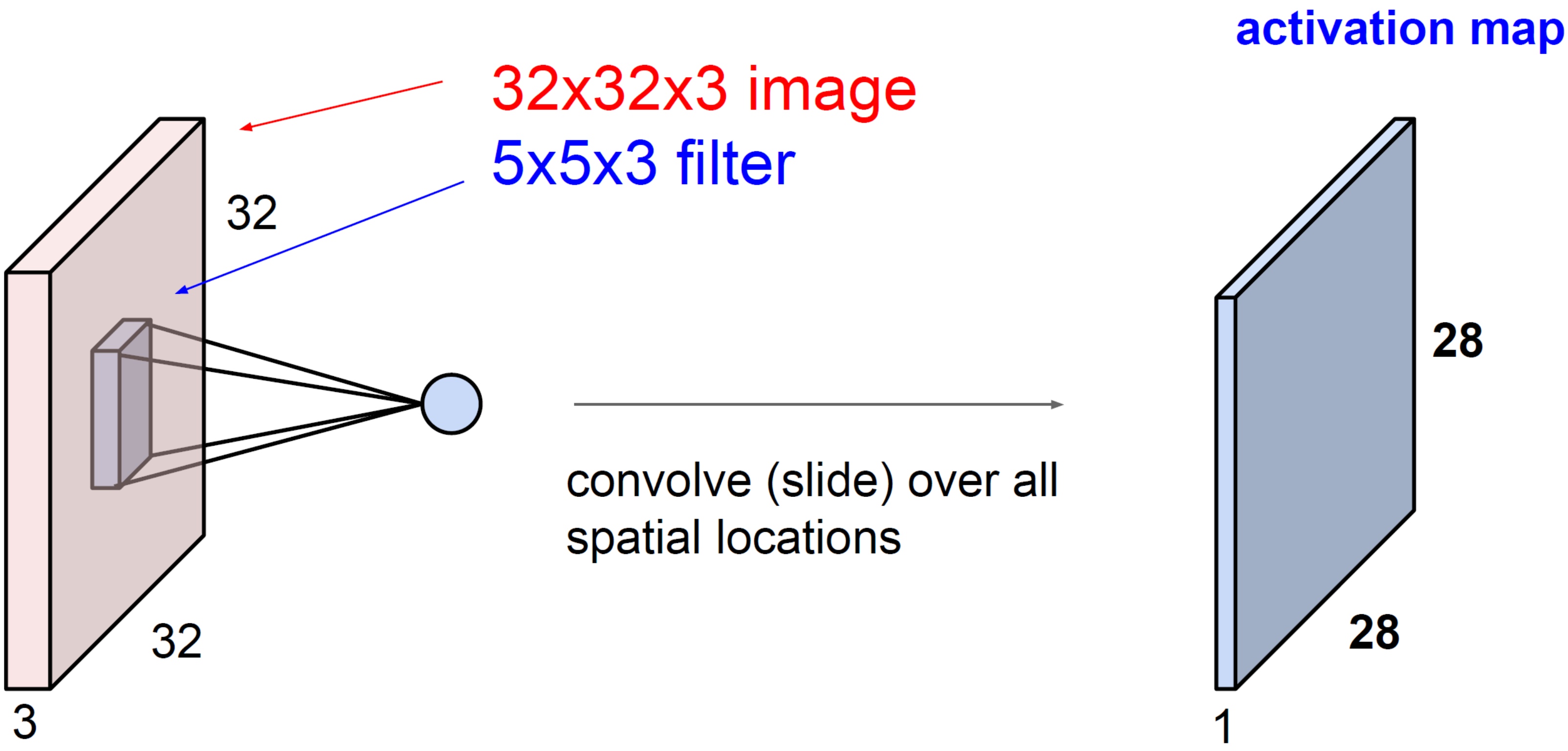



**1 number:**
the result of taking a dot product between the filter and a small 5x5x3 chunk of the image
(i.e. 5*5*3 = 75-dimensional dot product + bias)

