Linear Algebra and Matrices

Methods for Dummies

21st October, 2009

Elvina Chu & Flavia Mancini

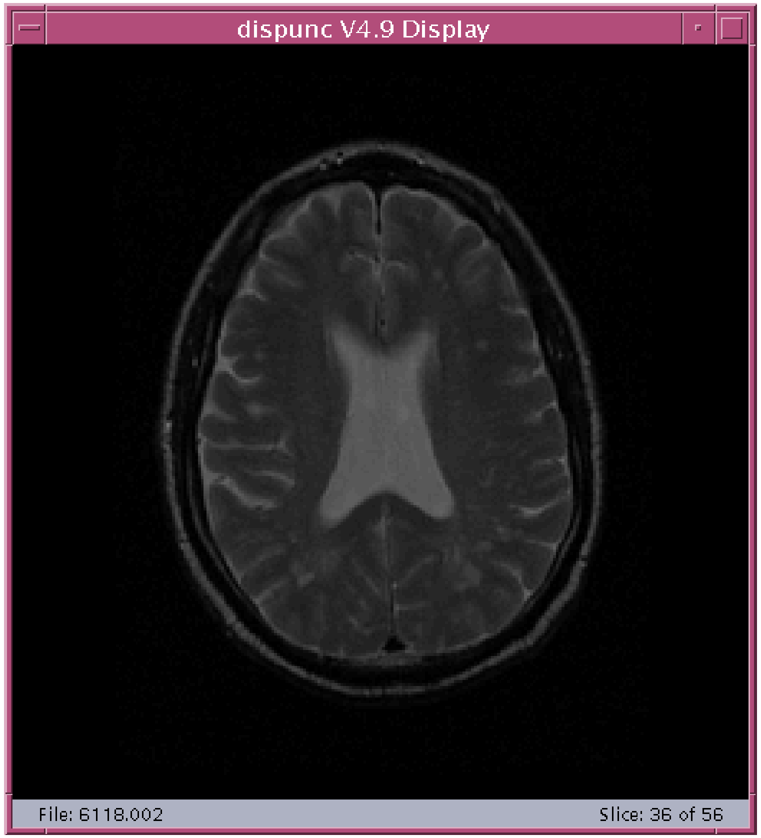
Talk Outline

- Scalars, vectors and matrices
- Vector and matrix calculations
- Identity, inverse matrices & determinants
- Solving simultaneous equations
- Relevance to SPM

Scalar

- Variable described by a single number

e.g. Intensity of each voxel in an MRI scan



Vector

- Not a physics vector (magnitude, direction)
- Column of numbers e.g. intensity of same voxel at different time points

$$\begin{bmatrix} x1 \\ x2 \\ x3 \end{bmatrix}$$

Matrices

- Rectangular display of vectors in rows and columns
- Can inform about the same vector intensity at different times or different voxels at the same time
- Vector is just a n x 1 matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 5 & 4 & 1 \\ 6 & 7 & 4 \end{bmatrix} \qquad \mathbf{C} = \begin{bmatrix} 1 & 4 \\ 2 & 7 \\ 3 & 8 \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} d_{11} & d_{12} & d_{13} \\ d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \end{bmatrix}$$

Square (3 x 3) Rectangular (3 x 2) $d_{i\,j}$: i^{th} row, j^{th} column

Defined as rows x columns (R x C)

Matrices in Matlab

- X=matrix
- ;=end of a row
- :=all row or column

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

Subscripting – each element of a matrix can be addressed with a pair of numbers; row first, column second (Roman Catholic)

