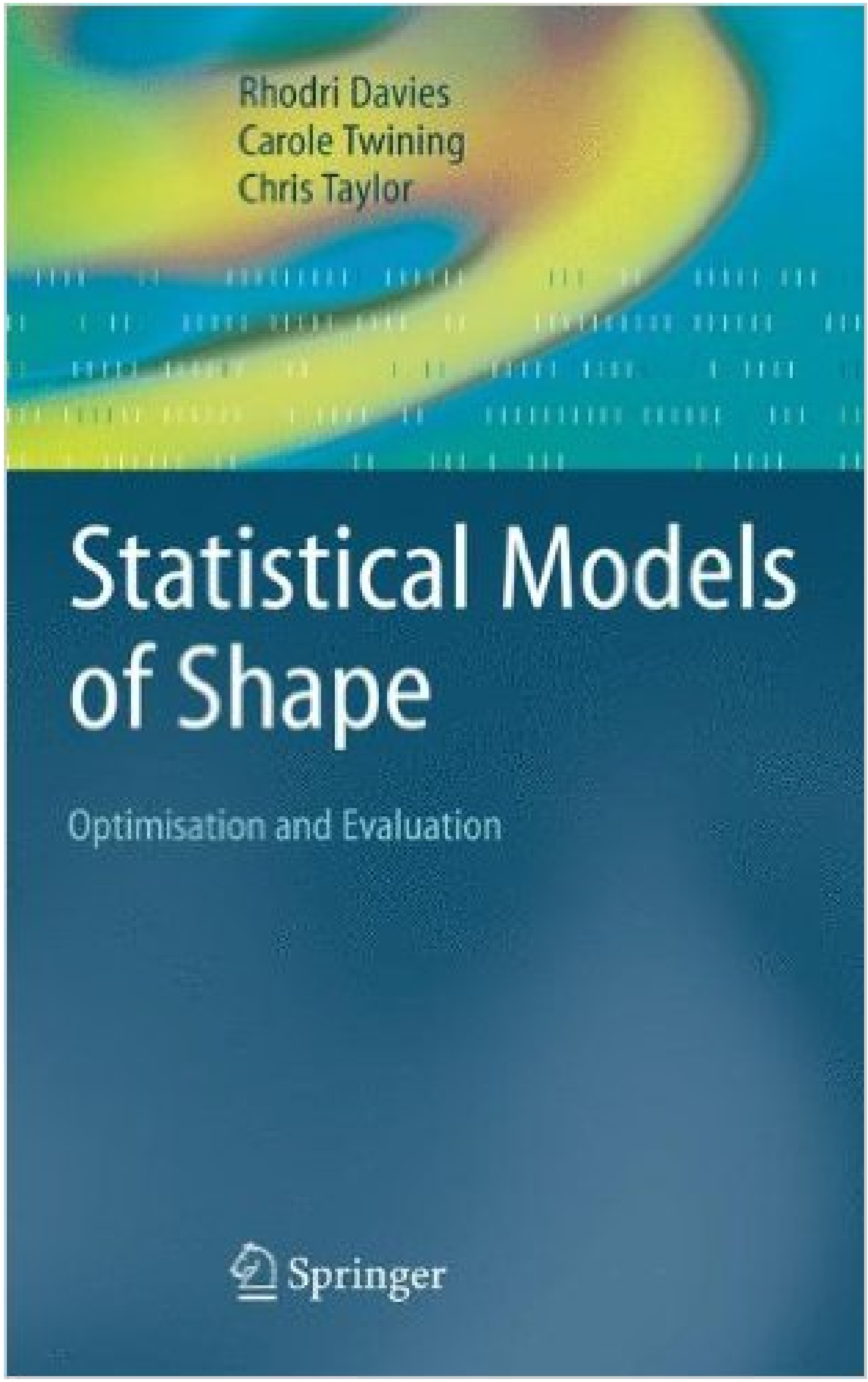
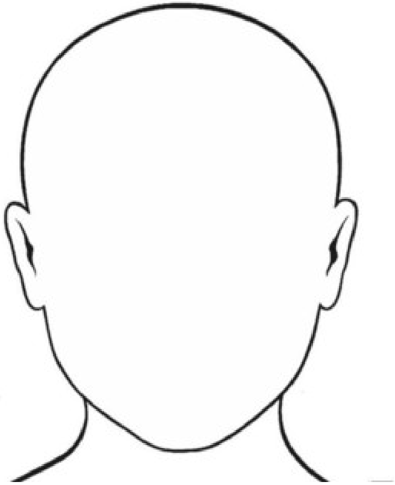
Statistical Shape Analysis

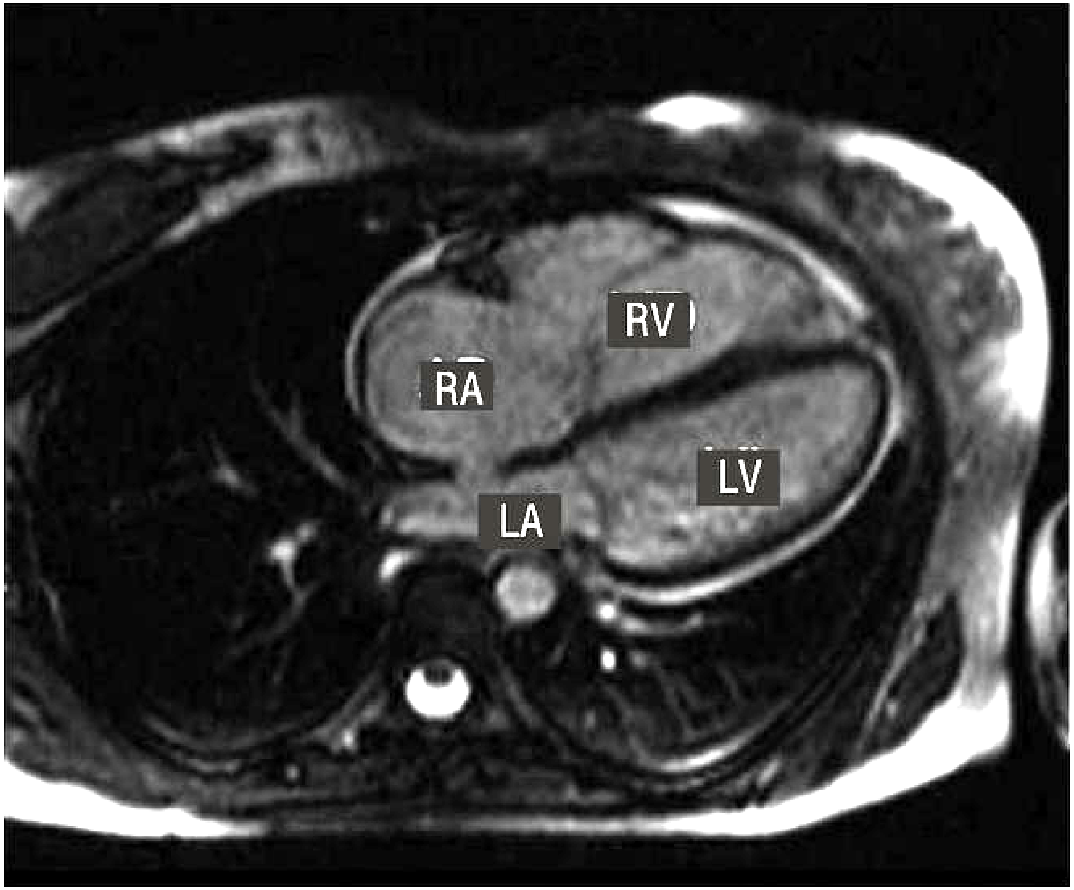


Suyash P. Awate

Shape

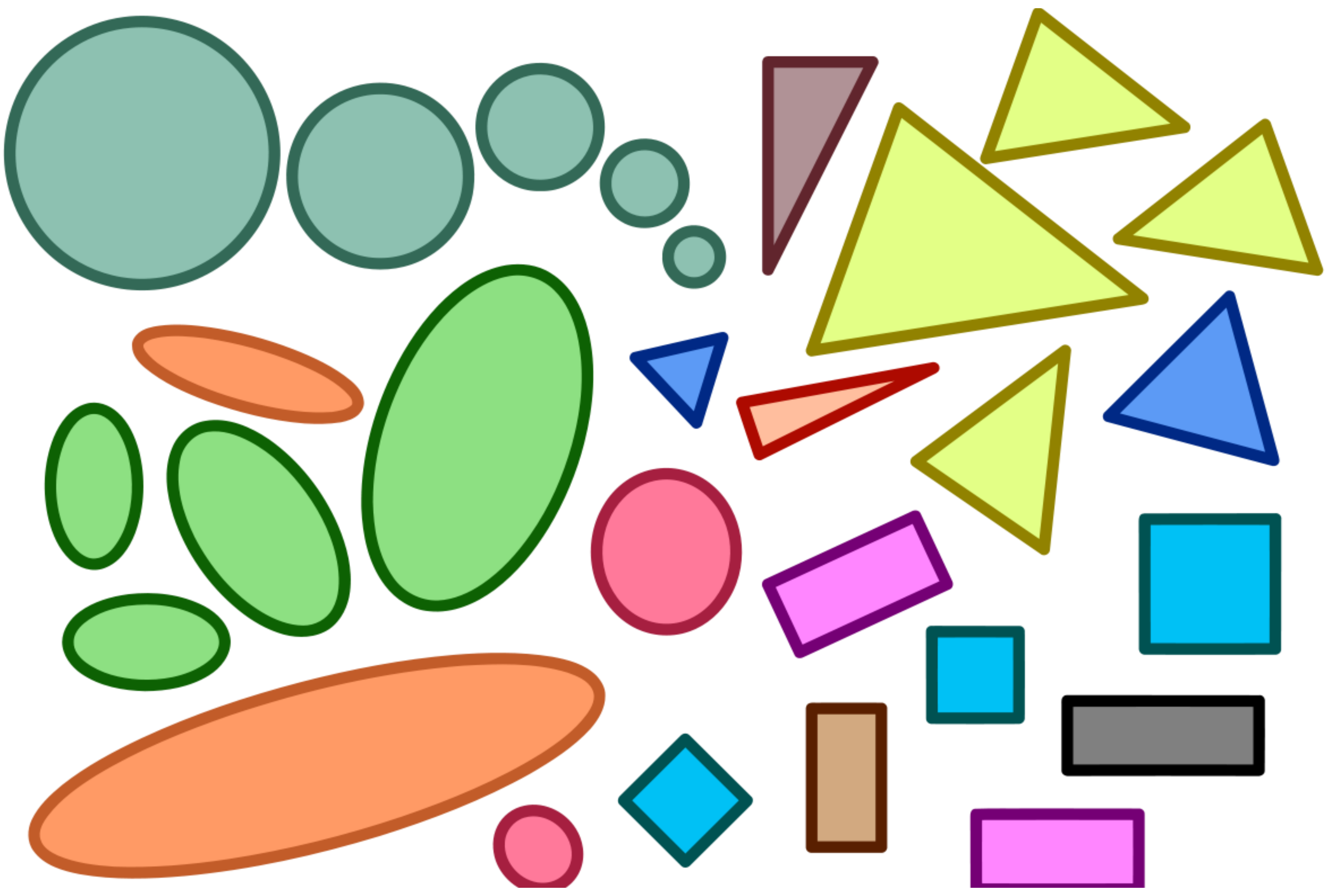
- **What is shape ?**
  - Shape [noun]: the external form, contours, or outline of someone or something



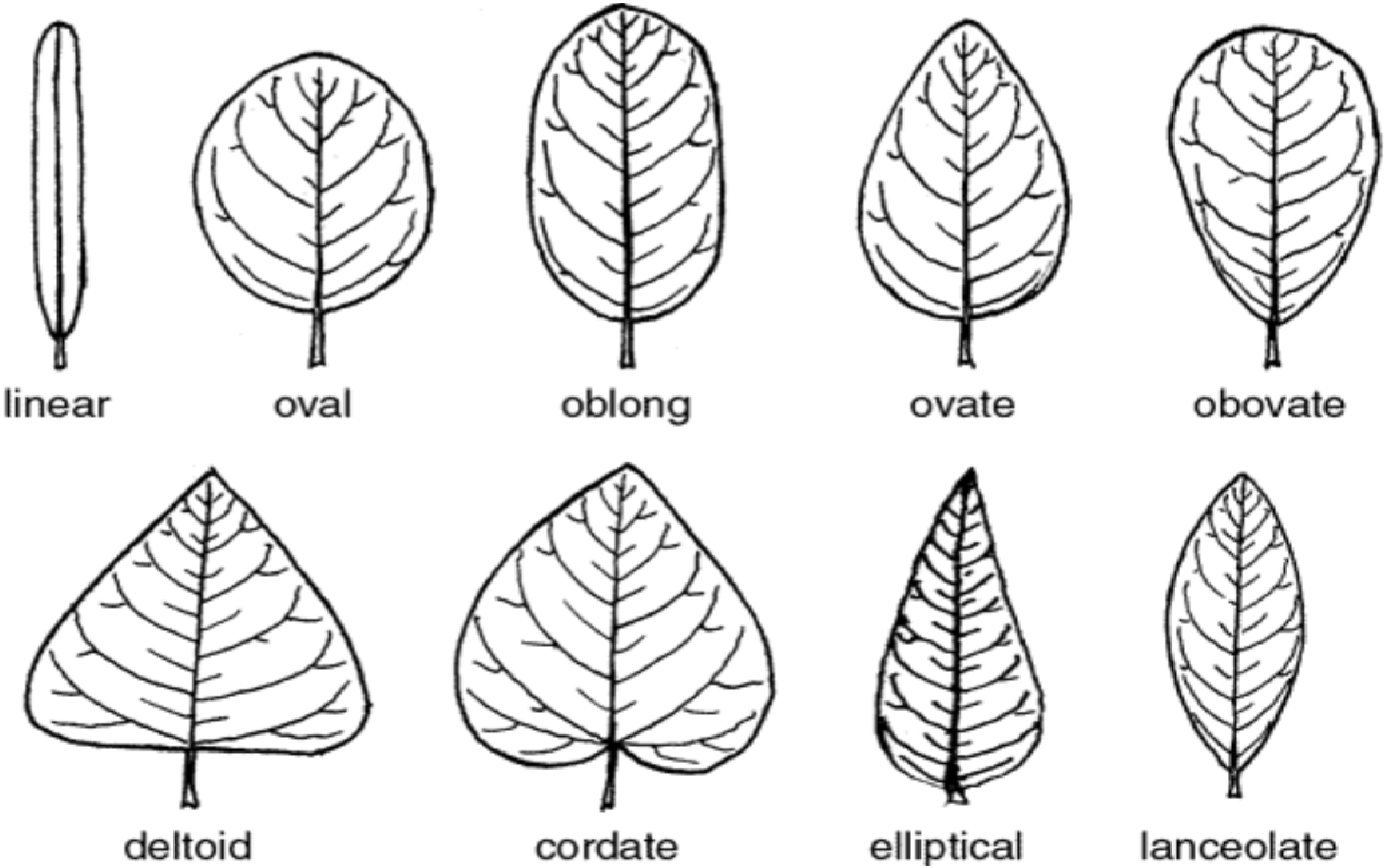


Shape

- Are these same shapes ?
  - Shape versus size
  - Shape versus pose / orientation