$$w^T x + b$$

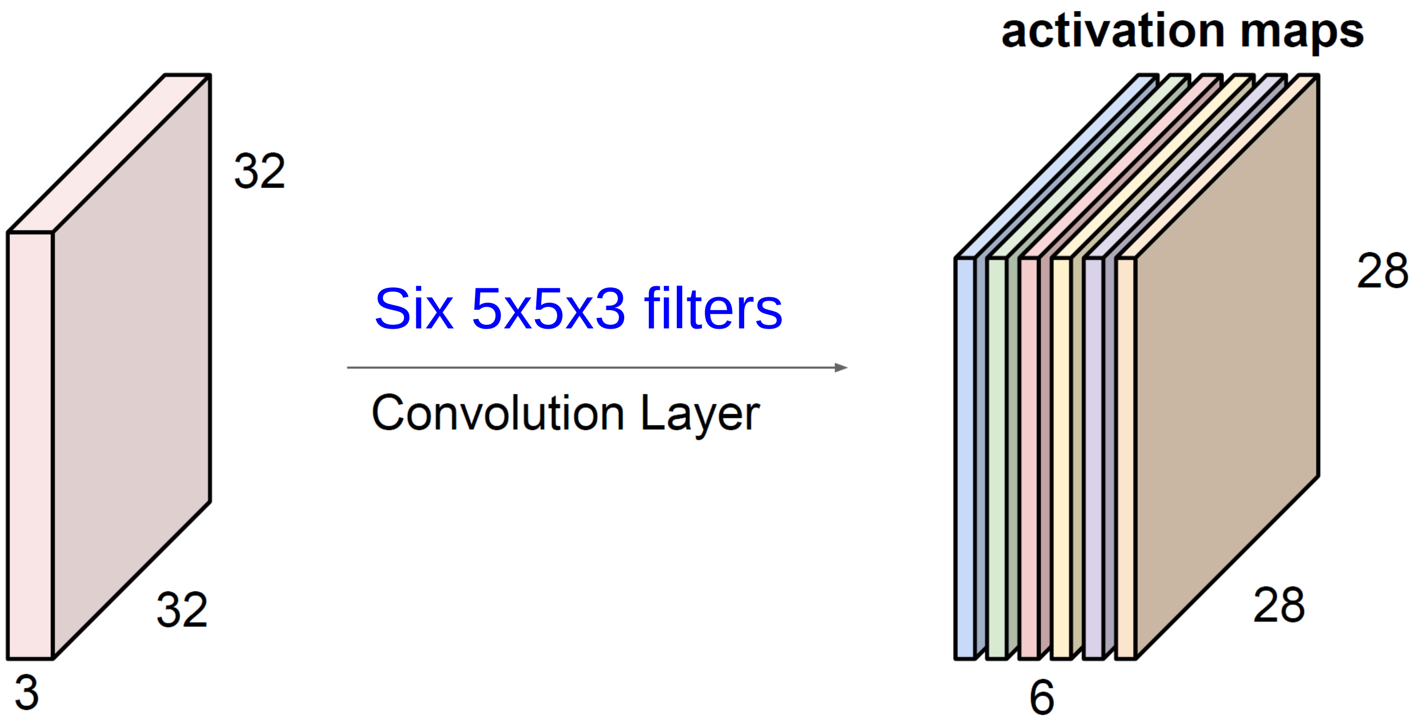
(Fei-Fei Li et al., CS231n)

# A closer look at spatial dimensions:




(Fei-Fei Li et al., CS231n)

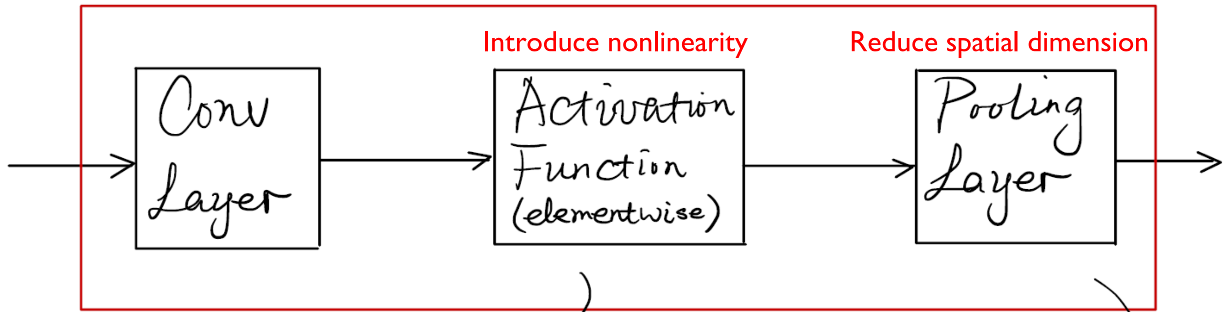
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:




We stack these up to get a "new image" of size 28x28x6!

