Multivariate Analysis (Slides 2)

- In today's class we will look at some important preliminary material that we need to cover before we look at many multivariate analysis methods.
- This material will include topics that you are likely to have seen in courses in probability and linear algebra.

Notation: observational unit

- A vector of observed values of each of m variables for observational unit i can be denoted as a column vector:

$$\mathbf{x}_i \quad = \quad \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{im} \end{pmatrix}$$

i.e., x_{ij} represents the value of variable j for observational unit i.

- Observations will generally be denoted by lower case letters.
- For univariate data $m = 1$.

Notation: multivariate data

- Multivariate data sets are generally denoted by a data matrix $\mathbf{X}$ with n rows and m columns (n = total number of observational units, m = number of variables).

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{pmatrix}$$

- The ith row of $\mathbf{X}$ is therefore $\mathbf{x}_i^T$.

Random variables

- A random variable (r.v.) is a mapping which assigns a real number to each outcome of a variable.
- Say our variable of interest is 'gender'. The outcomes of this variable are therefore 'male' and 'female'. The random variable X assigns a number to these outcomes, *i.e.*,

$$X = \begin{cases} 1 & \text{if female} \\ 0 & \text{if male.} \end{cases}$$

- A random variables whose value is unknown will generally be denoted by upper case letters.

Expectation of a Random Variable

- If X is a discrete random variable with probability *mass* function $P(X)$, then the expected value of X (also known as its mean) is defined as $\mu = \mathbb{E}[X] = \sum_x xP(X = x)$.
- If X is a continuous random variable with probability *density* function $f(x)$ defined on the space $\mathbb{R}$, then $\mu = \mathbb{E}[X] = \int_{-\infty}^{\infty} xf(x)dx$.
- The expectation of a function $u(X)$ is given by:

  a) $\mu = \mathbb{E}[u(X)] = \sum_x u(x)P(X = x)$ for a discrete r.v.

  b) $\mu = \mathbb{E}[u(X)] = \int_{-\infty}^{\infty} u(x)f(x)dx$ for a continuous r.v.

Variance, Covariance and Correlation

- Let's consider random variables $X_1, X_2, \ldots, X_m$.
- The variance of X_i is defined to be $\mathrm{Var}[X_i] = \mathbb{E}[(X_i - \mathbb{E}[X_i])^2] = \mathbb{E}[X_i^2] - (\mathbb{E}[X_i])^2$.
- The covariance of X_i and X_j is defined to be $\mathrm{Cov}[X_i, X_j] = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])]$.
- The correlation of X_i and X_j is defined to be

$$\mathrm{Cor}[X_i, X_j] = \frac{\mathrm{Cov}[X_i, X_j]}{\sqrt{\mathrm{Var}[X_i]\mathrm{Var}[X_j]}}.$$

- Correlation is hence a 'normalized' form of covariance, with equality between the two existing if the random variables have unit variance.

Covariance Matrix

- Frequently, it is convenient to record the variance and covariance of a set of random variables $\mathbf{X} = (X_1, X_2, \ldots, X_m)$ using a matrix

$$\mathbf{\Sigma} = \begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1m} \\ s_{21} & s_{22} & \cdots & s_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ s_{m1} & s_{m2} & \cdots & s_{mm} \end{pmatrix},$$

  where $s_{ij} = \mathrm{Cov}[X_i, X_j]$ and $s_{ii} = \mathrm{Var}[X_i]$.

- We call this matrix a *covariance matrix.*

- $\Sigma = \mathrm{Cov}[\mathbf{X}] = \mathrm{Var}[\mathbf{X}]$ (usually referred to by former equality).

Independence

- Two random variables X_1 and X_2 are said to be **independent** if and only if:

$$P(X_1 = x_1, X_2 = x_2) = P(X_1 = x_1)P(X_2 = x_2)$$

- For two independent random variables X_1 and X_2:

$$\mathbb{E}[X_1 X_2] = \mathbb{E}[X_1]\mathbb{E}[X_2]$$

- Proof: Exercise (refer to the definition).

Linear Combinations

- Suppose that a and b are constants and the random variable X has expected value μ and variance σ^2, then

  a) $\mathbb{E}[aX + b] = a\mathbb{E}[X] + b = a\mu + b$

  b) $\mathrm{Var}[aX + b] = a^2\mathrm{Var}[X] = a^2\sigma^2$.