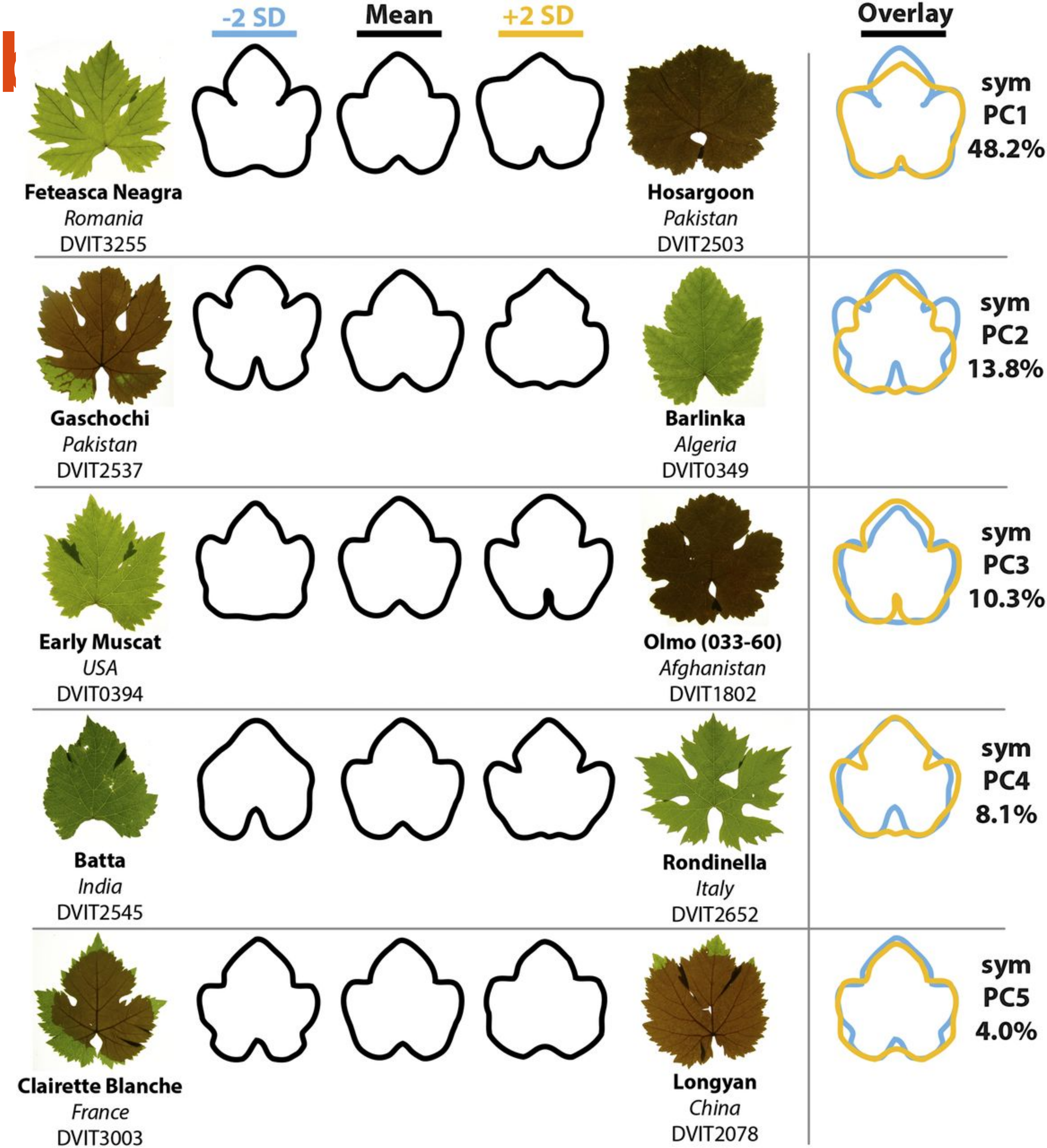


Shape Variability



Shape Variat

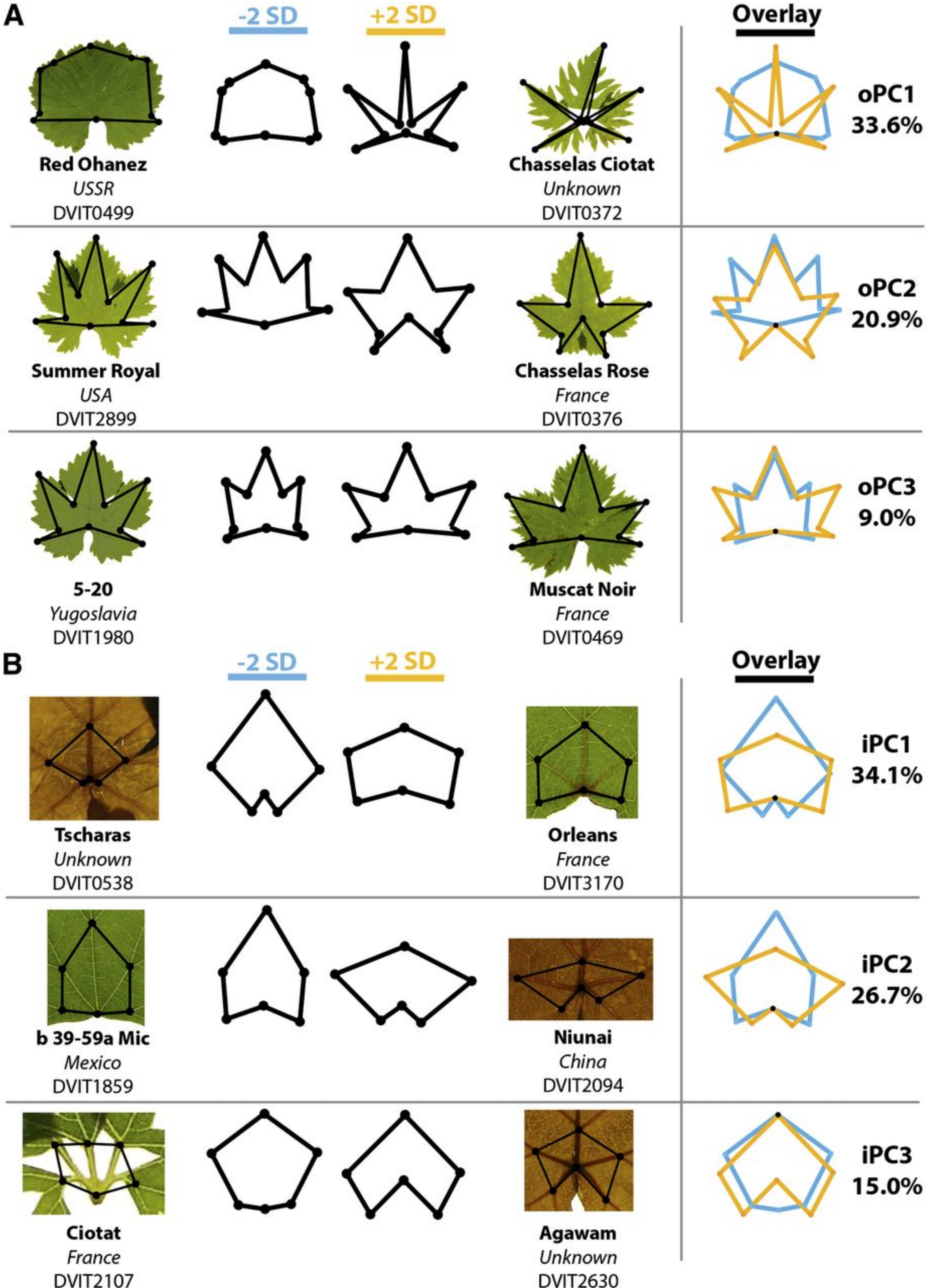
- Grape leaf shapes
  - Genetic similarities
    - PCA on elliptic Fourier descriptor



http://www.plantphysiol.org/content/164/1/259

Shape Variability

- Grape leaf shapes
  - Genetic similarities
    - GPA on landmarks



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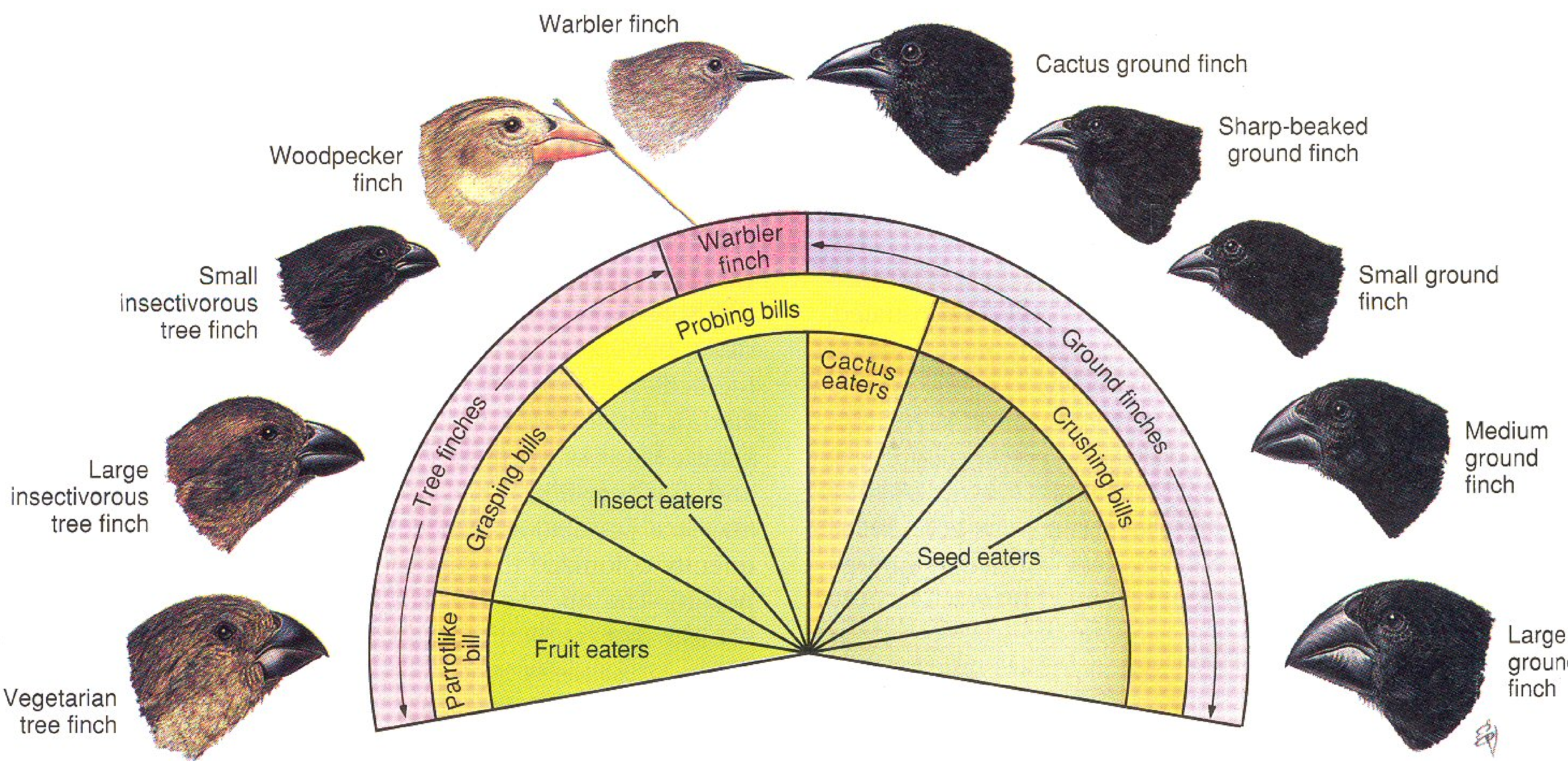
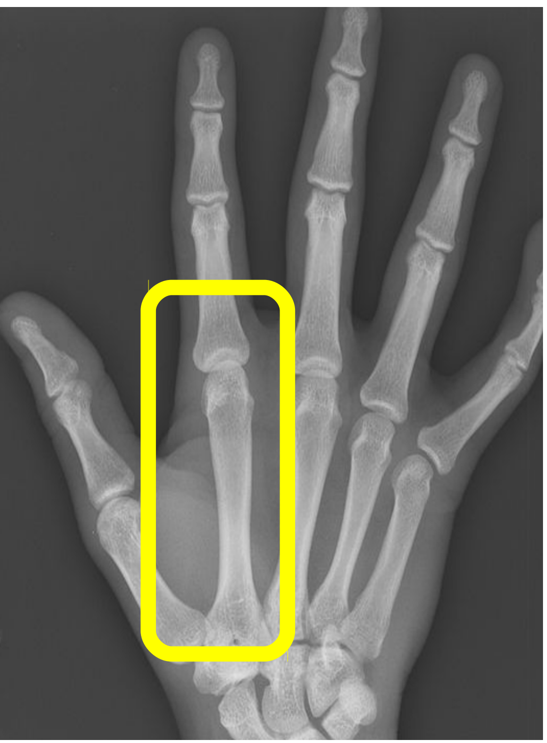
Shape Variability

- Darwin's finches
  - Variation of beak's shape and size



Statistical Shape Analysis

- Normal / abnormal variation of shape of structure
  - What is the mean (typical) shape?
  - What is the variability of shapes around the mean shape?



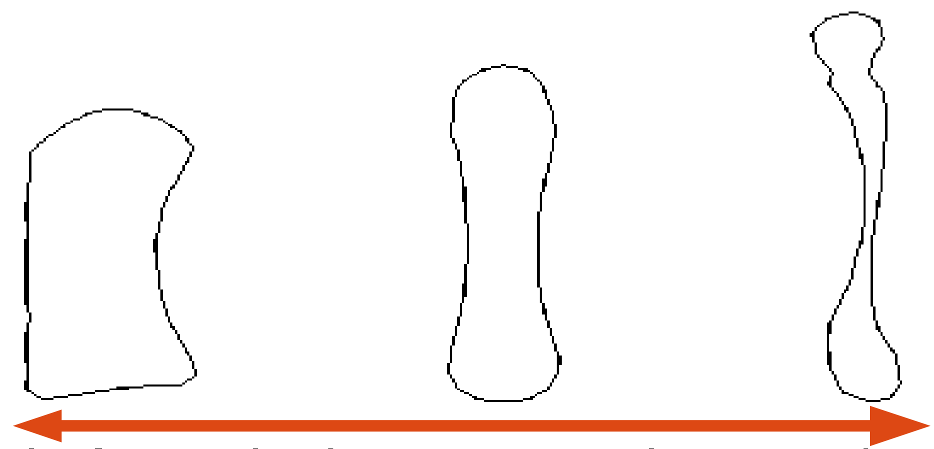
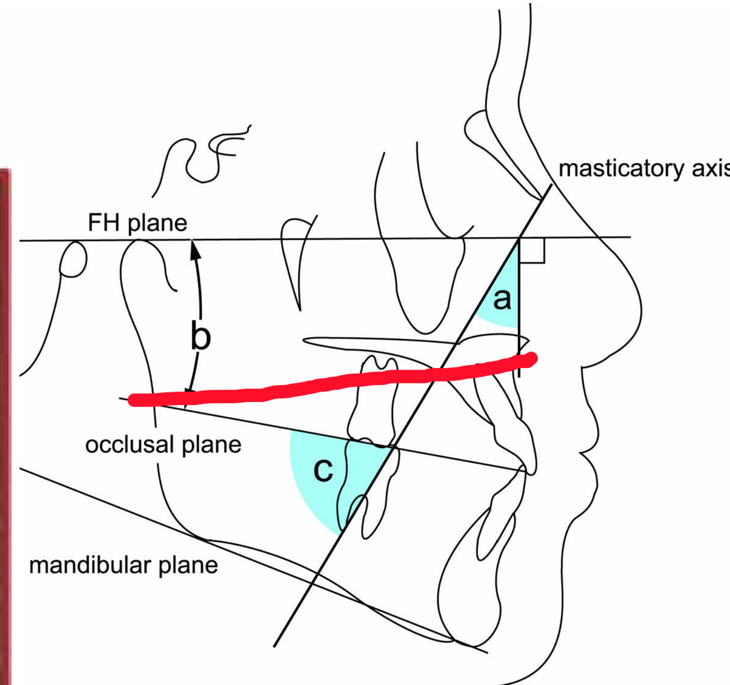