(Fei-Fei Li et al., CS231n)

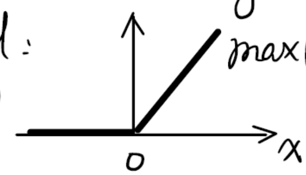
# Building Block for Modern CNN




(Rectified Linear Unit)

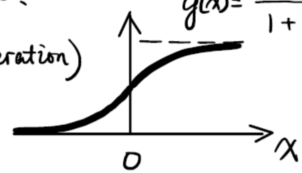
ReLU: (modern)

$g(x) = \max(0, x)$




Logistic: (prior generation)

$g(x) = \frac{1}{1+e^{-x}}$




Ex: 

| | |
|---|---|
| $x_{11}$ | $x_{12}$ |
| $x_{21}$ | $x_{22}$ |

: $\{x_{ij}\}_{i,j=1}^{2}$

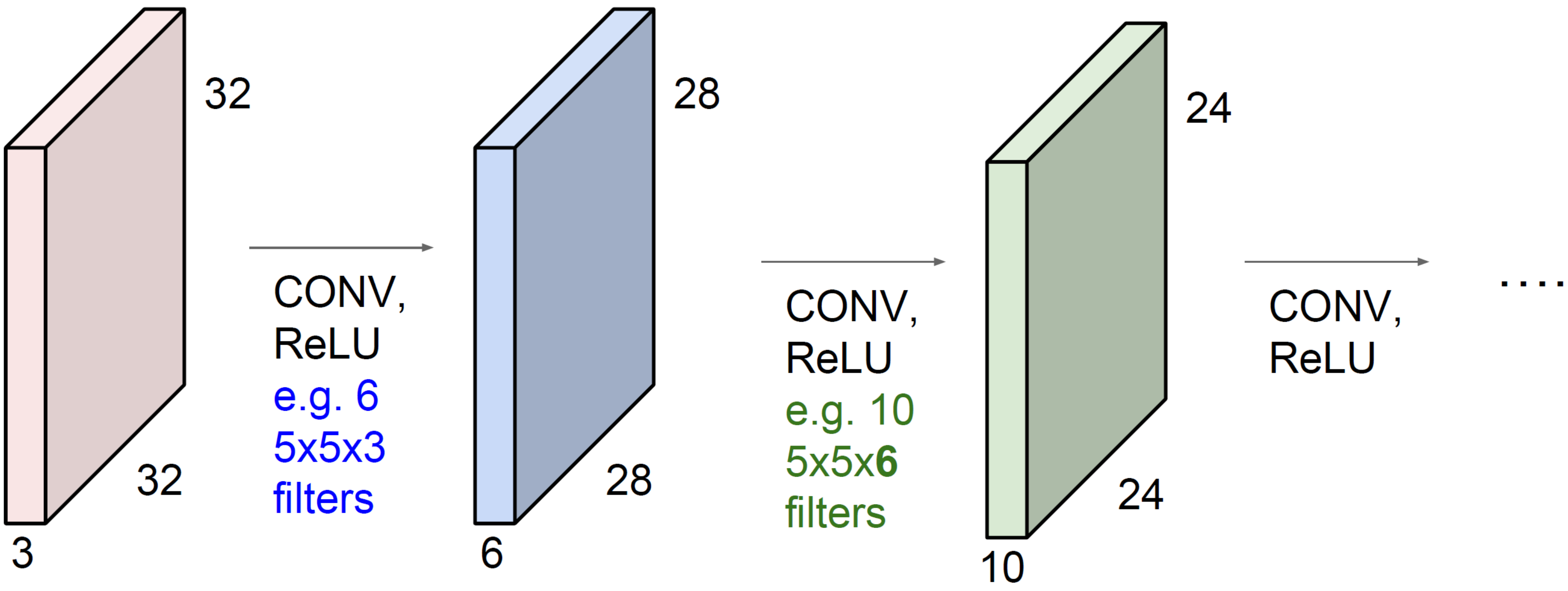
Max pooling:

$$g(\{x_{ij}\}) = \max(\{x_{ij}\})$$

Average pooling:

$$g(\{x_{ij}\}) = \frac{1}{|\{x_{ij}\}|} \sum_{i,j} x_{ij}$$

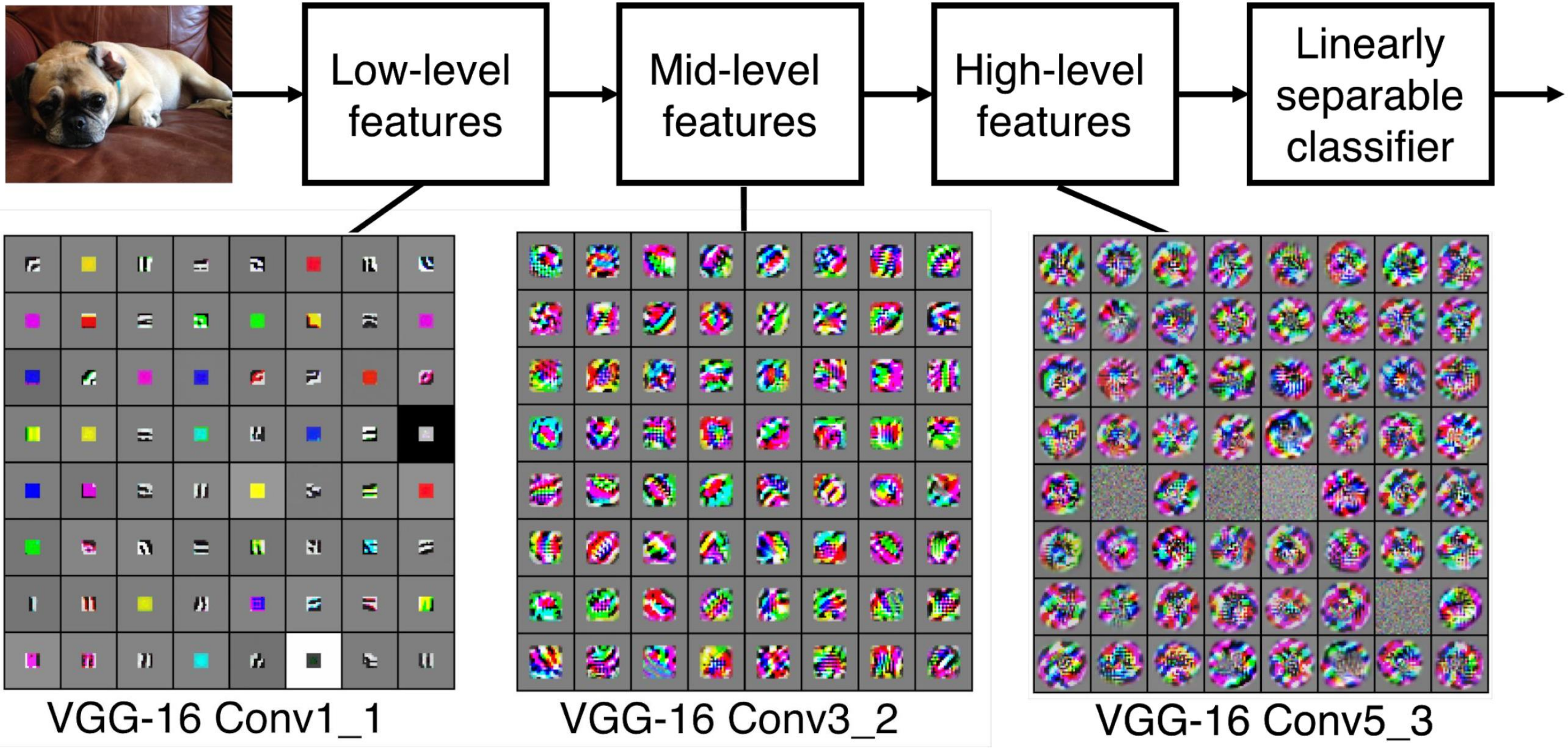
# CNN is composed of a sequence of convolutional layers, interspersed with activation functions (ReLU, in most cases).




(Fei-Fei Li et al., CS231n)

[Zeiler and Fergus 2013]

Visualization of VGG-16 by Lane McIntosh. VGG-16 architecture from [Simonyan and Zisserman 2014].

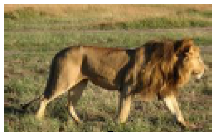



(Fei-Fei Li et al., CS231n)

# IMAGENET Large Scale Visual Recognition Challenge

## Year 2010

### NEC-UIUC



Dense descriptor grid: HOG, LBP

↓

Coding: local coordinate, super-vector

↓

Pooling, SPM

↓

Linear SVM

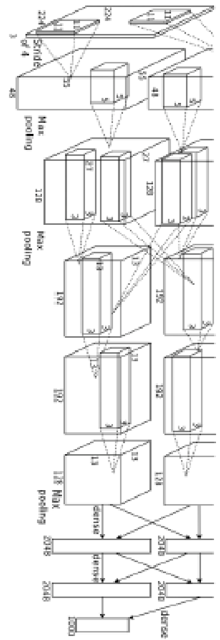
[Lin CVPR 2011]