- Let X_1 and X_2 denote two **independent** random variables with respective means μ_1 and μ_2 and variances σ_1^2 and σ_2^2. If a_1 and a_2 are constants, then

  c) $\mathbb{E}[a_1X_1 + a_2X_2] = a_1\mathbb{E}[X_1] + a_2\mathbb{E}[X_2] = a_1\mu_1 + a_2\mu_2$.

  d) $\mathrm{Var}[a_1X_1 + a_2X_2] = a_1^2\mathrm{Var}[X_1] + a_2^2\mathrm{Var}[X_2] = a_1^2\sigma_1^2 + a_2^2\sigma_2^2$.

- If X_1 and X_2 are **not independent** then c) above still holds but d) is replaced by

  e) $\mathrm{Var}[a_1X_1 + a_2X_2] = a_1^2\mathrm{Var}[X_1] + a_2^2\mathrm{Var}[X_2] + 2a_1a_2\mathrm{Cov}[X_1, X_2]$.

- Proofs: Exercise (return to the definitions).

Linear Combinations for Covariance

Suppose that a, b, c and d are constants and X, Y, W and Z are random variables with non-zero variance, then

a) $\text{Cov}[aX + b, cY + d] = ac\text{Cov}[X, Y]$

b) $\text{Cov}[aX + bY, cW + dZ] =$
$ac\text{Cov}[X, W] + ad\text{Cov}[X, Z] + bc\text{Cov}[Y, W] + bd\text{Cov}[Y, Z]$.

- Proofs: Exercise (as with the rest, manipulation of algebra from the definitions).

Matrix representation: Expected Value

- Similar ideas follow in the more general $a_1X_1 + \cdots + a_mX_m$ case.
- Remember $\mathbb{E}[a_1X_1 + a_2X_2 + \cdots + a_mX_m] = a_1\mu_1 + a_2\mu_2 + \cdots a_m\mu_m$.
- Let $\mathbf{a} = (a_1, a_2, \ldots, a_m)^T$ be a vector of constants and $\mathbf{X} = (X_1, X_2, \ldots, X_m)^T$ be a vector of random variables.
- Then we can write

$$a_1X_1 + a_2X_2 + \ldots a_mX_m = (a_1, a_2, \cdots, a_m)\begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_m \end{pmatrix} = \mathbf{a}^T\mathbf{X}$$

- Hence we can write $\mathbb{E}[\mathbf{a}^T\mathbf{X}] = \mathbf{a}^T\mu$, where $\mu = (\mu_1, \mu_2, \ldots, \mu_m)^T$.

Matrix representation: Variance

- Similarly $\mathrm{Var}[a_1X_1 + a_2X_2 + \cdots + a_mX_m] = \mathrm{Var}[\mathbf{a}^T\mathbf{X}]$, and

$$
\begin{aligned}
\mathrm{Var}[\mathbf{a}^T\mathbf{X}] &= a_1^2\mathrm{Var}[X_1] + a_2^2\mathrm{Var}[X_2] + \cdots + a_m^2\mathrm{Var}[X_m] \\
&\quad + a_1a_2\mathrm{Cov}[X_1, X_2] + \cdots + a_1a_m\mathrm{Cov}[X_1, X_m] \\
&\quad + \cdots + a_{m-1}a_m\mathrm{Cov}[X_{m-1}, X_m] \\
&= \sum_{i=1}^{m} a_i^2\mathrm{Var}[X_i] + \sum_{i=1}^{m}\sum_{j\neq i}^{m} a_ia_j\mathrm{Cov}[X_i, X_j] \\
&= \sum_{i=1}^{m} a_i^2 s_{ii} + \sum_{i=1}^{m}\sum_{j\neq i}^{m} a_ia_js_{ij} \\
&= \mathbf{a}^T\mathbf{\Sigma}\mathbf{a}
\end{aligned}
$$

Matrix representation: Covariance

- Suppose that $U = \mathbf{a}^T\mathbf{X}$ and $V = \mathbf{b}^T\mathbf{X}$.

$$\mathrm{Cov}[U, V] = \sum_{i=1}^{m} a_i b_i s_{ii} + \sum_{i=1}^{m} \sum_{j \neq i}^{m} a_i b_j s_{ij}.$$