Figure 8.14 *The first mode of variation;* $-2.5\lambda_1$, *mean shape,* $2.5\lambda_1$. *Courtesy N.D. Efford, School of Computer Studies, University of Leeds.*

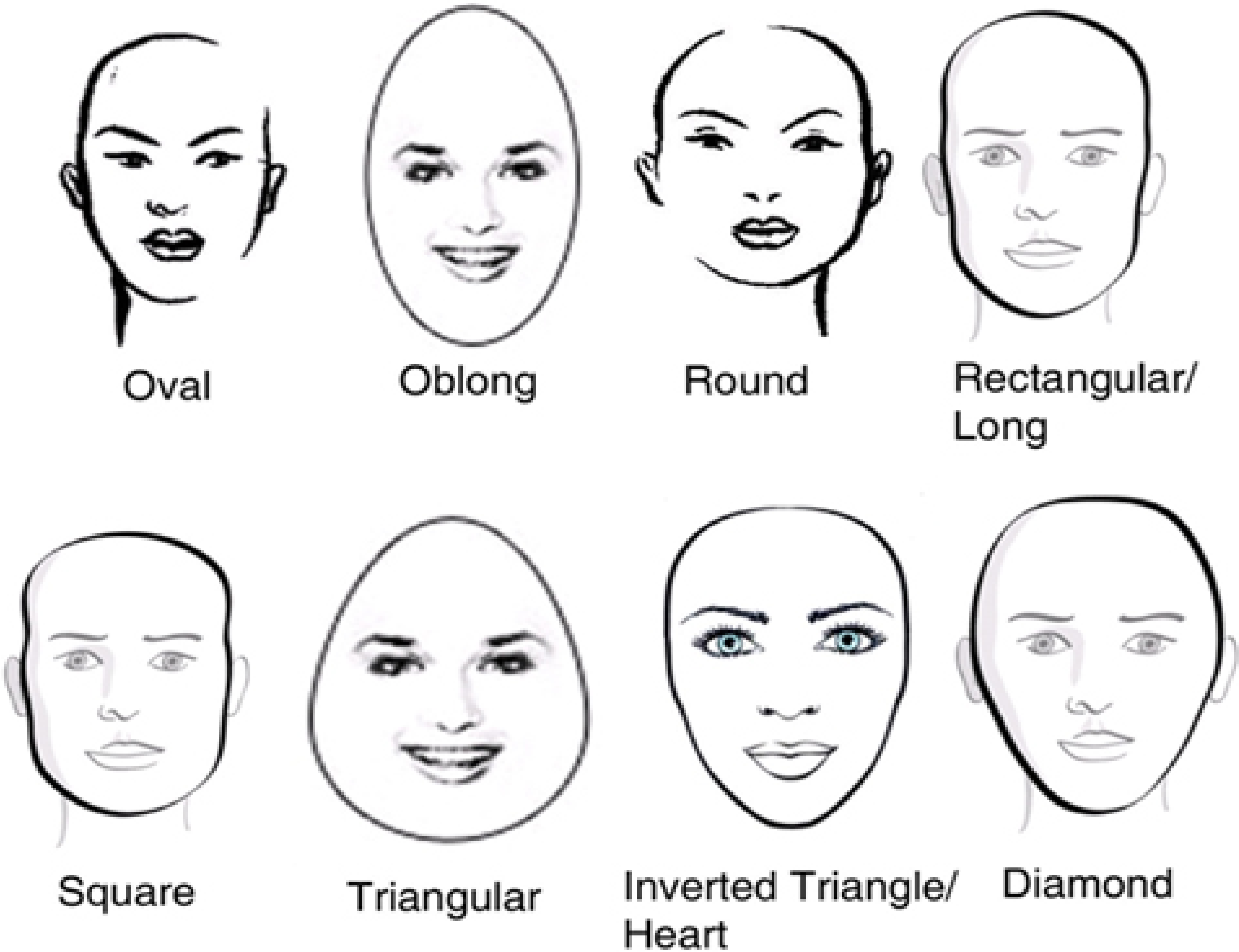
Statistical Shape Analys

Mode 1: Concavity

Mode 2: Inclination

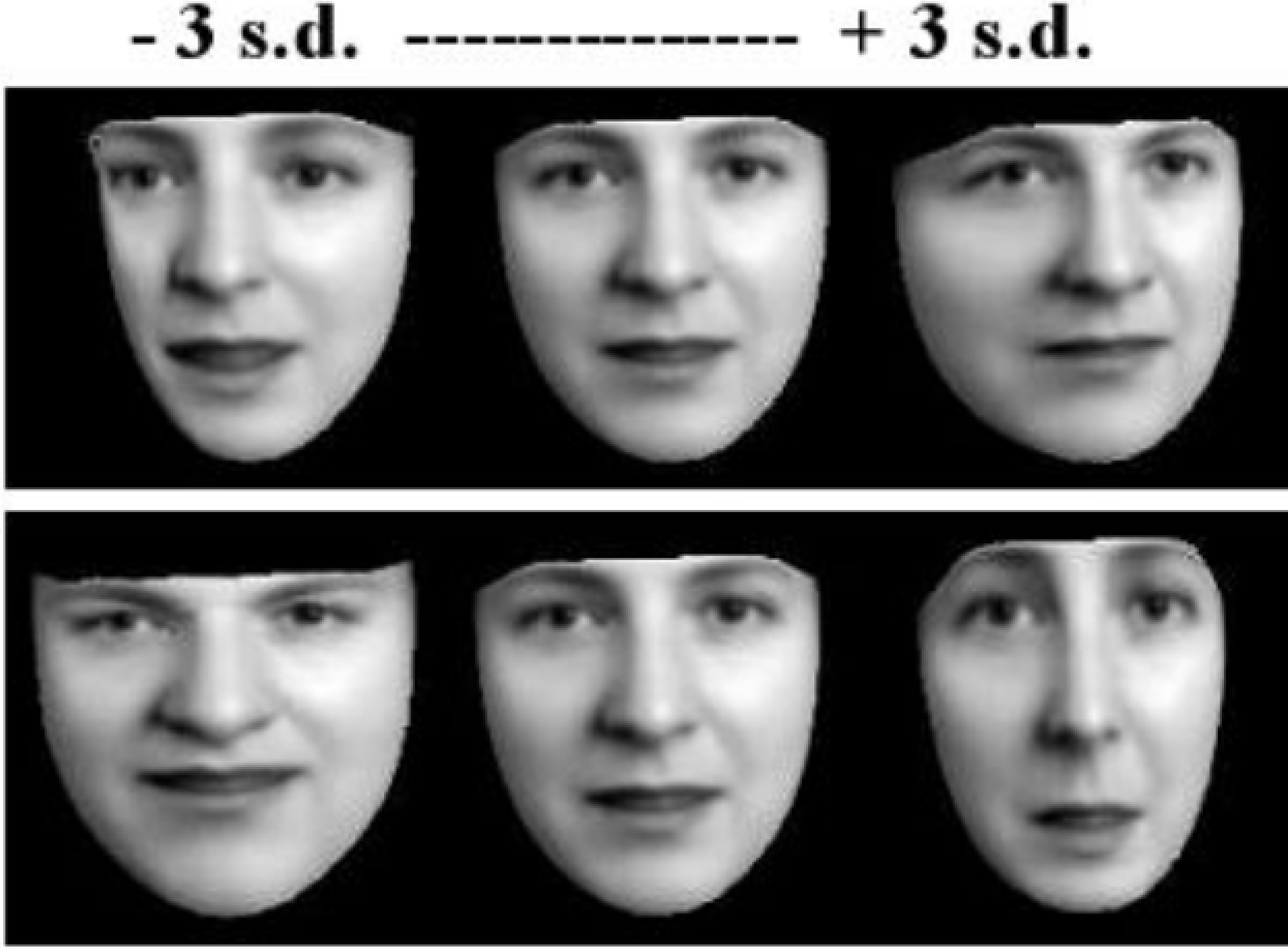


Shape Variability



Statistical Shape Analysis

- Normal / abnormal variation of shape of structure



First two modes of shape variation

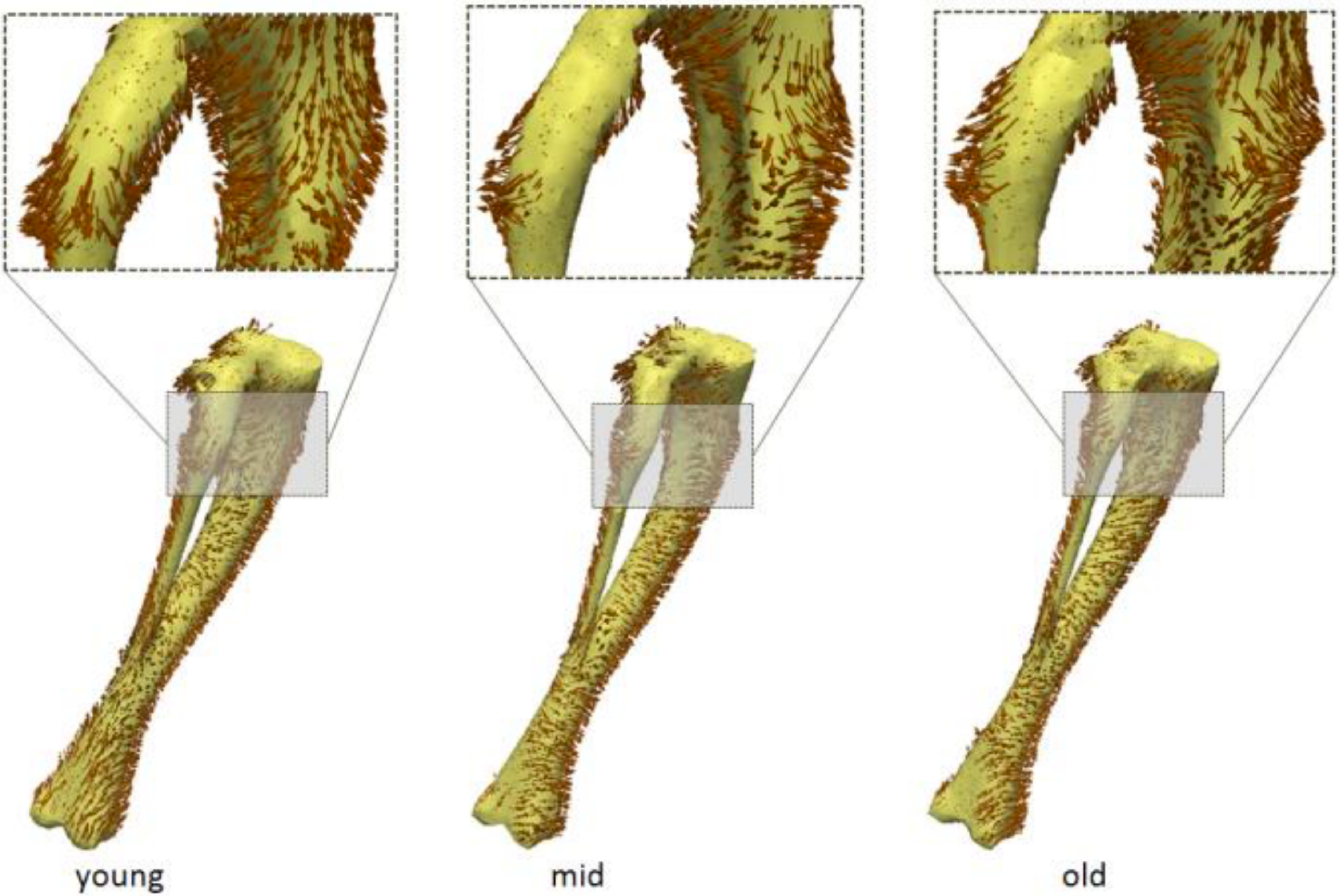
Statistical Shape Analysis

First two modes of shape variation

First two modes of gray-level variation

First four modes of appearance variation

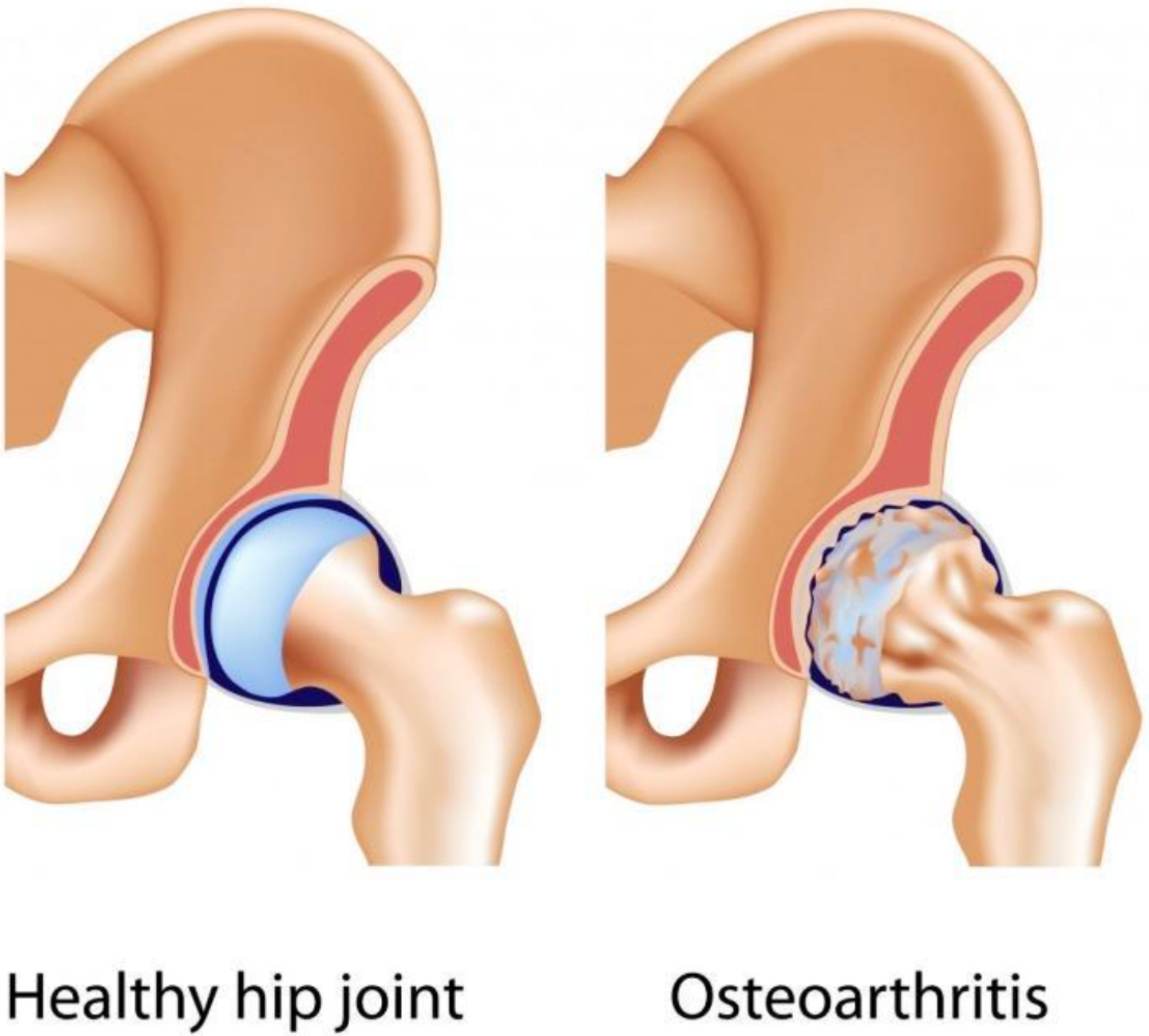
Shape Variability



Group Differences

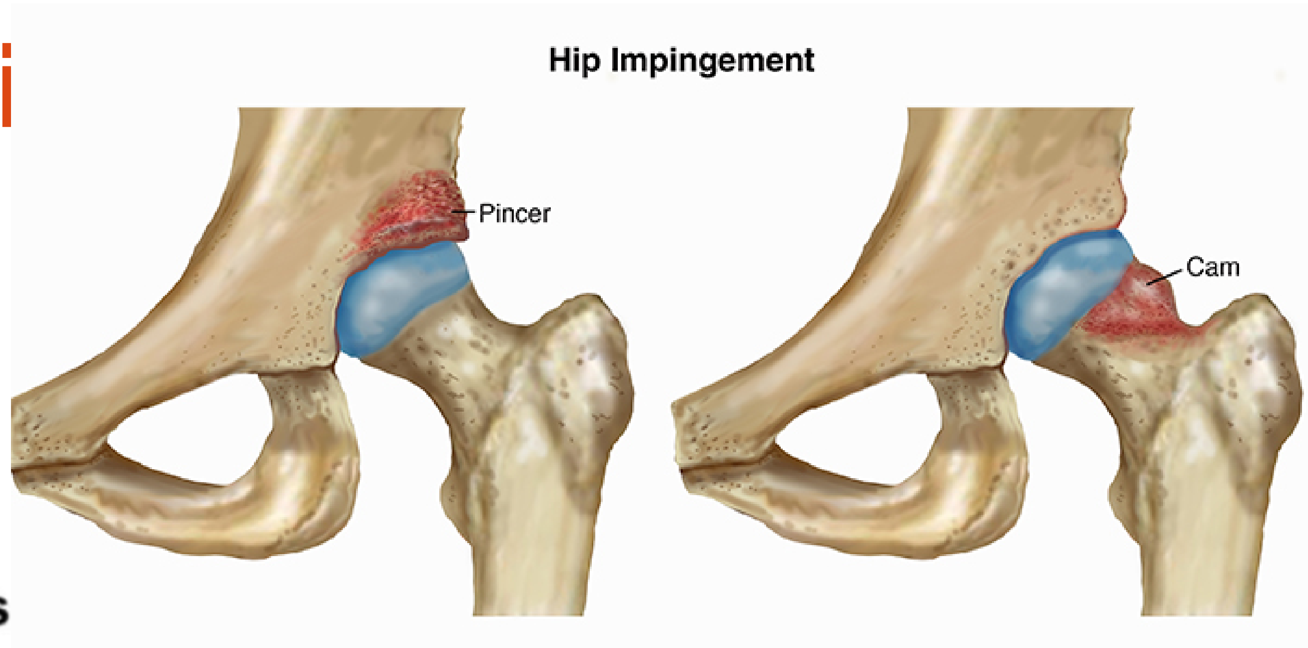
Dr. Kevin Jones, M.D.
Huntsman Cancer Institute
Department of Orthopedics
University of Utah

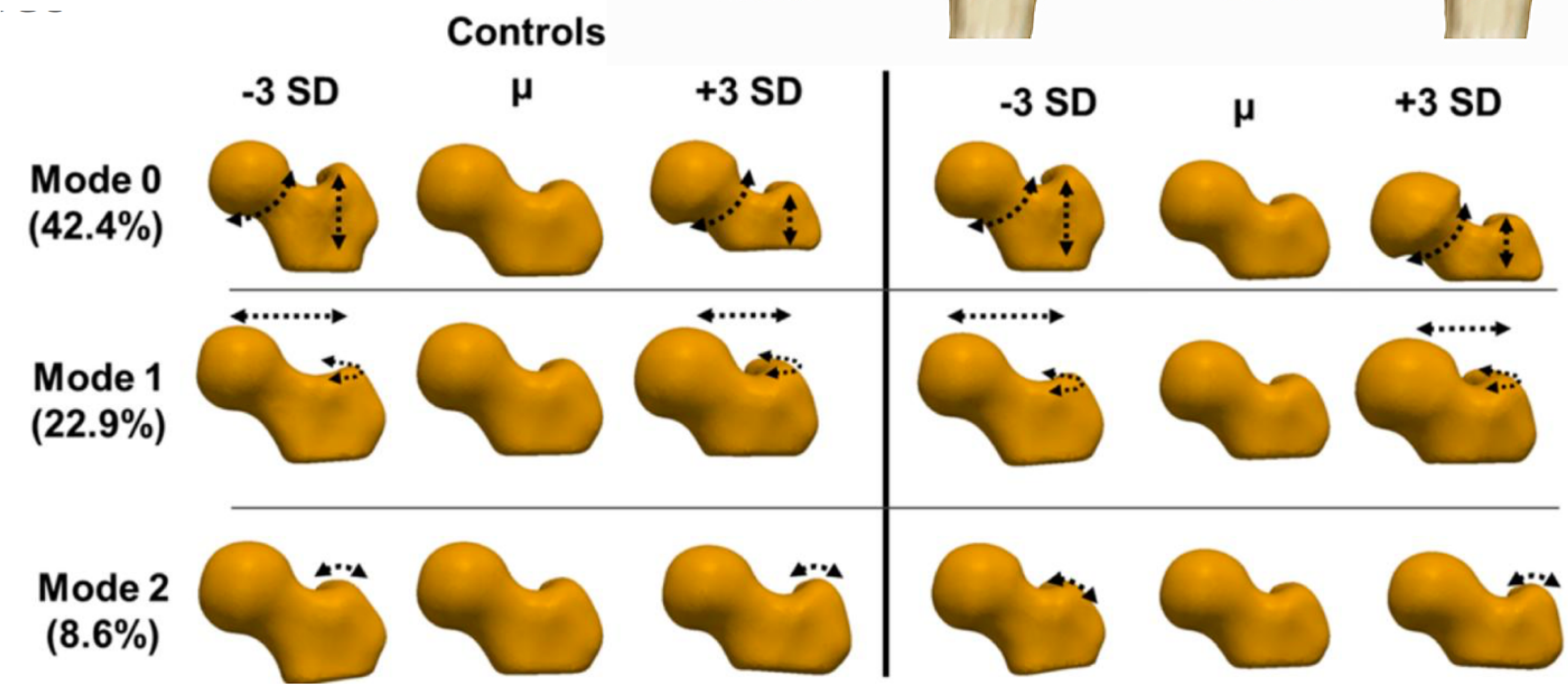
Shape Variability



Shape Variabili

- Shape variation in normal population & diseased population





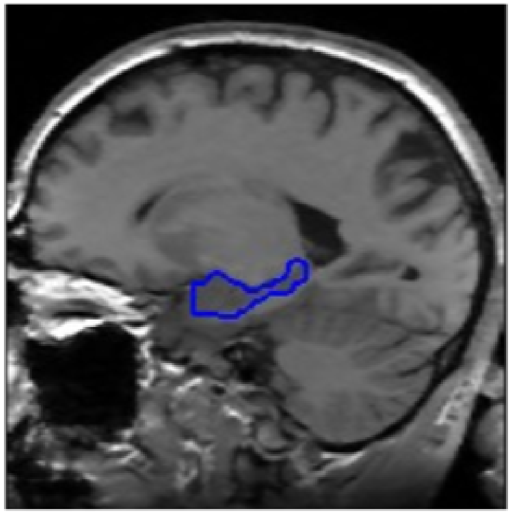
Variability in population

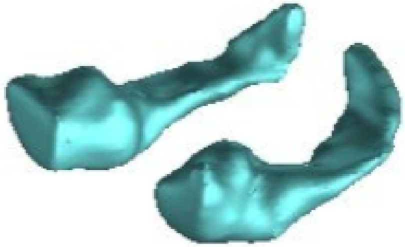
Statistical Shape Analysis

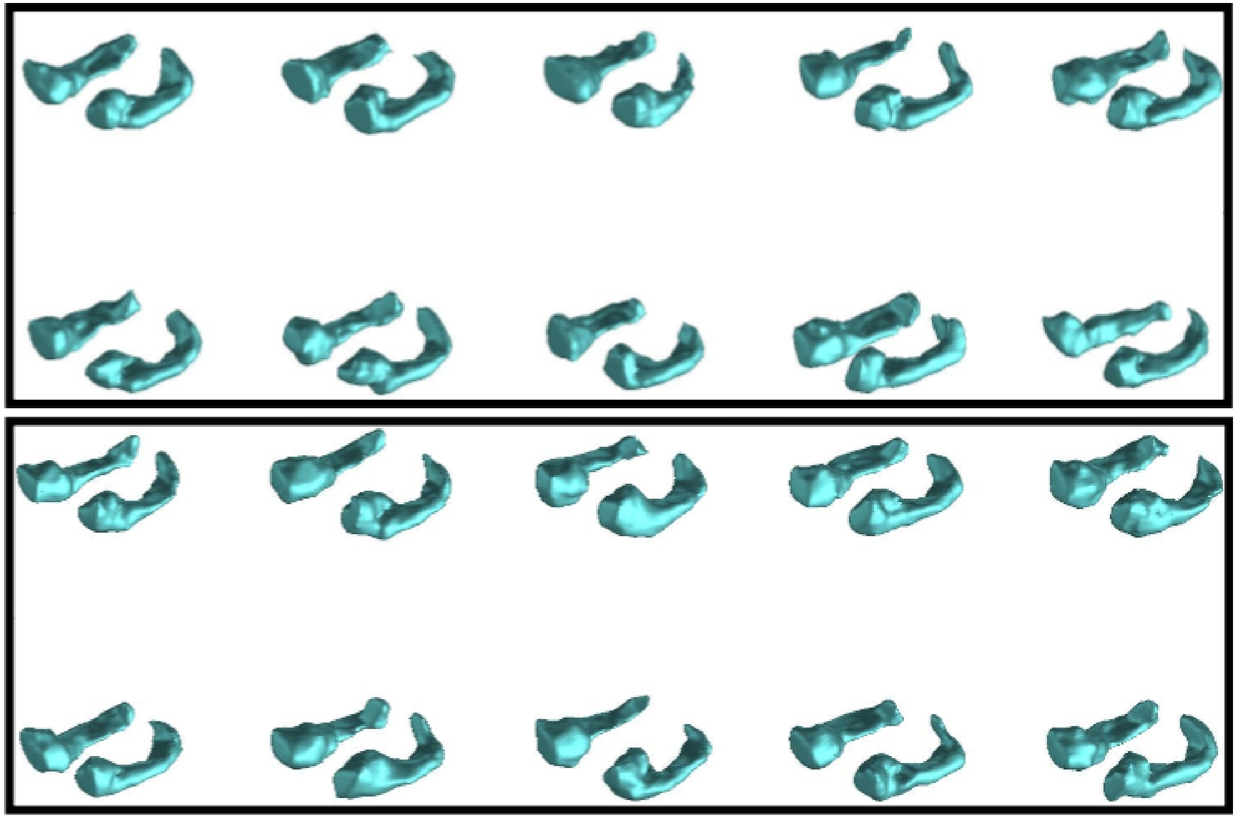