e.g. **X(2,3) = 6**

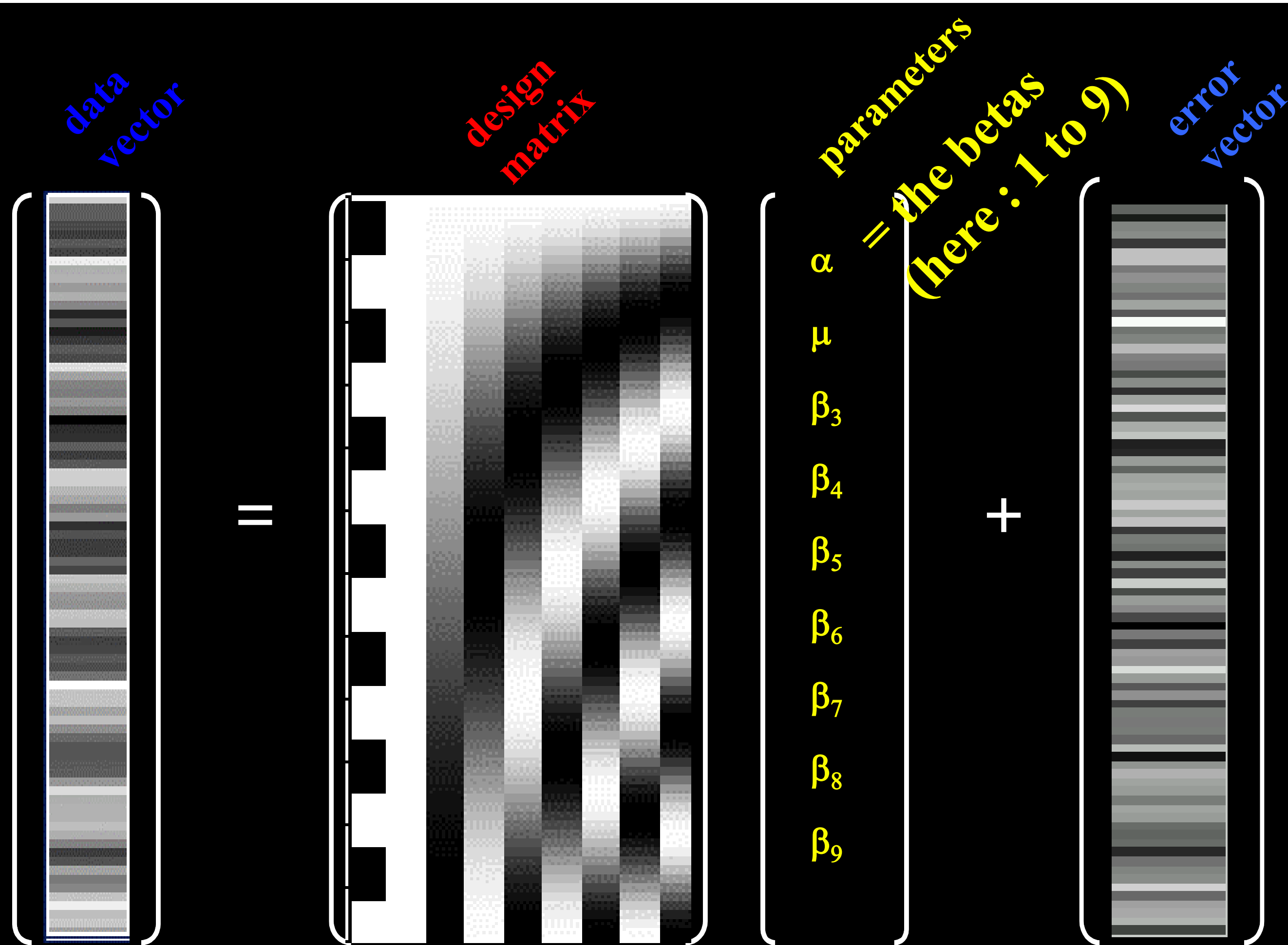
X(3, :) = $\begin{pmatrix} 7 & 8 & 9 \end{pmatrix}$

X([2 3], 2) = $\begin{pmatrix} 5 \\ 8 \end{pmatrix}$

"Special" matrix commands:

- `zeros(3,1)` = $\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$
- `ones(2)` = $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$
- `magic(3)` = $\begin{pmatrix} 8 & 1 & 6 \\ 3 & 5 & 7 \\ 4 & 9 & 2 \end{pmatrix}$

Design matrix



$$Y = X \times \beta + \varepsilon$$

Transposition

$$\mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix} \qquad \mathbf{b}^T = \begin{bmatrix} 1 & 1 & 2 \end{bmatrix} \qquad \mathbf{d} = \begin{bmatrix} 3 & 4 & 9 \end{bmatrix} \qquad \mathbf{d}^T = \begin{bmatrix} 3 \\ 4 \\ 9 \end{bmatrix}$$

column $\longrightarrow$ row   row $\longrightarrow$ column

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 5 & 4 & 1 \\ 6 & 7 & 4 \end{bmatrix} \qquad \mathbf{A}^T = \begin{bmatrix} 1 & 5 & 6 \\ 2 & 4 & 7 \\ 3 & 1 & 4 \end{bmatrix}$$

Matrix Calculations

Addition

– Commutative: **A**+**B**=**B**+**A**

– Associative: (**A**+**B**)+**C**=**A**+(**B**+**C**)

$$\mathbf{A}+\mathbf{B}=\begin{bmatrix}2 & 4\\ 2 & 5\end{bmatrix}+\begin{bmatrix}1 & 0\\ 3 & 1\end{bmatrix}=\begin{bmatrix}2+1 & 4+0\\ 2+3 & 5+1\end{bmatrix}\begin{bmatrix}3 & 4\\ 5 & 6\end{bmatrix}$$

Subtraction

- By adding a negative matrix

$$\mathbf{A}-\mathbf{B}=\begin{bmatrix}2 & 4\\ 5 & 3\end{bmatrix}-\begin{bmatrix}1 & 2\\ 3 & 4\end{bmatrix}=\begin{bmatrix}2 & 4\\ 5 & 3\end{bmatrix}+\begin{bmatrix}-1 & -2\\ -3 & -4\end{bmatrix}=\begin{bmatrix}1 & 2\\ 2 & -1\end{bmatrix}$$