- In matrix notation,

$$\mathrm{Cov}[U, V] = \mathbf{a}^T\boldsymbol{\Sigma}\mathbf{b} = \mathbf{b}^T\boldsymbol{\Sigma}\mathbf{a}.$$

- Proof: Exercise

Example

- Let $\mathbb{E}[X_1] = 2$, $\mathrm{Var}[X_1] = 4$, $\mathbb{E}[X_2] = 0$, $\mathrm{Var}[X_2] = 1$ and $\mathrm{Cor}[X_1, X_2] = 1/3$.
- **Exercise:**
  - What is the expected value and variance of $X_1 + X_2$?
  - What is the expected value and variance of $X_1 - X_2$?

Eigenvalues and Eigenvectors

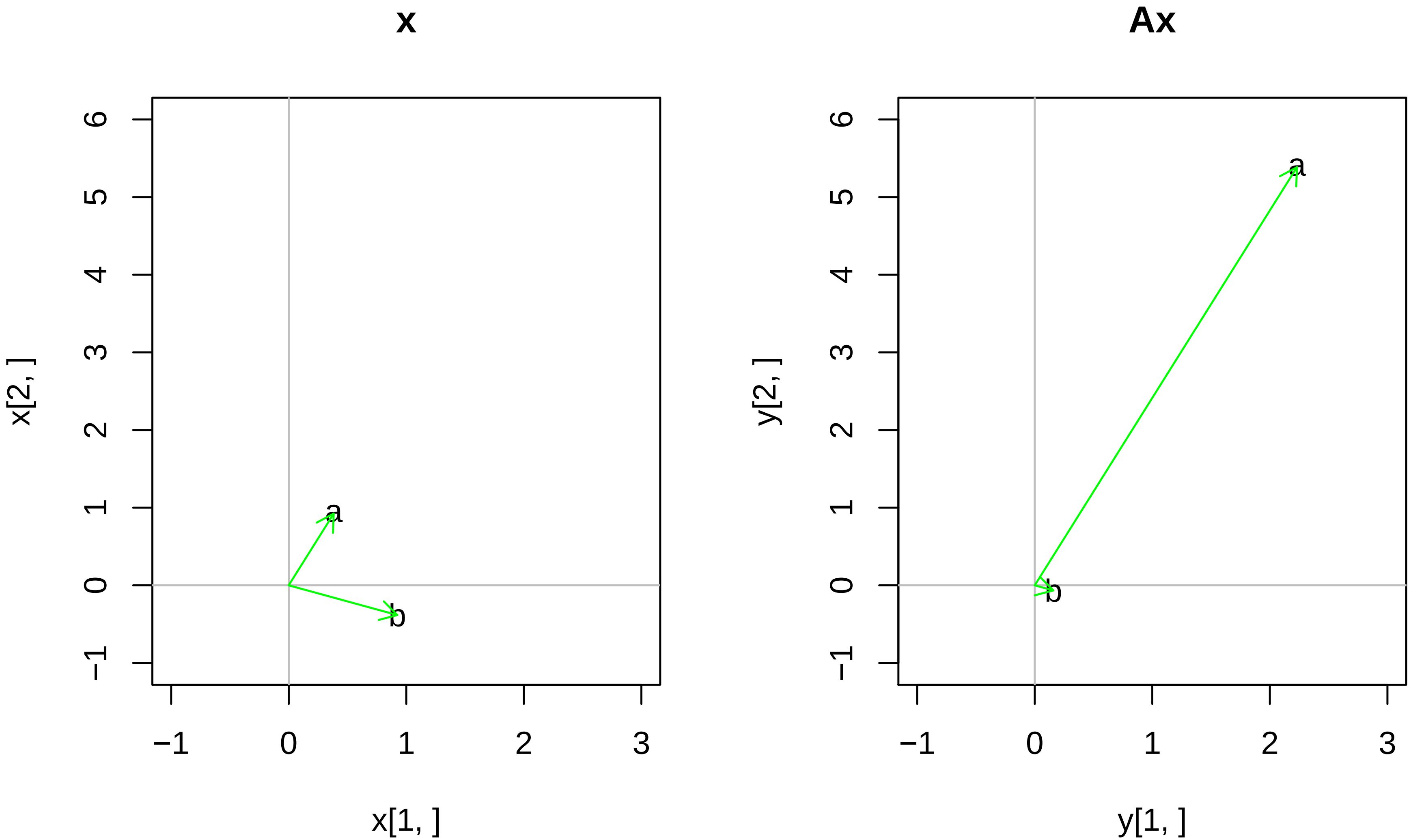
- Suppose that we have a $m \times m$ matrix $\mathbf{A}$.
- **Definition:** λ is an *eigenvalue* of $\mathbf{A}$ if there exists a non-zero vector $\mathbf{v}$ such that
$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}.$$
- The vector $\mathbf{v}$ is said to be an *eigenvector* of $\mathbf{A}$ corresponding to the eigenvalue λ.
- We can find eigenvalues by solving the equation,
$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0.$$