- Normal / abnormal variation of shape of structure
  - Need the notion of a “**mean**” shape
  - Need the notion of “**covariance**” of shapes
    - Principal **modes of variation**
  - Need a way to **represent** shape that allows us to visualize the mean and modes of variation

Statistical Shape Analysis

- Dementia
  - Shape of hippocampus







Polina Golland. MIT. 2001

Hip pain may be 'hangover from evolution'

By Smitha Mundasad
Health reporter, BBC News

27 December 2016 | Health

Share

Scientists at the University of Oxford say a hangover from evolution could help explain why humans get so much shoulder, hip and knee pain.

Bones from the skeleton of the 3.2m-year-old hominid Lucy

Pain in the ...

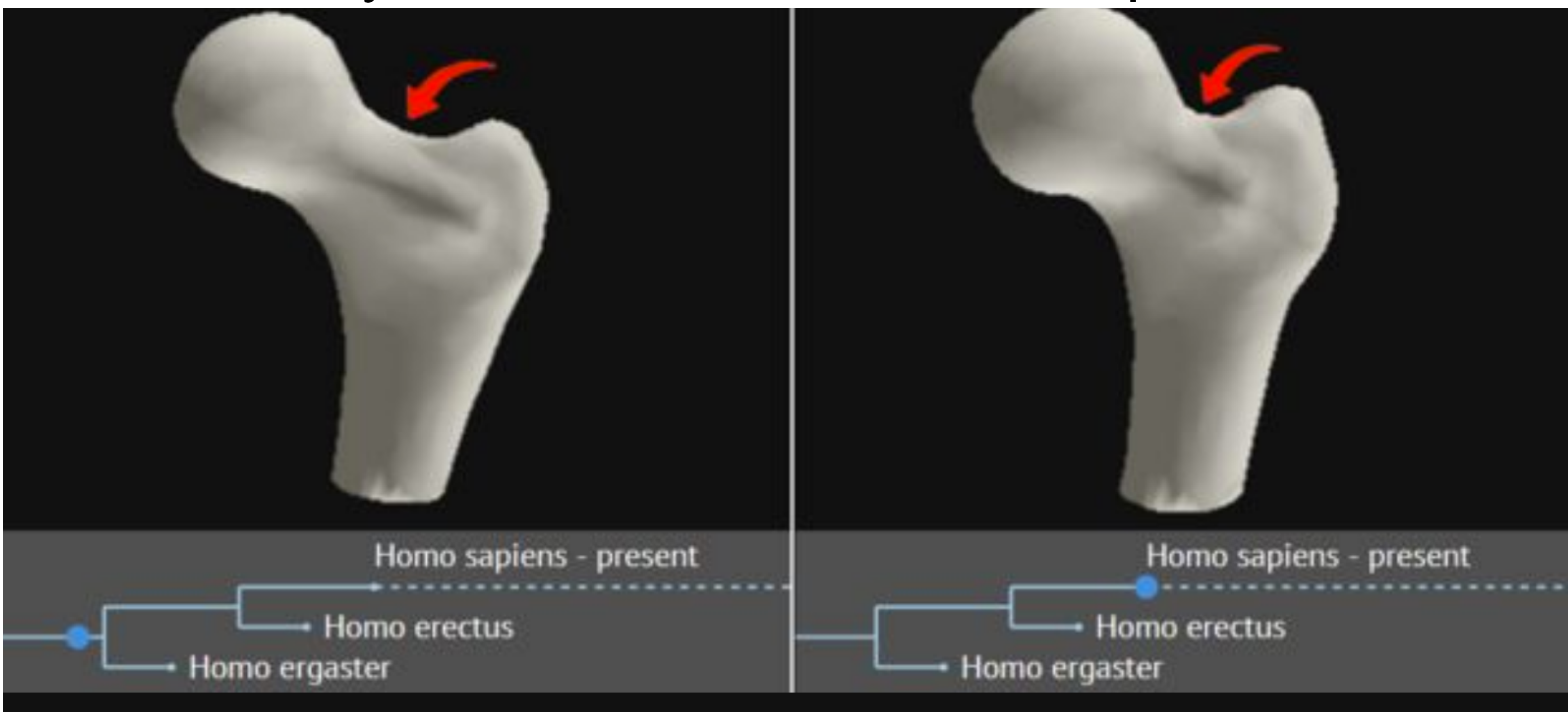
- Typical observations in hospitals:
  - Pain in the shoulder with reaching overhead
  - Pain in the front of the knee
  - Arthritis of the hip
  - In younger people, joints that have a tendency to pop out
- "We wondered how on earth we have ended up with this bizarre arrangement of bones and joints that allows people to have these problems.
- "And it struck us that the way to answer that is to look backwards through evolution."