Scalar multiplication

- Scalar x matrix = scalar multiplication

$$\lambda \begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix} = \begin{pmatrix} \lambda a & \lambda b & \lambda c \\ \lambda d & \lambda e & \lambda f \end{pmatrix}$$

Matrix Multiplication

*"When **A** is a **m**x**n** matrix & **B** is a **k**x**l** matrix, **AB** is only possible if **n=k**. The result will be an **mxl** matrix"*

$$
\begin{array}{c}
\begin{array}{cc} & \xrightarrow{\textbf{n}} \\ \textbf{m}\ \big\downarrow & \begin{matrix} A_1 & A_2 & A_3 \\ A_4 & A_5 & A_6 \\ A_7 & A_8 & A_9 \\ A_{10} & A_{11} & A_{12} \end{matrix} \end{array}
\quad \times \quad
\begin{array}{cc} \xrightarrow{\textbf{l}} & \\ \begin{matrix} B_{13} & B_{14} \\ B_{15} & B_{16} \\ B_{17} & B_{18} \end{matrix} & \big\downarrow\ \textbf{k} \end{array}
\quad = \textbf{m} \times \textbf{l} \text{ matrix}
\end{array}
$$

Number of columns in A = Number of rows in B

Matrix multiplication

- Multiplication method:

Sum over product of respective <u>rows</u> and <u>columns</u>

$$\begin{pmatrix} 1 & 0 \\ 2 & 3 \end{pmatrix} \times \begin{pmatrix} 2 & 1 \\ 3 & 1 \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$$

A **B**

Define output matrix

$$= \begin{bmatrix} (1\times 2)+(0\times 3) & (1\times 1)+(0\times 1) \\ (2\times 2)+(3\times 3) & (2\times 1)+(3\times 1) \end{bmatrix}$$

$$= \begin{pmatrix} \mathbf{2} & \mathbf{1} \\ \mathbf{13} & \mathbf{5} \end{pmatrix}$$

- Matlab does all this for you!
- Simply type: C = A * B

Matrix multiplication

- Matrix multiplication is NOT commutative
- $AB \neq BA$
- Matrix multiplication IS associative
- $A(BC)=(AB)C$
- Matrix multiplication IS distributive
- $A(B+C)=AB+AC$
- $(A+B)C=AC+BC$

Vector Products

Two vectors:

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

Inner product = scalar

Inner product $X^T Y$ is a scalar
(1xn) (nx1)

$$\mathbf{x}^T \mathbf{y} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = x_1 y_1 + x_2 y_2 + x_3 y_3 = \sum_{i=1}^{3} x_i y_i$$

Outer product = matrix

$$xy^T = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & x_1 y_3 \\ x_2 y_1 & x_2 y_2 & x_2 y_3 \\ x_3 y_1 & x_3 y_2 & x_3 y_3 \end{bmatrix}$$

Outer product XY^T is a matrix
(nx1) (1xn)

Identity matrix

Is there a matrix which plays a similar role as the number 1 in number multiplication?

Consider the nxn matrix:

$$I_n = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}.$$

For any nxn matrix $\boldsymbol{A}$, we have $\boldsymbol{A}\,\boldsymbol{I}_n = \boldsymbol{I}_n\,\boldsymbol{A} = \boldsymbol{A}$

For any nxm matrix $\boldsymbol{A}$, we have $\boldsymbol{I}_n\,\boldsymbol{A} = \boldsymbol{A}$, and $\boldsymbol{A}\,\boldsymbol{I}_m = \boldsymbol{A}$ (so 2 possible matrices)

Identity matrix

Worked example
$\boldsymbol{A I_3 = A}$
for a 3x3 matrix:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1+0+0 & 0+2+0 & 0+0+3 \\ 4+0+0 & 0+5+0 & 0+0+6 \\ 7+0+0 & 0+8+0 & 0+0+9 \end{bmatrix}$$

- In Matlab: **eye(r, c)** produces an r x c identity matrix

Matrix inverse

- **Definition.** A matrix $\boldsymbol{A}$ is called **nonsingular** or **invertible** if there exists a matrix $\boldsymbol{B}$ such that:

$$\boxed{AB = BA = I_n}$$

$$\begin{bmatrix} 1 & 1 \\ -1 & 2 \end{bmatrix} \times \begin{bmatrix} \frac{2}{3} & \frac{-1}{3} \\ \frac{1}{3} & \frac{1}{3} \end{bmatrix} = \begin{bmatrix} \frac{2}{3}+\frac{1}{3} & \frac{-1}{3}+\frac{1}{3} \\ \frac{-2}{3}+\frac{2}{3} & \frac{1}{3}+\frac{2}{3} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