Finding Eigenvalues

- If $\mathbf{v}$ is an eigenvector of $\mathbf{A}$ with eigenvalue λ, then $\mathbf{A}\mathbf{v} - \lambda\mathbf{I}\mathbf{v} = \mathbf{0}$.
- Hence $(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}$.
- If there exists an inverse $(\mathbf{A} - \lambda\mathbf{I})^{-1}$ then the trivial solution $\mathbf{v} = \mathbf{0}$ is obtained.
- When there does not exist a trivial solution there is no inverse and hence $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$.

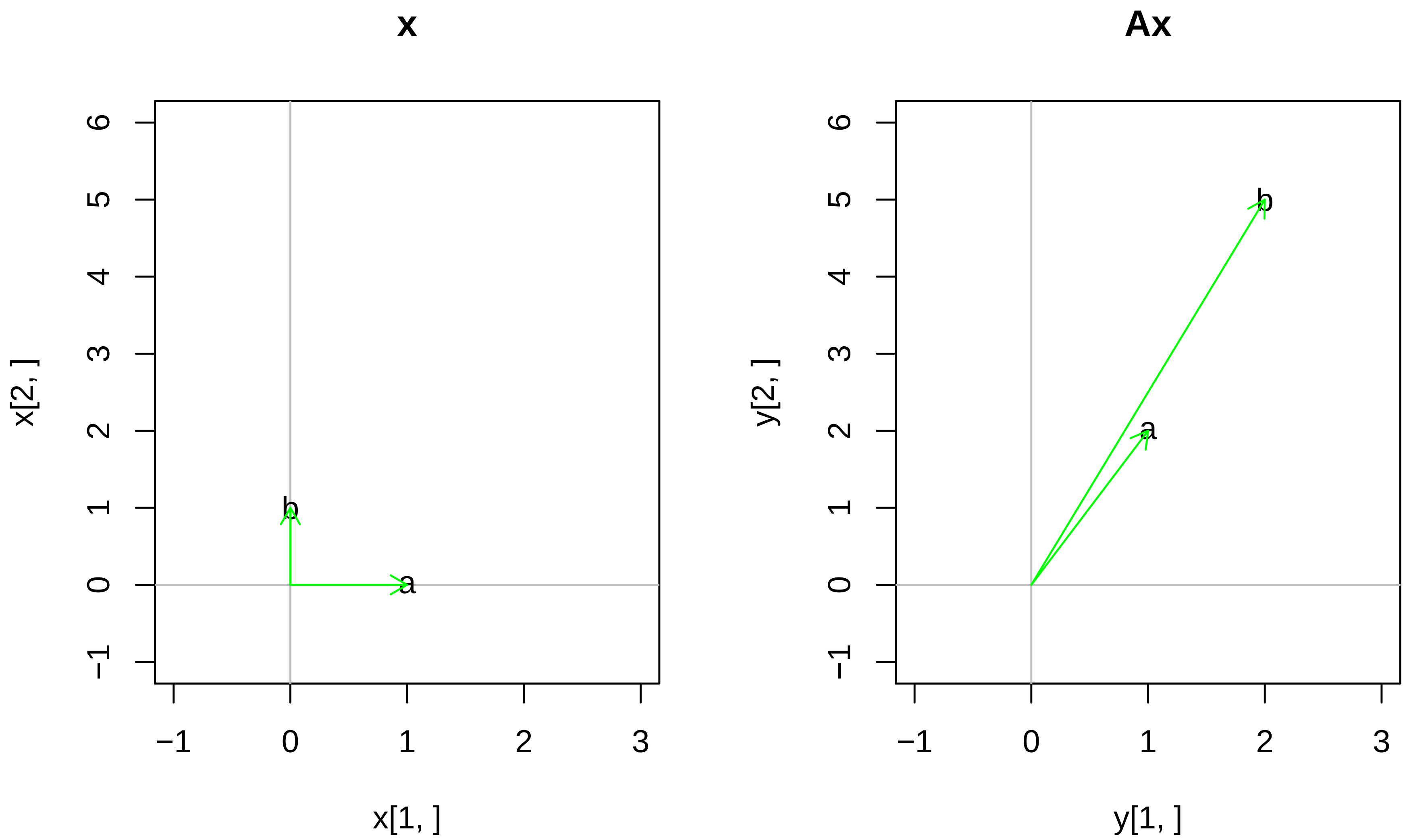
Picture

- The eigenvectors are only scaled by the matrix $\mathbf{A}$.



Picture II

- Other vectors are rotated and scaled by the matrix **A**.



Unit Eigenvectors

- **Property:** If $\mathbf{v}$ is an eigenvector corresponding to eigenvalue λ, then $\mathbf{u} = \alpha \mathbf{v}$ will also be an eigenvector corresponding to λ.
- **Definition:** The eigenvector $\mathbf{v}$ is a *unit eigenvector* if $\sum_{i=1}^{m} v_i^2 = \mathbf{v}^T \mathbf{v} = 1$.
- We can turn any eigenvector $\mathbf{v}$ into a unit eigenvector by multiplying it by the value $\alpha = \frac{1}{\sqrt{\mathbf{v}^T \mathbf{v}}}$.

Orthogonal and Orthonormal Vectors

- **Definition:** Two vectors $\mathbf{u}$ and $\mathbf{v}$ are *orthogonal* if $\mathbf{u}^T\mathbf{v} = 0 = \mathbf{v}^T\mathbf{u}$.

- **Definition:** Two vectors $\mathbf{u}$ and $\mathbf{v}$ are *orthonormal* if they are orthogonal and $\mathbf{u}^T\mathbf{u} = 1$ and $\mathbf{v}^T\mathbf{v} = 1$.

Eigenvalues of Covariance Matrices