Pain in the ...

- CT scans of 300 ancient specimens, from different species, spanning 400 million years
  - Natural History Museum in London and Oxford
  - Smithsonian Institution, Washington
- Study how bones changed subtly over millennia

Pain in the ...

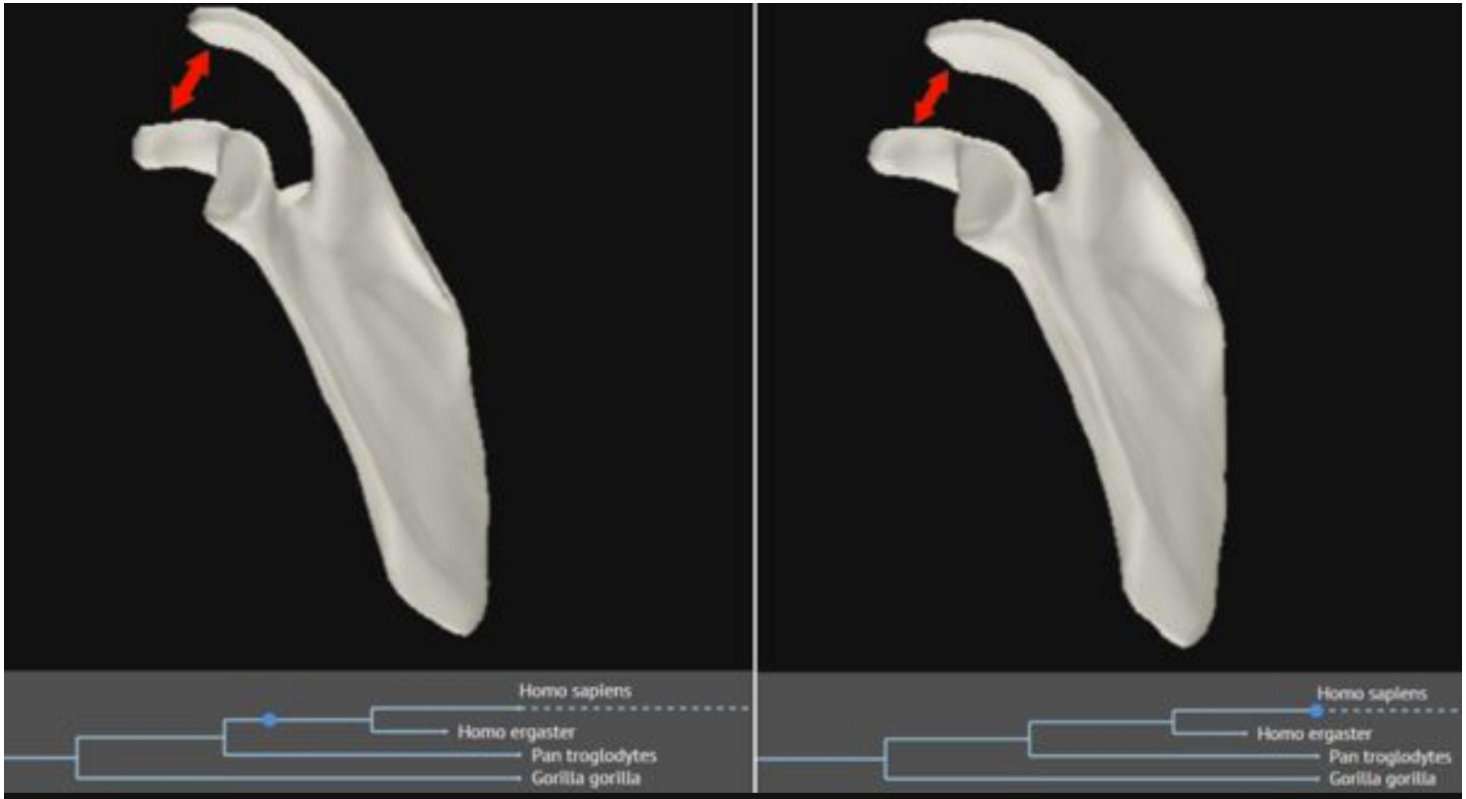
- As species evolved from moving around on 4 legs to standing up on 2,
  neck of the thigh bone grew broader to support extra weight
- Studies show that the thicker the neck of the thigh bone, the more likely it is that arthritis will develop



The thigh bone changing over time

Pain in the ...

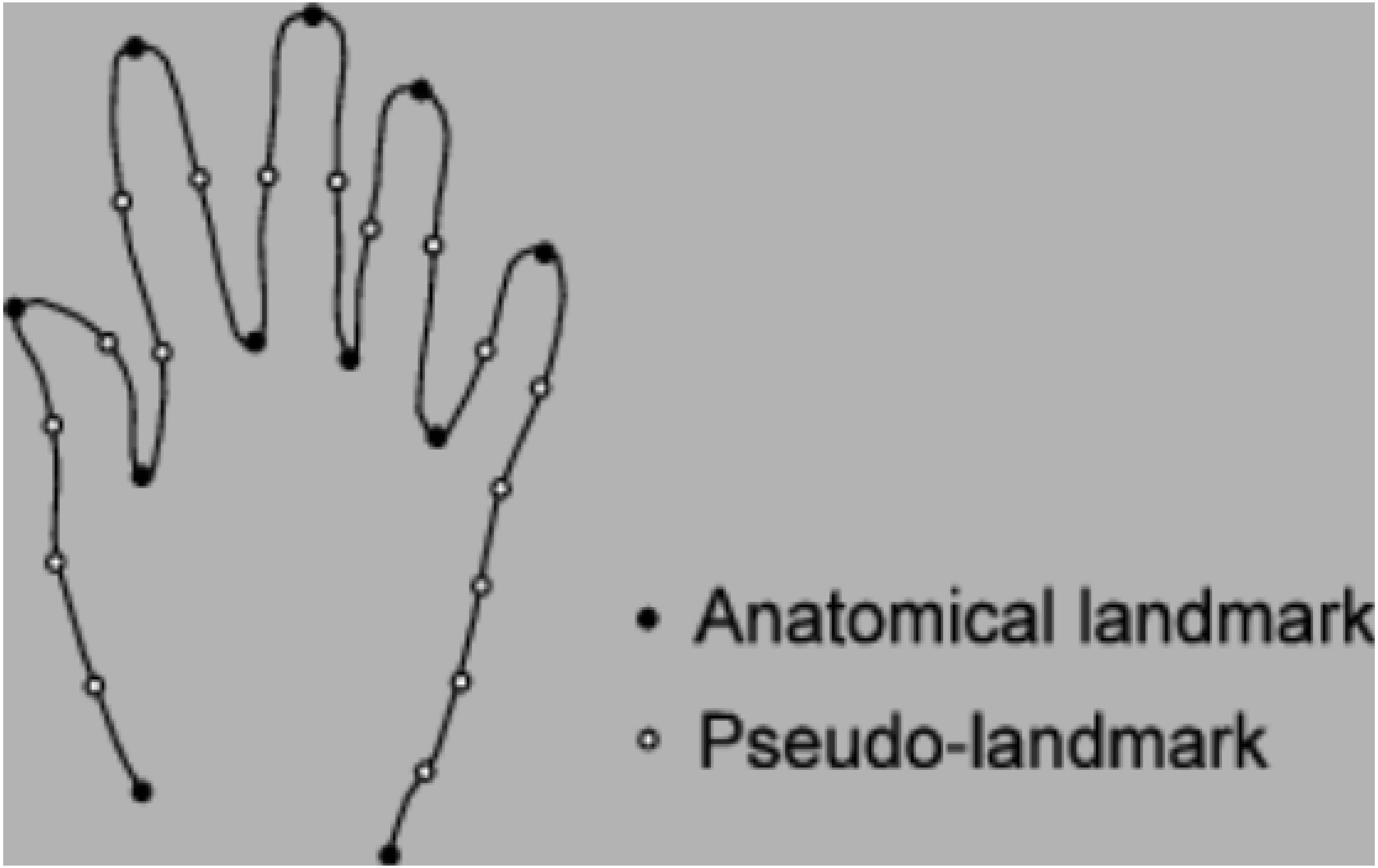
- In the shoulder, scientists found that a natural gap - which tendons and blood vessels normally pass through - got narrower over evolution
- The narrower space makes it more difficult for tendons to move and might help explain why some people experience pain when they reach overhead



The shape of the shoulder changing over time.

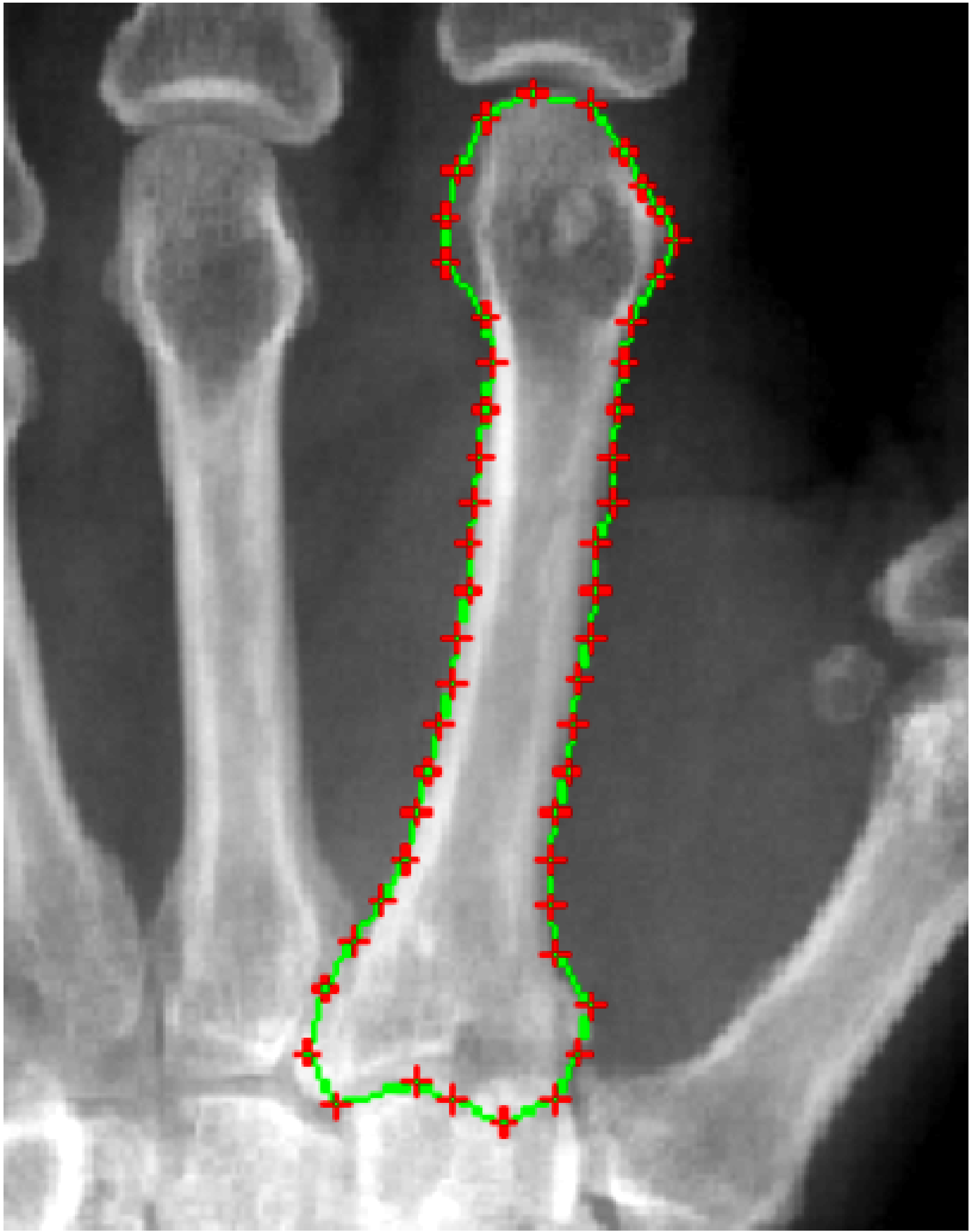
Shape Representation

- **Shape represented as a pointset**
  - Where to place the points ?