- **Notation.** A common notation for the inverse of a matrix $\boldsymbol{A}$ is $\boldsymbol{A}^{-1}$. So:

$$\boxed{AA^{-1} = A^{-1}A = I_n\,.}$$

- The inverse matrix is unique when it exists. So if $\boldsymbol{A}$ is invertible, then $\boldsymbol{A}^{-1}$ is also invertible and then $(A^T)^{-1} = (A^{-1})^T$

• In Matlab: $\boldsymbol{A}^{-1}$ = **inv(A)**

•Matrix division: A/B= $\boldsymbol{A}*\boldsymbol{B}^{-1}$

Matrix inverse

- For a XxX square matrix: $A = \begin{pmatrix} x_{1,1} & \dots & x_{1,j} \\ \vdots & \ddots & \vdots \\ x_{i,1} & \dots & x_{i,j} \end{pmatrix}$
- The inverse matrix is: $A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} \operatorname{cof}(A, x_{1,1}) & \dots & \operatorname{cof}(A, x_{1,j}) \\ \vdots & \ddots & \vdots \\ \operatorname{cof}(A, x_{i,1}) & \dots & \operatorname{cof}(A, x_{i,j}) \end{pmatrix}^T$
- E.g.: 2x2 matrix $\mathbf{A}^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$

Determinants

• Determinants are mathematical objects that are very useful in the analysis and solution of systems of linear equations (i.e. GLMs).

• The **determinant** is a function that associates a scalar det(A) to every square matrix A.

- Input is nxn matrix
- Output is a single number (real or complex) called the determinant

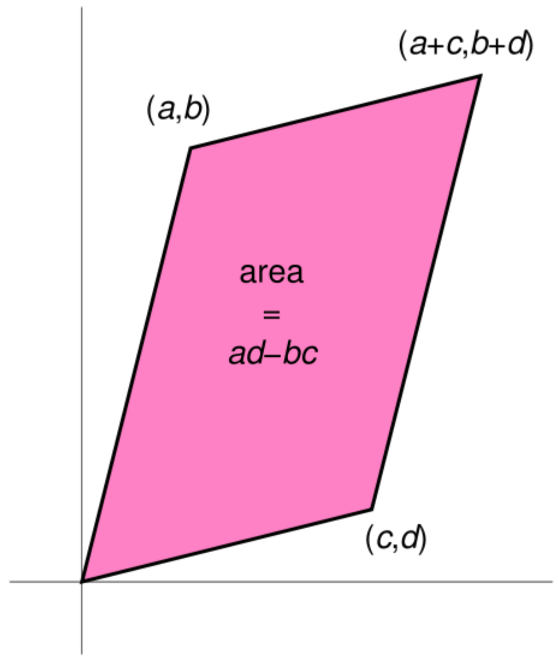
$$\det(M) = \begin{vmatrix} M_{11} & M_{12} & \cdots & M_{1n} \\ M_{21} & M_{22} & \cdots & M_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ M_{n1} & M_{n2} & \cdots & M_{nn} \end{vmatrix} = \sum_{x} \operatorname{sgn}(x) M_{1x_1} M_{2x_2} \cdots M_{nx_n}$$

Determinants

•Determinants can only be found for square matrices.

•For a 2x2 matrix A, **det(A) = ad-bc.** Lets have at closer look at that:

$$\det(A) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$$



• In Matlab: ***det(A)*** = `det(A)`

• A matrix A has an inverse matrix A^{-1} if and only if **det(A)≠0.**

Solving simultaneous equations

For one linear equation ***ax=b*** where the unknown is *x* and *a* and *b* are constants,

3 possibilities:

- If $\boxed{a \neq 0}$ then $x = \dfrac{b}{a} \equiv a^{-1}b$ thus there is single solution
- If $\boxed{a = 0\,,\ b = 0}$ then the equation $ax = b$ becomes $0 = 0$ and any value of x will do
- If $\boxed{a = 0\,,\ b \neq 0}$ then $ax = b$ becomes $0 = b$ which is a contradiction

With >1 equation and >1 unknown

- Can use solution $x = a^{-1}b$ from the single equation to solve
- For example $$2x_1 + 3x_2 = 5$$ $$x_1 - 2x_2 = -1$$
- In matrix form $$\begin{bmatrix} 2 & 3 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 4 \end{bmatrix}$$

A X = B

$$X = A^{-1}B$$

- X = A⁻¹B
- To find A^{-1}

$$A^{-1} = \frac{1}{\det(A)} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