AlexNet

## Year 2012

### SuperVision

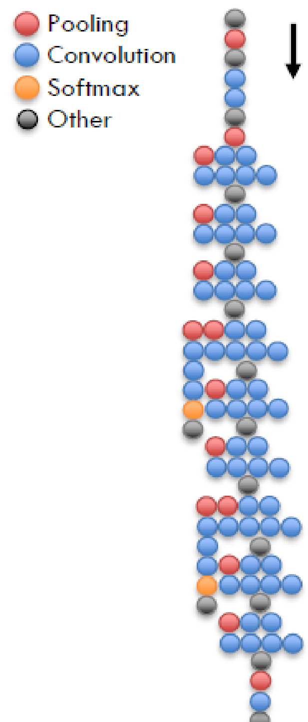


[Krizhevsky NIPS 2012]



## Year 2014

### GoogLeNet




[Szegedy arxiv 2014]

### VGG

Image

conv-64
conv-64
maxpool

conv-128
conv-128
maxpool

conv-256
conv-256
maxpool

conv-512
conv-512
maxpool

conv-512
conv-512
maxpool

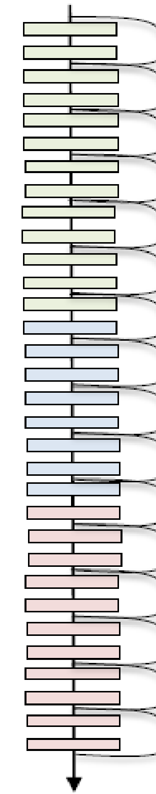
fc-4096
fc-4096
fc-1000
softmax

[Simonyan arxiv 2014]

ResNet

## Year 2015

### MSRA

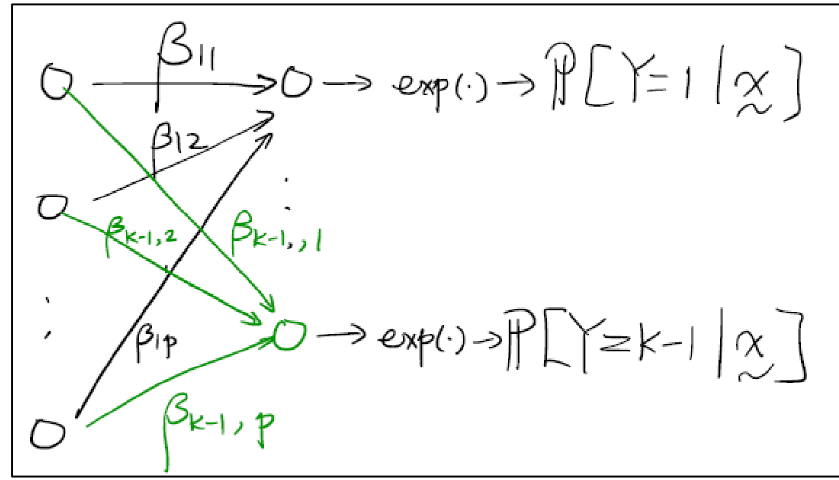


[He ICCV 2015]

(Fei-Fei Li et al., CS231n)

# One Last Thing: When Output is Categorical

- A **softmax layer** is needed:




- Softmax function:

$$\sigma_i(\underset{\sim}{z}) = \frac{e^{\beta z_i}}{\sum_{j=1}^{K} e^{\beta z_j}}$$

- Ex:

$$K=2 \qquad \sigma_1 = \frac{e^{\beta z_1}}{e^{\beta z_1} + e^{\beta z_2}}$$

$$= \frac{1}{1+e^{\beta(z_2 - z_1)}}$$

When $\beta$ very large,

$z_2 > z_1$ leads to $\begin{cases} \sigma_1 = 0 \\ \sigma_2 = 1 \end{cases}$

Winner takes all!

# Machine Learning (ML) and Data Science (DS)

- Follow-up machine learning / data science courses:
  - ECE 411 Intro to Machine Learning
  - ECE 542 Neural Nets and Intro to Deep Learning
  - ECE 592-61 Data Science
  - ECE 759 Pattern Recognition and Machine Learning
  - ECE 763 Computer Vision
  - ECE 792-41 Statistical Foundations for Signal Processing & Machine Learning
  - Any courses/videos on YouTube, Coursera, etc.
- Data science competitions: kaggle.com
- Programming languages for ML/DS: Python, R, Matlab