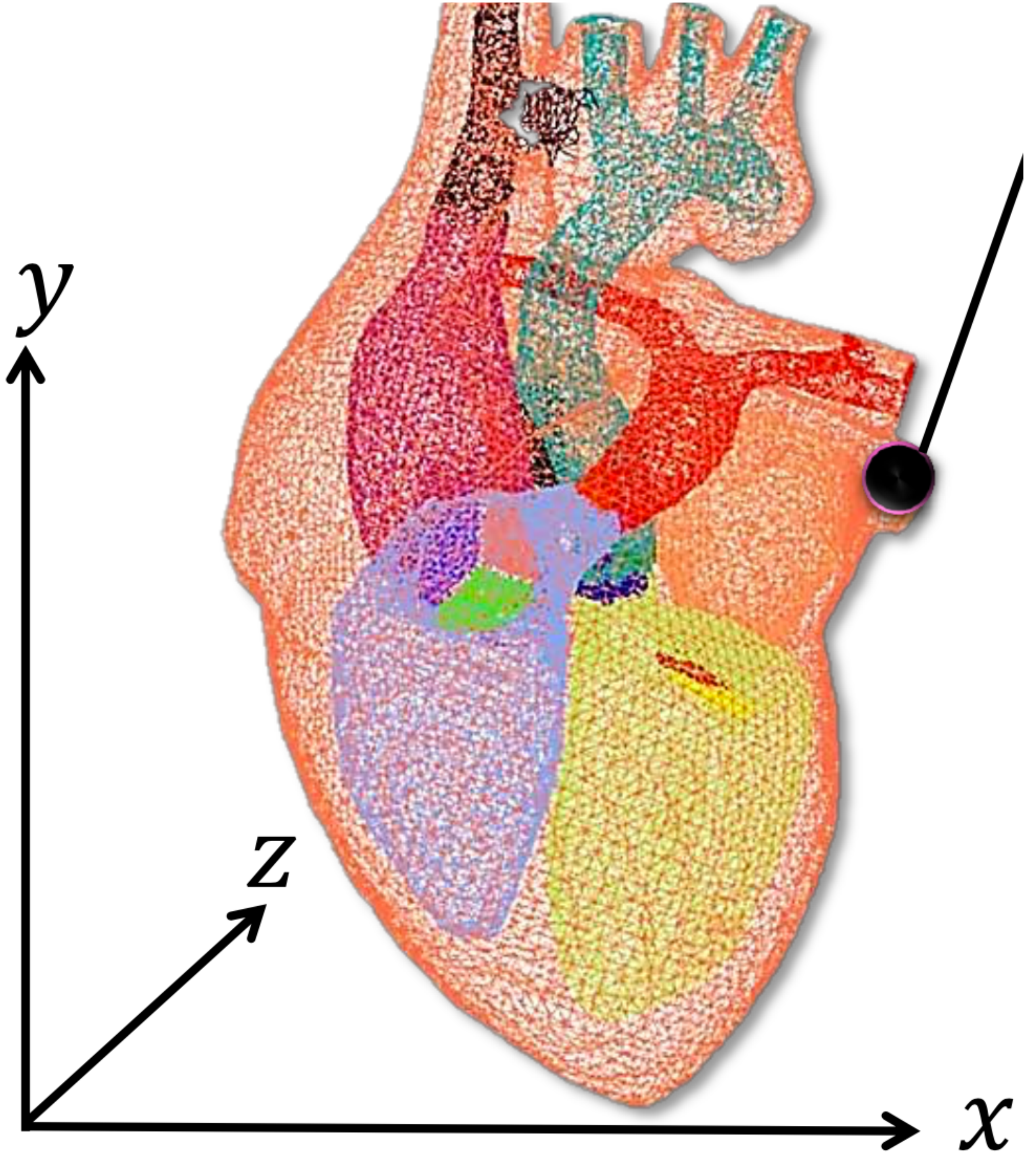
Shape Representation

- Shape represented as a pointset
  - Where to place the points ?
    - 2D case



Shape Representation

- Shape represented as a pointset
  - Where to place the points ?
    - 3D case



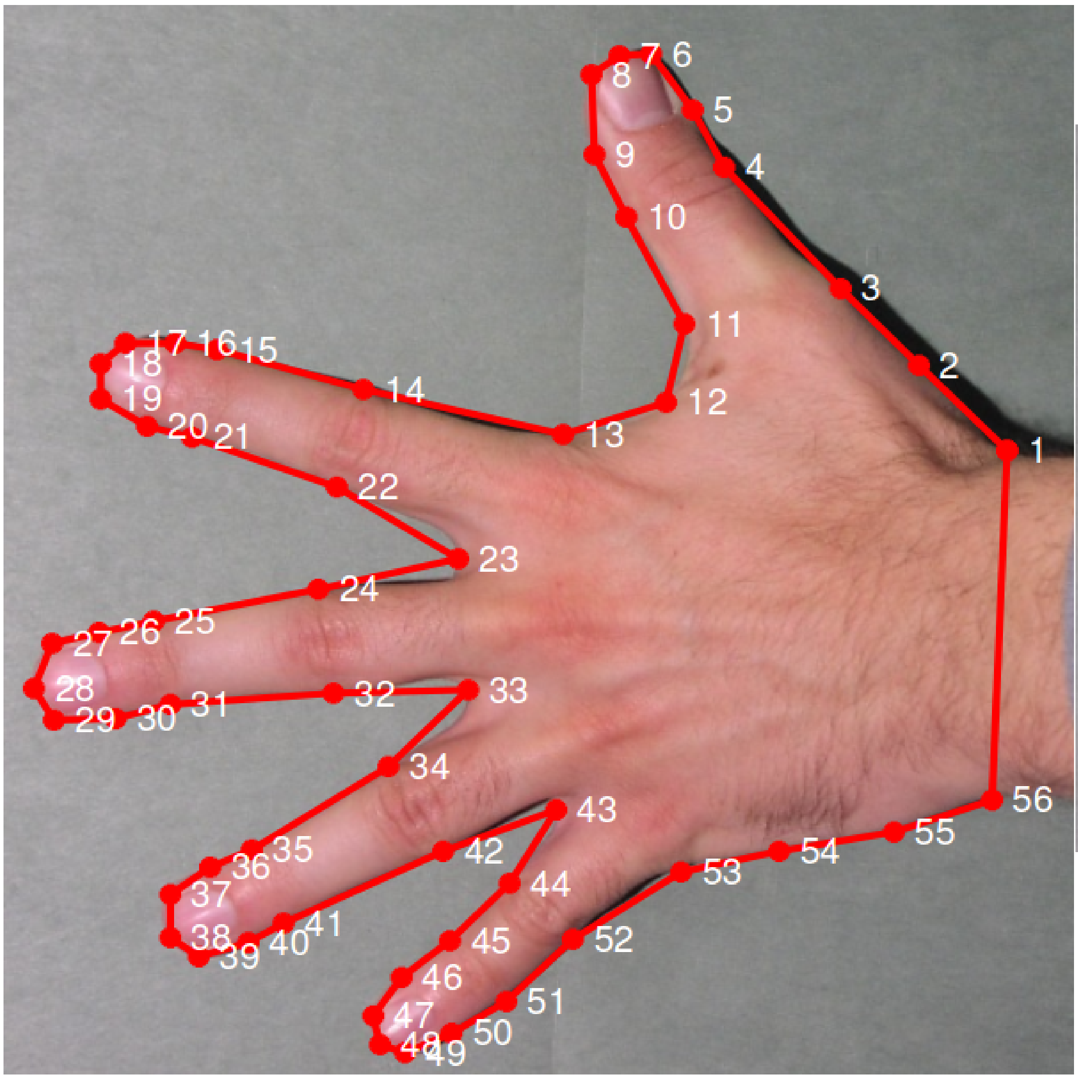
Shape Analysis

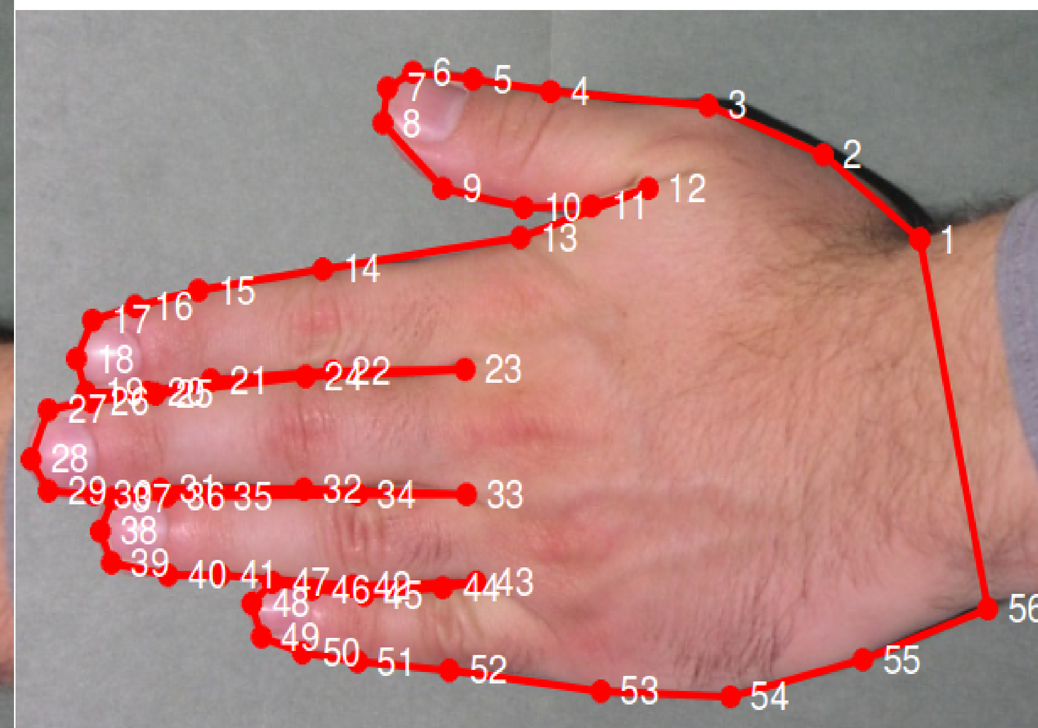
- **Measuring similarity / distance between shapes**
  - Assume representation = pointset
  - Distance between these shapes → equals … ?

  - Must account for following variations in pointsets:
    - Translation (coordinate-frame origin)
    - Rotation (pose)
    - Scale (size)
      - Uniformly / isotropic scaling; enlarging / shrinking
  - How ?

Shape Analysis

- **Correspondences of points across pointsets**
  - Outline represented as an ordered fixed-size pointset
  - We will work within this correspondence-based regime





Shape Analysis

- Shape representation
  - In this correspondence-based regime, we can Choose an ordering on the points → Vector of N point coordinates
    - Assuming points are in 2D
    - $\text{Shape}_1 = z_1$
      $= [\, z_{11} \dots z_{1N} \,] = [\; x_{11}\, y_{11} \quad x_{12}\, y_{12} \quad \dots \dots \quad x_{1N}\, y_{1N} \;]$
    - $\text{Shape}_2 = z_2$
      $= [\, z_{21} \dots z_{2N} \,] = [\; x_{21}\, y_{21} \quad x_{22}\, y_{22} \quad \dots \dots \quad x_{2N}\, y_{2N} \;]$

Shape Analysis

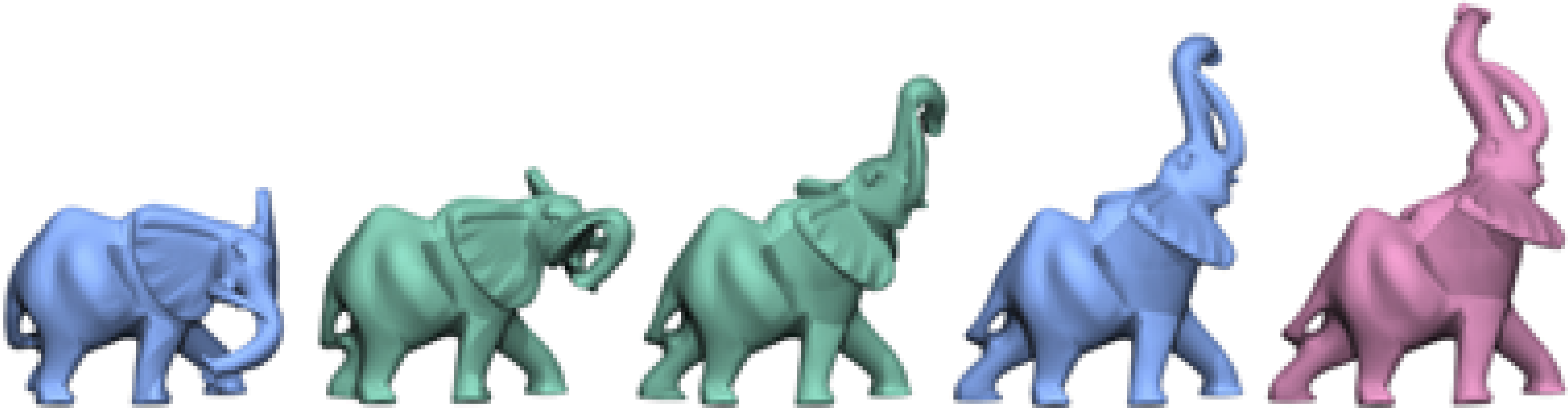
- Pointset transformations
  - (Special) Similarity Transform
    - Linear coordinate transformation comprising :
      - Translation : T = [tx ty]'
      - Scaling (identical scaling of all coordinates; NO shear) : “s > 0”
      - Rotation
        - $M_\theta = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$
        - Orthogonal matrix of determinant +1
      - **NO** reflection allowed (hence, “special”)
        - Reflection matrix has determinant -1
        - $M_\theta = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}$ (reflection about line at angle θ/2)
      - Let point a = [x1 y1]'

        Then, similarity transformation is : $b \leftarrow s\, M_\theta\, a + T$

        where point b = [x2 y2]'

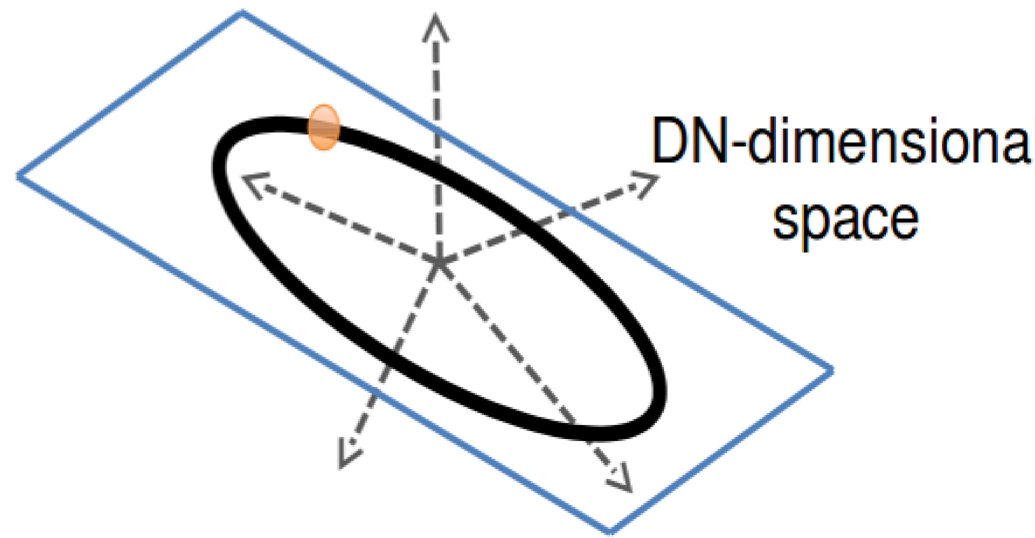
Shape Analysis

- Are these (3D) shapes the same ?



Shape Analysis

- **Shape space**
  - Pointset
    - { x_n in R^D : n=1,...,N }
    - Vector of length DN
  - Degrees of freedom < DN
    - Translation reduces D
    - Scale reduces 1
    - Preshape space = hypersphere resulting from factoring out translation + scale
    - Rotation reduces more
      - Degrees of freedom in an orthogonal matrix
      - D*D - (D + D_choose_2) = D(D-1)/2



Shape Analysis

- **Shape distance** (squared) between pointsets z_1, z_2 in **preshape** shape

  $= \min_\theta \; d^2 (z_1, \mathrm{Rot} (z_2; \theta))$

  - For z_1, z_2: Translation (tx, ty) is chosen s.t. centroids match
    - Puts pointsets on *same* **hyperplane**
  - For z_1, z_2: Scale (s) is chosen s.t. norms match (a constant)
    - Puts pointsets on *same* **hypersphere**
  - Rotation is explicitly optimized (in terms of θ)
    - Rotation about the centroid
  - d(.,.) is measured, modulo rotation, in preshape space, via:
    - (1) Geodesic distance on hypersphere, or
    - (2) Approximated by Euclidean (chord) distance (**Procrustes distance**)

Shape Analysis

- **Procrustes analysis for shape matching / alignment**

  (1) Align w.r.t. Location

  - Compute centroid of each pointset
  - Subtract centroid from each point in pointset

  (2) Align w.r.t. Scale

  - Re-scale each shape to have same size
  - Size = norm of vector (= some fixed pre-decided number)

  (3) Align w.r.t. Rotation

  - We'll see next

  (4) Procrustes 'Distance' / dissimilarity = Euclidean distance between optimally-transformed shapes

    - Actually, 'distance' metric only when pointsets lie in shape space

Shape Analysis

- Procrustes analysis for shape matching
  - Given: N data points in 2 shapes (say, z_1 and z_2) in 2D
  - Goal: Find transformation parameters
    - Rotation: 1 variable
    - Cootes et al. 1995 CVIU (Active Shape Models) solved also for:
      - Translation: 2 variables
      - Scale: 1 variable
      - Assuming z_1 , z_2 don't lie in preshape space
      - Procrustes 'distance' / dissimilarity between z1, z2
        $= \min_{\theta,T,s} \; d^2 \, (z_1, \text{SimilarityTransform} \, (z_2; \theta, T, s) \,)$

Procrustes

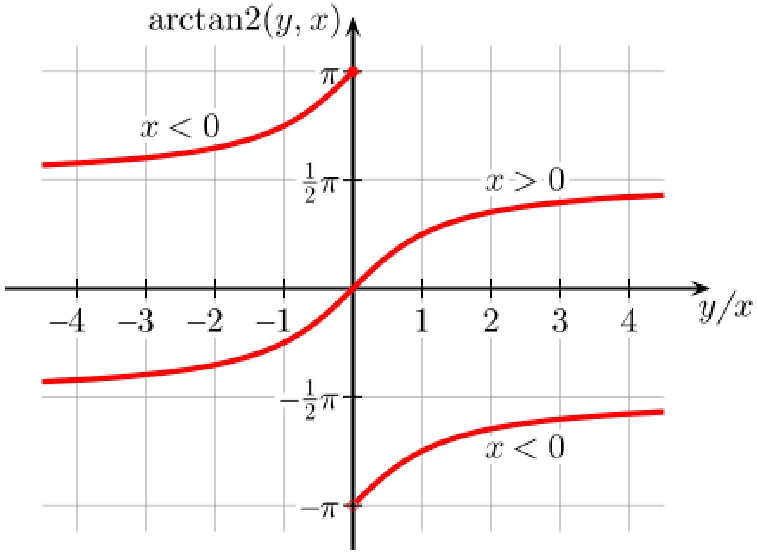
- Greek mythology
  - “the stretcher
    [who hammers out the metal]”
- Procrustes
  - Had an infamous bed
  - Invited travelers to spend the night in his home
  - If the guest proved too tall, …
  - If the guest proved too short, …
  - End: Theseus captured P, “fitted” him to his own bed

Shape Analysis

- Procrustes analysis for shape matching
  - Strategy:
    $\text{Minimize}_{\{T,\, s,\, \theta\}} \sum_{n = 1,\ldots,N} \| z_{1n} - s\, M_\theta\, z_{2n} - T \|^2$
    - How will you optimize ?