- Need to find determinant of matrix A

$$\det(A) = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

- From earlier

$$\begin{bmatrix} 2 & 3 \\ 1 & -2 \end{bmatrix}$$

(2 -2) – (3 1) = -4 – 3 = -7

- So determinant is -7

$$A^{-1} = \frac{1}{(-7)}\begin{bmatrix} -2 & -3 \\ -1 & 2 \end{bmatrix} = \frac{1}{7}\begin{bmatrix} 2 & 3 \\ 1 & -2 \end{bmatrix}$$

if B is $\begin{bmatrix} 1 \\ 4 \end{bmatrix}$

$$x = a^{-1}b$$

$$X = \frac{1}{7}\begin{bmatrix} 2 & 3 \\ 1 & -2 \end{bmatrix}\begin{bmatrix} 1 \\ 4 \end{bmatrix} = \frac{1}{7}\begin{bmatrix} 14 \\ -7 \end{bmatrix} = \frac{2}{-1}$$

So $\boxed{\begin{array}{l} x_1 = 2 \\ x_2 = -1 \end{array}}$

How are matrices relevant to fMRI data?

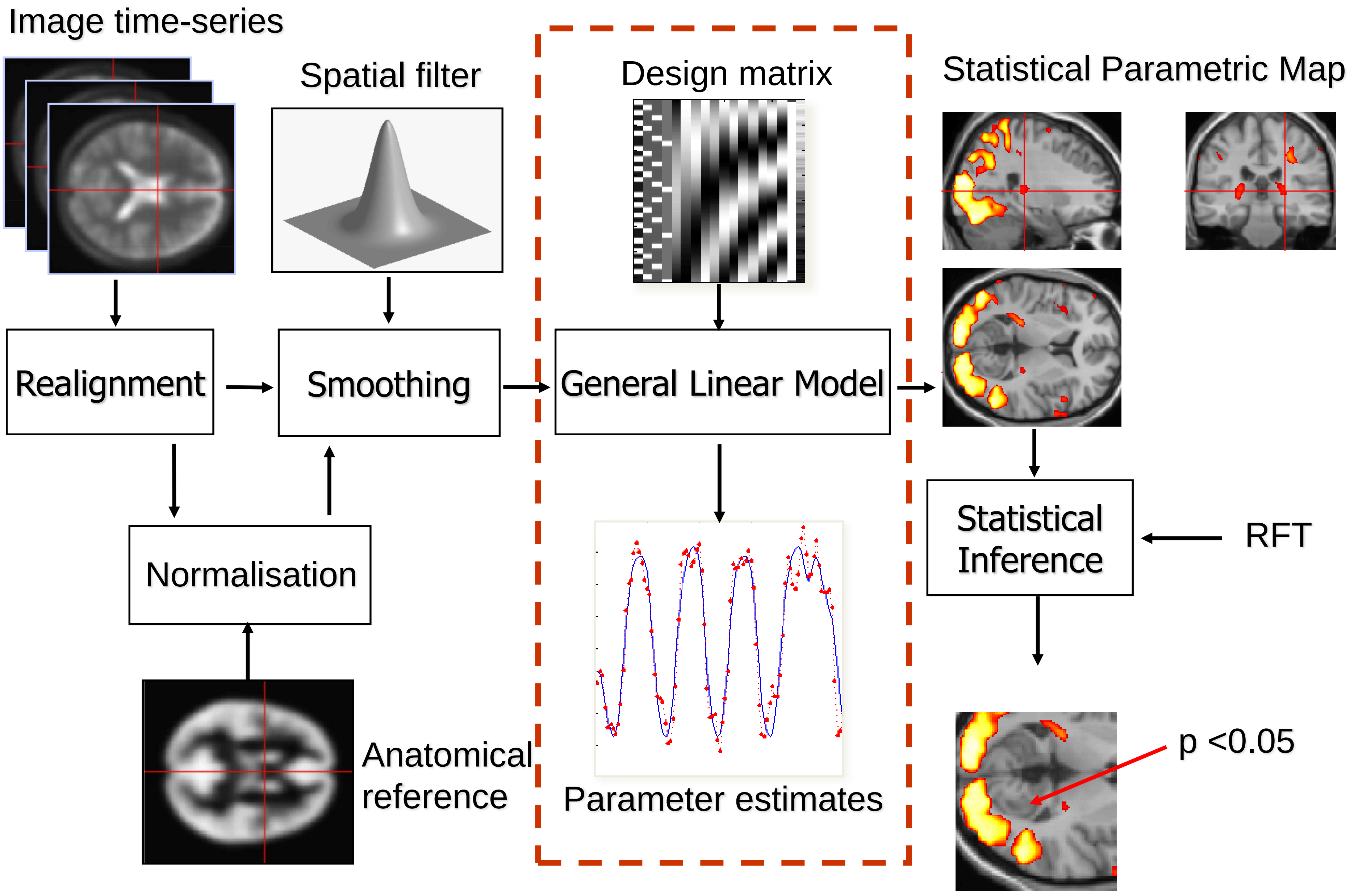
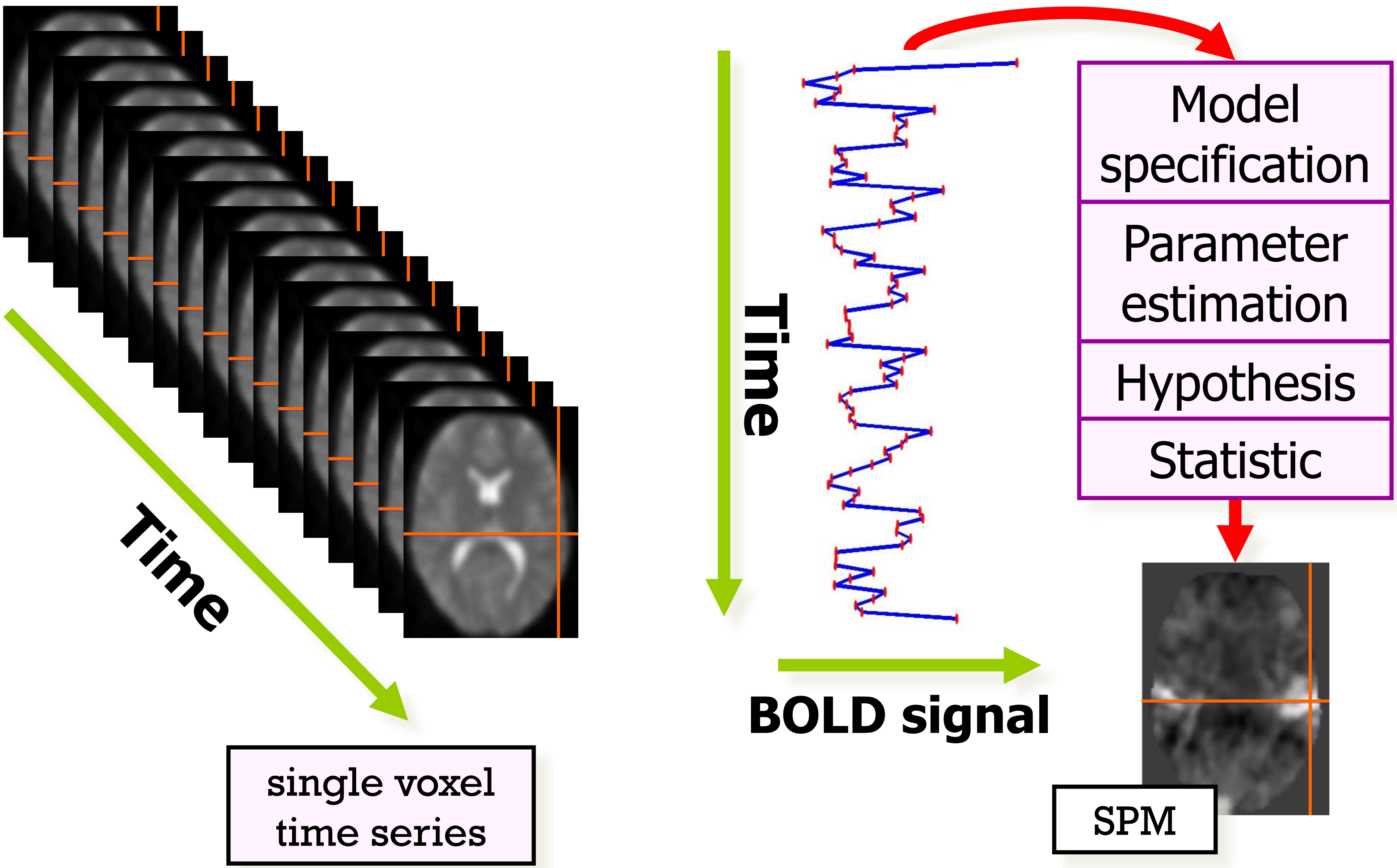