- **Fact:** The eigenvalues of a covariance matrix $\mathbf{\Sigma}$ are non-negative.
- If λ is an eigenvalue of $\mathbf{\Sigma}$, then

$$\mathbf{\Sigma v} = \lambda \mathbf{v},$$

  where $\mathbf{v}$ is an eigenvector corresponding to λ.

- Hence,

$$\mathbf{v}^T \mathbf{\Sigma v} = \mathbf{v}^T \lambda \mathbf{v} = \lambda \mathbf{v}^T \mathbf{v}$$

$$\Rightarrow \lambda = \frac{\mathbf{v}^T \mathbf{\Sigma v}}{\mathbf{v}^T \mathbf{v}}.$$

- The numerator and denominator are both non-negative (why?), so λ must be non-negative.

Eigenvectors of Covariance Matrices

- **Fact:** An $m \times m$ covariance matrix $\mathbf{\Sigma}$ has m orthonormal eigenvectors.
- Proof Omitted, but uses Spectral Decomposition (or similar theorem) of a symmetric matrix.
- This result will be used when developing principal components analysis.

Example

- Suppose that we have the matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}.$$

- **Question:** What are the eigenvalues and corresponding eigenvectors of $\mathbf{A}$?

Example

- **Answer:** The eigenvalues are 5.83 and 0.17 (2dp) and the corresponding eigenvectors are

$$\begin{pmatrix} 0.38 \\ 0.92 \end{pmatrix} \text{ and } \begin{pmatrix} 0.92 \\ -0.38 \end{pmatrix}.$$

Example: Frog Cranial Measurements

- **Example:** The cranial length and cranial breath of 35 female frogs are believed to have expected value $(23, 24)^T$ and covariance matrix

$$\begin{pmatrix} 17.7 & 20.3 \\ 20.3 & 24.4 \end{pmatrix}$$

- **Question:** What are the eigenvalues and eigenvectors of the covariance matrix?