Shape Analysis

- Procrustes analysis for shape matching
  - Strategy : Minimize $\sum_{n=1,\ldots,N} || z_{1n} - s\, M_\theta\, z_{2n} - T ||^2$
    - Optimization algorithm (by Cootes 1995)
      - First substitute $a = s \cos\theta$, $b = s \sin\theta$ and solve for { tx, ty, a, b }. How ?
        - **Quadratic** in { tx, ty, a, b } → **convex**
        - Many ways to optimize
          - e.g., gradient descent, Newton's method
          - Initialization doesn't matter
        - Closed-form solutions by solving a **linear system of equations**
        - https://doi.org/10.1006/cviu.1995.1004
      - Then, solve for $s > 0$ and θ, given a and b
        - $s = \mathrm{sqrt}(a*a + b*b)$
        - So, $s > a$ and $s > b$
        - So,
          $|\cos\theta| = |a/s| < 1$,
          $|\sin\theta| = |b/s| < 1$
        - $\theta = \mathrm{atan2}(b, a)$



Shape Analysis

- Procrustes analysis for shape matching
  - Strategy : Minimize $\sum_{n=1,\ldots,N} || z_{1n} - s\, M_\theta\, z_{2n} - T ||^2$
    - Optimal translation T turns out to be … ?
      - For any given s,θ: optimal T = displacement between centroids
      - Begin with centroids at origin because, once centroid is at origin, changing scale and rotation doesn't change centroid
    - Optimal scale “s” is slightly different !
      - Previously, transformed pointset z_2 was ensured to be unit norm
      - If unconstrained minimization over “s”, that guarantee is lost !
    - What happens in 3D ?
      - Optimizing for rotation in 3D → Coming up next ...
      - Optimization algorithm: Alternating minimization
        - Optimize T to match centroids → make centroids at origin
        - Given T,s: optimize θ.   Given T,θ: optimize s.   Repeat.

Shape Analysis

- **Optimizing for rotation**
  - Given: 'n' points in 2 pointsets
    $\{ x_i : i = 1,...,n \}$ and $\{ y_i : i = 1,...,n \}$
  - Goal: Find rotation R to best align pointsets

$$\underset{R}{\operatorname{argmin}} \sum_{i=1}^{n} w_i \left\| R\mathbf{x}_i - \mathbf{y}_i \right\|^2$$

$$= \underset{R}{\operatorname{argmin}} \sum_{i=1}^{n} w_i (\mathbf{x}_i^T \mathbf{x}_i - 2\mathbf{y}_i^T R\mathbf{x}_i + \mathbf{y}_i^T \mathbf{y}_i)$$

Because $R^T R$ = Identity

$$= \underset{R}{\operatorname{argmax}} \sum_{i=1}^{n} w_i \mathbf{y}_i^T R\mathbf{x}_i$$

  - How to optimize ?
    - What if we set derivative to zero ? Does it work ?

Shape Analysis

- Optimizing for rotation
  - [Kabsch 1976]
    - https://en.wikipedia.org/wiki/Kabsch_algorithm

$$\sum_{i=1}^{n} w_i \mathbf{y}_i^T R \mathbf{x}_i = tr\left(WY^T RX\right)$$

$$\begin{bmatrix} w_1 & & & \\ & w_2 & & \\ & & \ddots & \\ & & & w_n \end{bmatrix} \begin{bmatrix} — & \mathbf{y}_1{}^T & — \\ — & \mathbf{y}_2{}^T & — \\ & \vdots & \\ — & \mathbf{y}_n{}^T & — \end{bmatrix} \begin{bmatrix} R \end{bmatrix} \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \\ | & | & & | \end{bmatrix}$$

Shape Analysis

- Optimizing for rotation
  - Property: Trace (AB) = Trace (BA)

$$tr\left(WY^TRX\right) = tr\left((WY^T)(RX)\right) = tr\left(RXWY^T\right)$$

  - XWY^T = (weighted) cross covariance matrix
  - Perform SVD of $XWY^T = U\Sigma V^T$

$$= tr\left(RU\Sigma V^T\right) = tr\left(\Sigma V^T RU\right)$$

  - Let $V^TRU \rightarrow M$

$$tr(\Sigma M) = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_d \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} & \dots & m_1 \\ m_{21} & m_{22} & \dots & m_2 \\ \vdots & \vdots & \vdots & \vdots \\ m_{d1} & m_{d2} & \dots & m_d \end{pmatrix}$$

Shape Analysis

- Optimizing for rotation
  - V,R,U = orthogonal matrices →
    M = orthogonal matrix →
    elements of M have magnitude <= 1

$$tr(\Sigma M) = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_d \end{pmatrix} \begin{pmatrix} m_{11} & m_{12} & \dots & m_{1d} \\ m_{21} & m_{22} & \dots & m_{2d} \\ \vdots & \vdots & \vdots & \vdots \\ m_{d1} & m_{d2} & \dots & m_{dd} \end{pmatrix} = \sum_{i=1}^{d} \sigma_i m_{ii} \leq \sum_{i=1}^{d} \sigma_i$$

  - How to maximize this quantity, over all orthogonal M ?
    - Set m_{ii} = 1, other elements = 0
    - M = Orthogonal ? Yes. So, R = Orthogonal
    - Thus, $I = M = V^T RU \;\Rightarrow\; V = RU \;\Rightarrow\; R = VU^T$
  - Are we done ? Is $R = VU^T$ a rotation matrix ?
  - If $\det(R) = \det(VU^T) = +1$ →We are done.

Shape Analysis

- Optimizing for rotation
  - If det(R) = det(VU^T) = -1, then …
  - **Objective function** = function of M that is a function of R

    $$tr(\Sigma M) = \sigma_1 m_{11} + \sigma_2 m_{22} + \ldots + \sigma_d m_{dd}$$

    = linear in variables m_{ii}
  - **Constraint set (for diagonal of M)** = cube = $[-1,1]^d$
    - But constraints on M → orthogonality and determinant = -1
    - This makes certain points within the cube as infeasible
  - [S Umeyama 1991 IEEE TPAMI]
    - Least-squares estimation of transformation parameters between two point patterns

Shape Analysis

- Optimizing for rotation
  - [Umeyama 1991 TPAMI] [Kanatani 1994 TPAMI] proved that next best location is at corner [1, ..., 1, -1], where objective function = $tr(\Sigma M) = \sigma_1 + \sigma_2 + \ldots + \sigma_{d-1} - \sigma_d$
  - Can M be orthogonal ? Yes. So, R = orthogonal
  - Is det(M) negated ? Yes. So, det(R) also negated
  - If det(R = VU^T) = -1, then …

$$M = V^T R U = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & -1 \end{pmatrix} \quad \Rightarrow \quad R = V \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & -1 \end{pmatrix} U^T$$

Shape Analysis

- What is the mean shape ?
  - How to define the mean ?
    - Karcher mean, Frechet mean
      - Mean = “center”
    - Assume a Gaussian distribution on shapes
      - Distance between shapes = Procrustes distance
      - For simplicity, assume the distribution is isotropic
        - No covariance matrix
        - Just variance (scalar)
    - Define mean as ML estimate
      - What objective function does this produce ?

Shape Analysis

- What is the mean shape ?
  - How to define the mean ?
    - Mean shape := pointset that minimizes sum of squared distances to all given pointsets
  - How to find the mean ?
    - Given: M pointsets (say, z_m), each having N points
    - Goal: Find the mean shape
      - But, distances depend on optimal transformations between each data pointset and mean !
      - So, must find transformation parameters !
    - Strategy
      - Optimize over mean + N sets of transformation parameters

Shape Analysis

- What is the mean shape ?
  - Optimize
    - Minimize: $\sum_{m = 1,\ldots,M} \sum_{n = 1,\ldots,N} || z_n - s_m M_{m\theta} z_{mn} - T_m ||^2$
      - z_m = observed pointset number 'm'
        - Each pointset has N points
      - z = mean pointset (unknown)
        - Must fix norm to 1; else trivial solution
        - Also fix centroid to origin
      - $\{ s_m, M_m, T_m \}$ = transformation parameters for each data shape
    - How to optimize ?
      - Alternating minimization

        (1) Given mean 'z', find optimal transformations
        - Can be solved independently for each data shape

        (2) Given all transformations, find optimal mean pointset 'z'
        - How to do that ?

Shape Analysis

- What is the mean shape ?
  - Minimize: $\sum_{n = 1,\ldots,N} || z_n - s_m M_{m\theta} z_{mn} - T_m ||^2$

    (1) Given mean, find optimal transformations

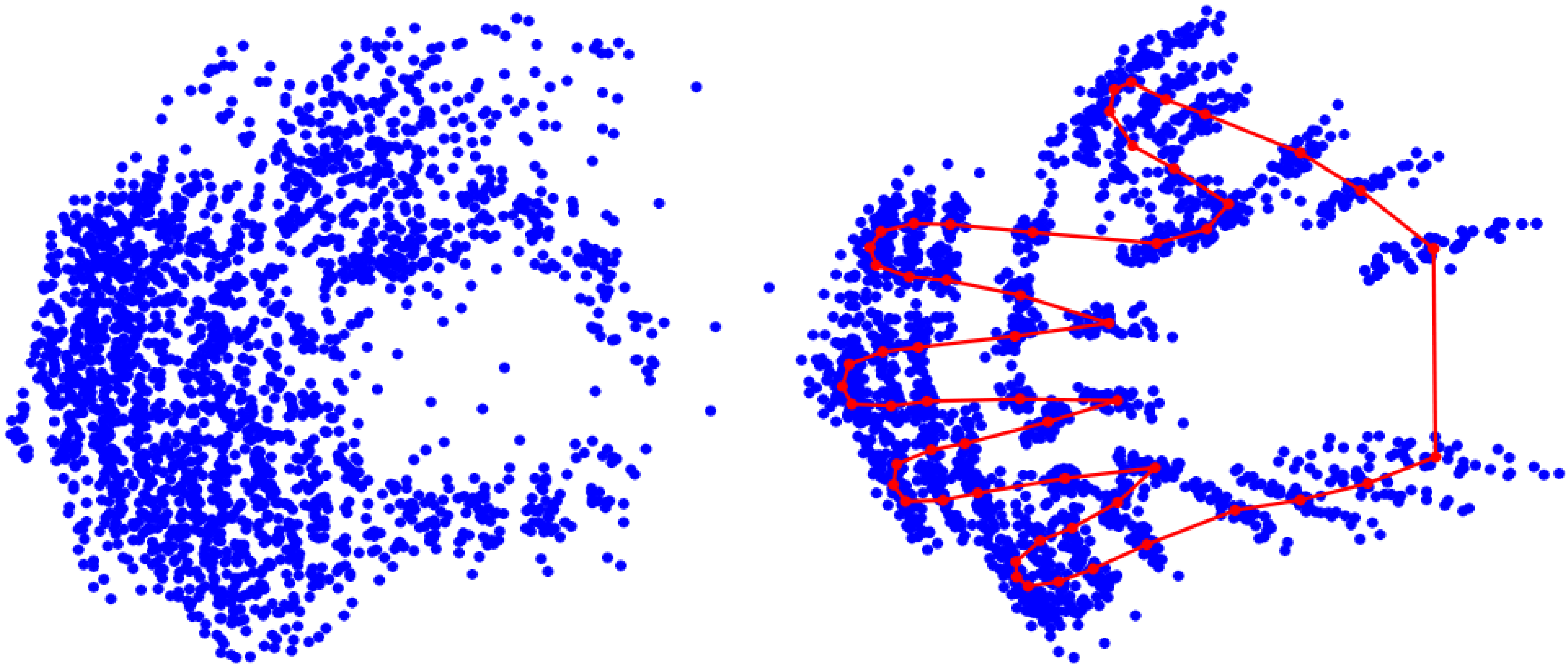
    (2) Given all transformations, find optimal mean pointset

    (A) Average all (aligned) pointsets
      - Similar to gradient descent
      - Resulting pointset guaranteed to have centroid at origin !
      - Why ?

    (B) Take resulting pointset and rescale (divide) by the norm
      - Projection onto constraint set

Shape Analysis

- What is the mean shape ?
  - Left: unaligned pointsets
  - Right: aligned pointsets + mean shape
  - http://graphics.stanford.edu/courses/cs164-09-spring/Handouts/paper_shape_spaces_imm403.pdf

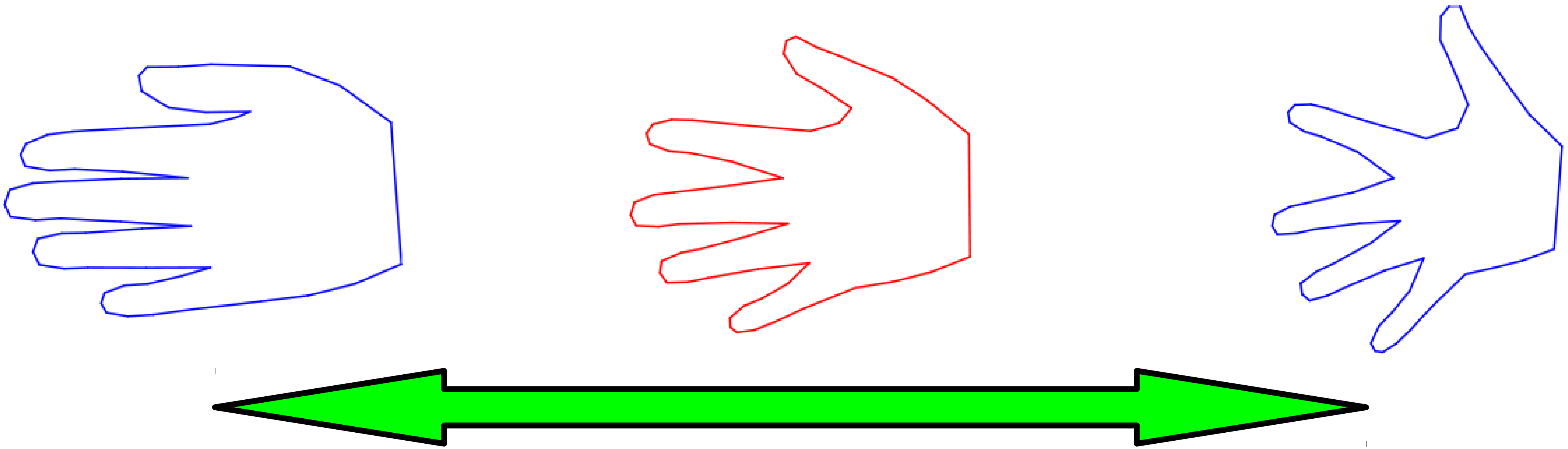


Shape Analysis

- How to learn shape variability ?
  - Assume: Shape mean is given
    - Optimized using previous approach
  - Estimate a covariance matrix
    - ML estimation
    - Now, assuming a Gaussian model with a covariance
    - This is just the sample covariance !