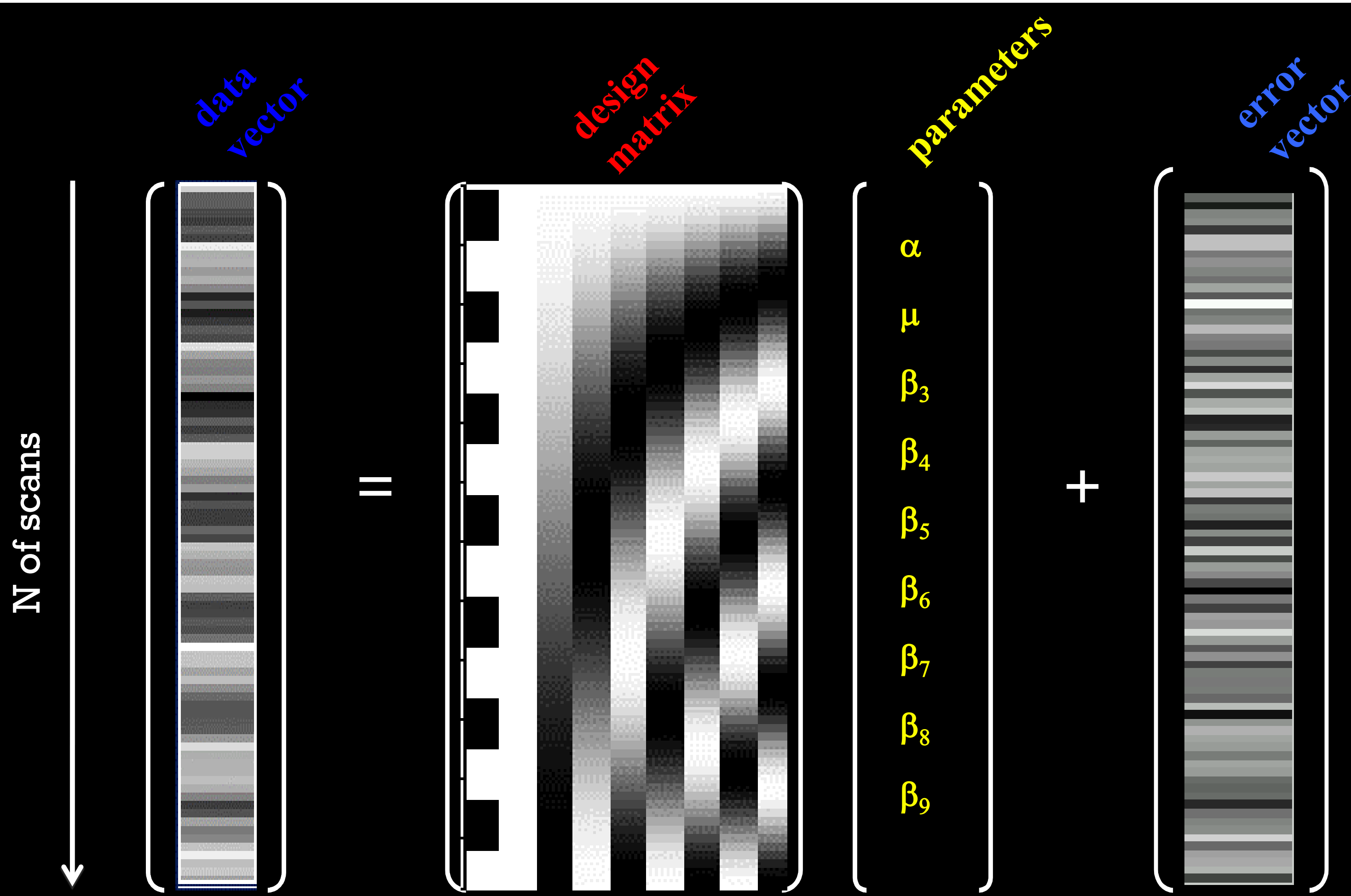
Image time-series
Spatial filter
Design matrix
Statistical Parametric Map
Realignment
Smoothing
General Linear Model
Normalisation
Anatomical reference
Parameter estimates
Statistical Inference
RFT
p <0.05

Voxel-wise time series analysis



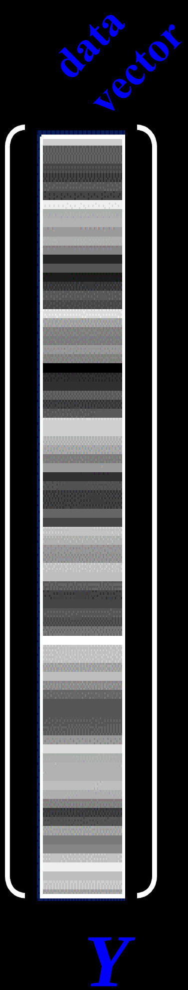
How are matrices relevant to fMRI data?

GLM equation



$$Y = X \times \beta + \varepsilon$$

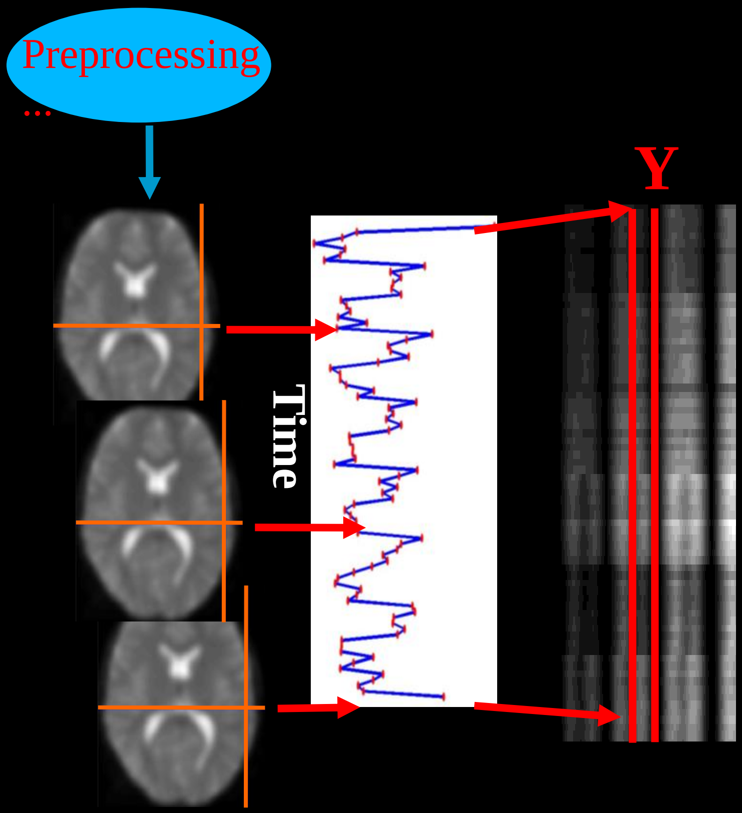
How are matrices relevant to fMRI data?



Response variable

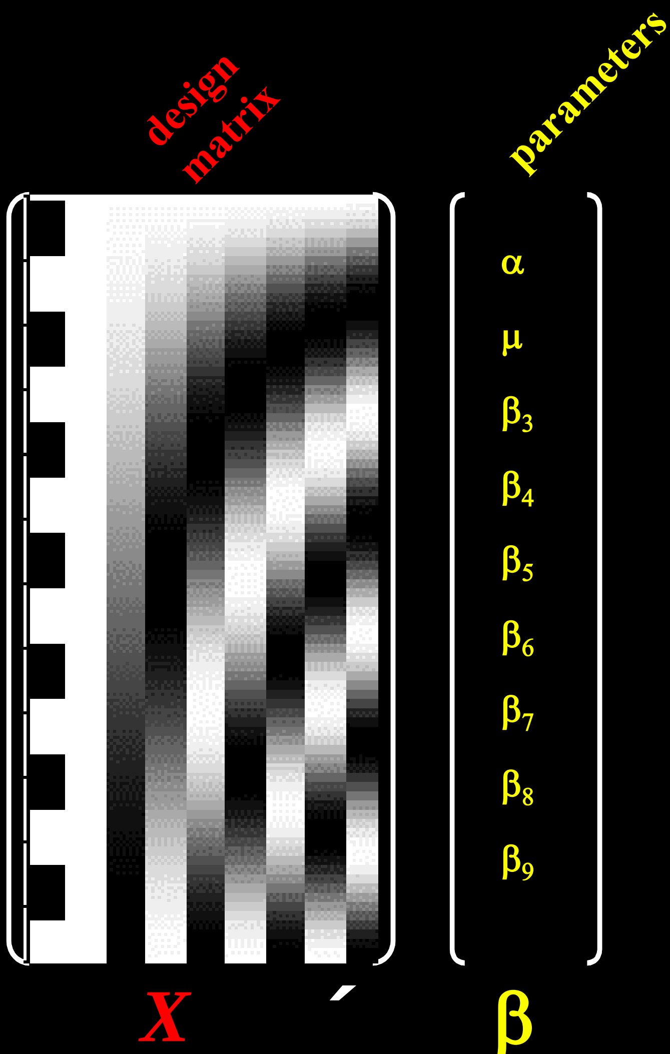
e.g BOLD signal at a particular voxel

A single voxel sampled at successive time points.
Each voxel is considered as independent observation.



$$Y = X \, . \, \beta + \varepsilon$$

How are matrices relevant to fMRI data?



Explanatory variables

- These are assumed to be measured without error.
- May be continuous;
- May be dummy, indicating levels of an experimental factor.

Solve equation for β – tells us how much of the BOLD signal is explained by X

$$Y = X \cdot \beta + \varepsilon$$

In Practice

- Estimate MAGNITUDE of signal changes
- MR INTENSITY levels for each voxel at various time points
- Relationship between experiment and voxel changes are established
- Calculation and notation require linear algebra

Summary

- SPM builds up data as a matrix.
- Manipulation of matrices enables unknown values to be calculated.

$$Y = X \cdot \beta + \varepsilon$$

Observed = Predictors * Parameters + Error

BOLD = Design Matrix * Betas + Error

References

- SPM course http://www.fil.ion.ucl.ac.uk/spm/course/
- Web Guides

http://mathworld.wolfram.com/LinearAlgebra.html

http://www.maths.surrey.ac.uk/explore/emmaspages/option1.html

http://www.inf.ed.ac.uk/teaching/courses/fmcs1/

(Formal Modelling in Cognitive Science course)

- http://www.wikipedia.org
- Previous MfD slides