Shape Analysis

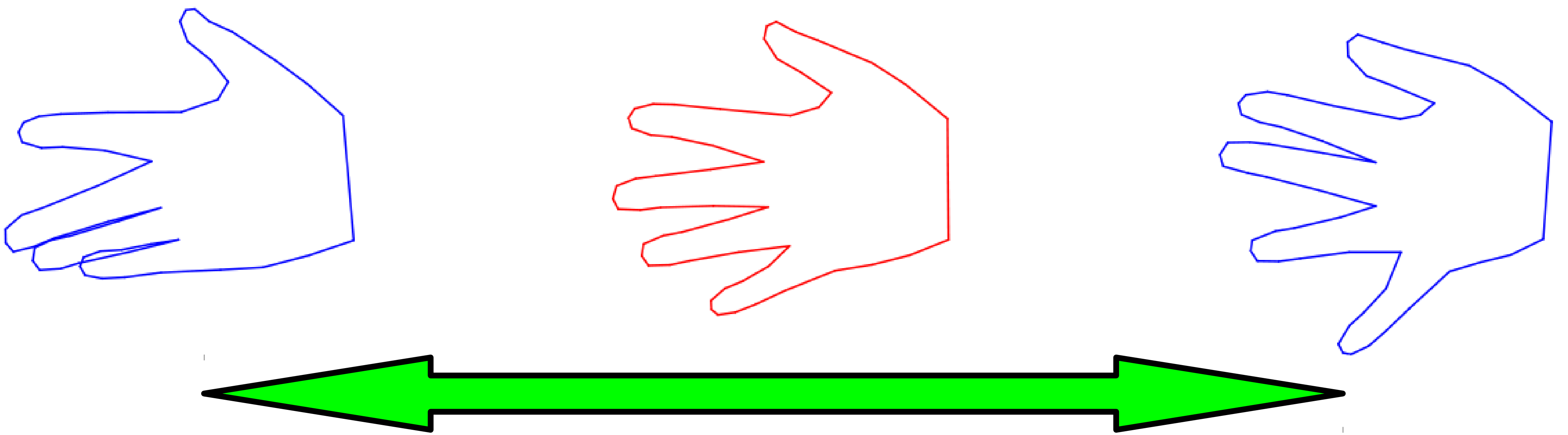
- How to learn modes of variation ?
  - Perform eigen analysis of covariance matrix
    - Principal eigenvectors give principal modes of variation
      - Eigenvector 1



(a) $b_1 = -3\sqrt{\lambda_1}$ **(b)** $b_1 = 0$ **(c)** $b_1 = +3\sqrt{\lambda_1}$

Shape Analysis

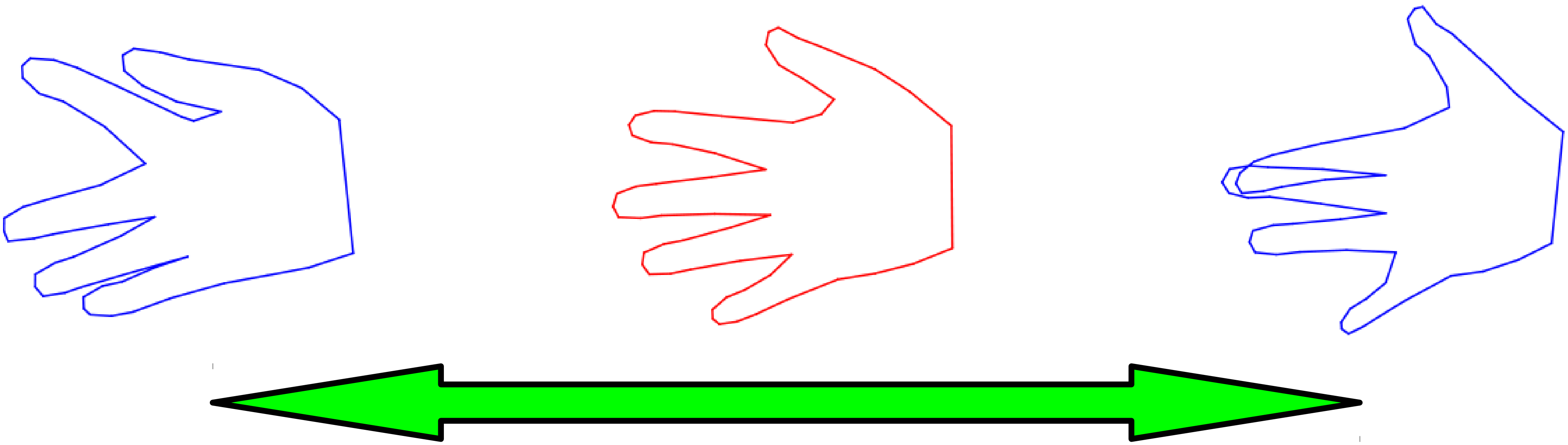
- How to learn modes of variation ?
  - Perform eigen analysis of covariance matrix
    - Principal eigenvectors give principal modes of variation
      - Eigenvector 2



(d) $b_2 = -3\sqrt{\lambda_2}$ (e) $b_2 = 0$ (f) $b_2 = +3\sqrt{\lambda_2}$

Shape Analysis

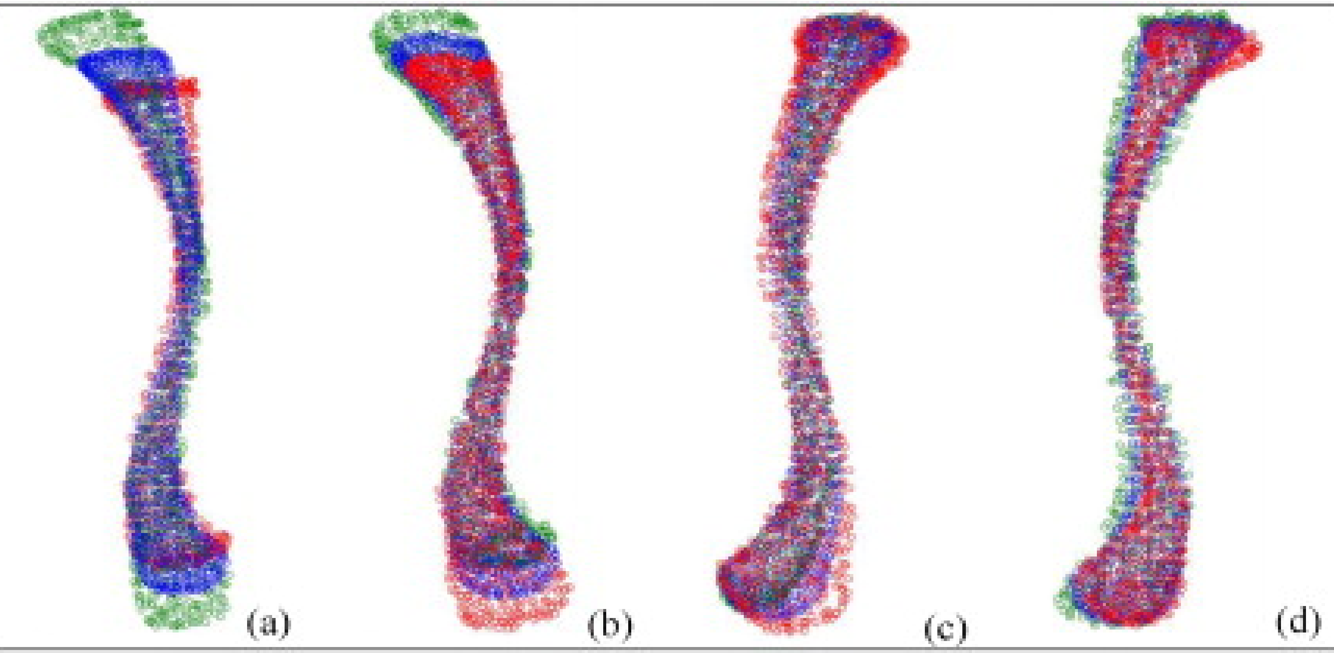
- How to learn modes of variation ?
  - Perform eigen analysis of covariance matrix
    - Principal eigenvectors give principal modes of variation
      - Eigenvector 3



(g) $b_3 = -3\sqrt{\lambda_3}$ **(h)** $b_3 = 0$ **(i)** $b_3 = +3\sqrt{\lambda_3}$

Shape Analysis

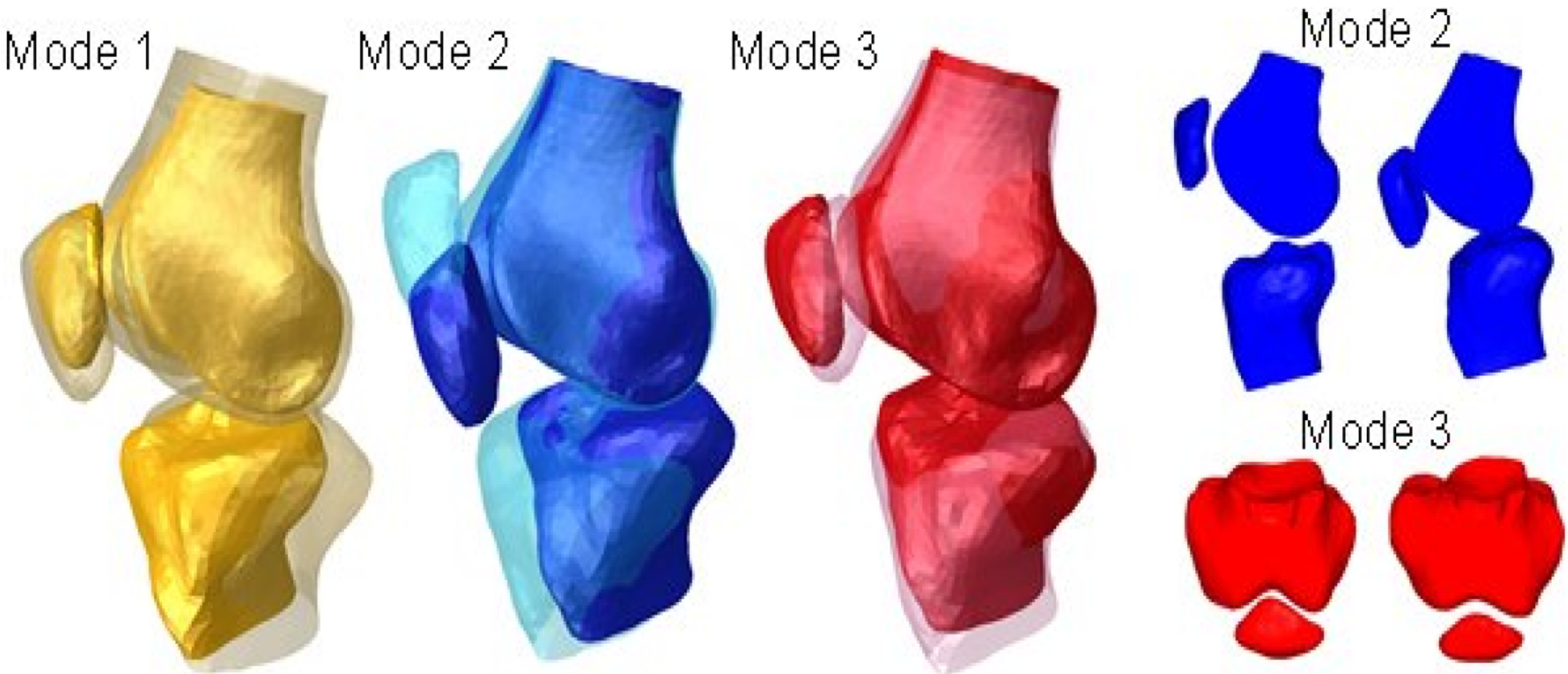
- How to learn modes of variation ?
  - Perform eigen analysis of covariance matrix
    - Principal eigenvectors give principal modes of variation
      - http://www.sciencedirect.com/science/article/pii/S0169260713001740

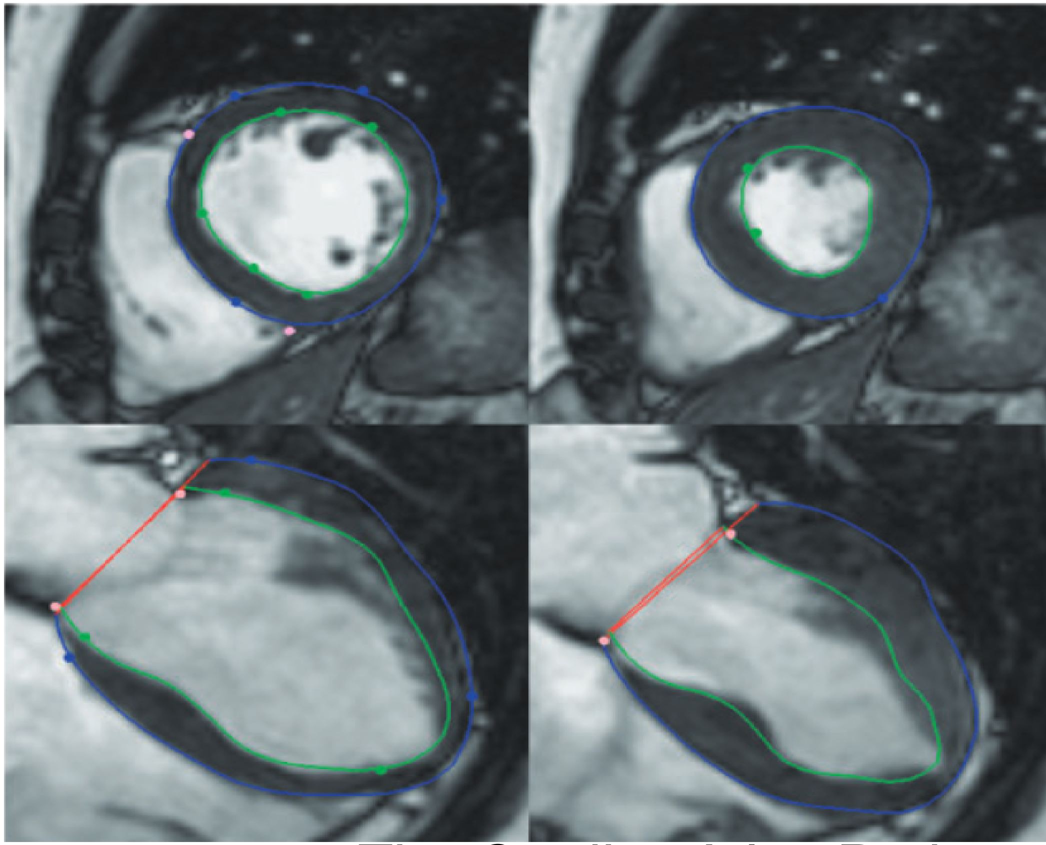
Mode	1	2	3	4
(-3SD, Mean Shape, +3SD)				
Percentage of Variance (%)	31.9	19.0	10.6	5.0
Description	Overall length (T_1)	Sternal diameter (T_2) and acromial diameter (T_3)	Medial curve radius (R_1) and inferior curve radius (R_2)	Overall diameter (T_4)

* The green, blue and red models represent the -3 SD, the median and the +3SD models

Shape Analysis

- How to learn modes of variation ?
  - Perform eigen analysis of covariance matrix
    - Principal eigenvectors give principal modes of variation
      - http://www.du.edu/rsecs/departments/mme/biomechanics/research/statisticalshapemodeling.html



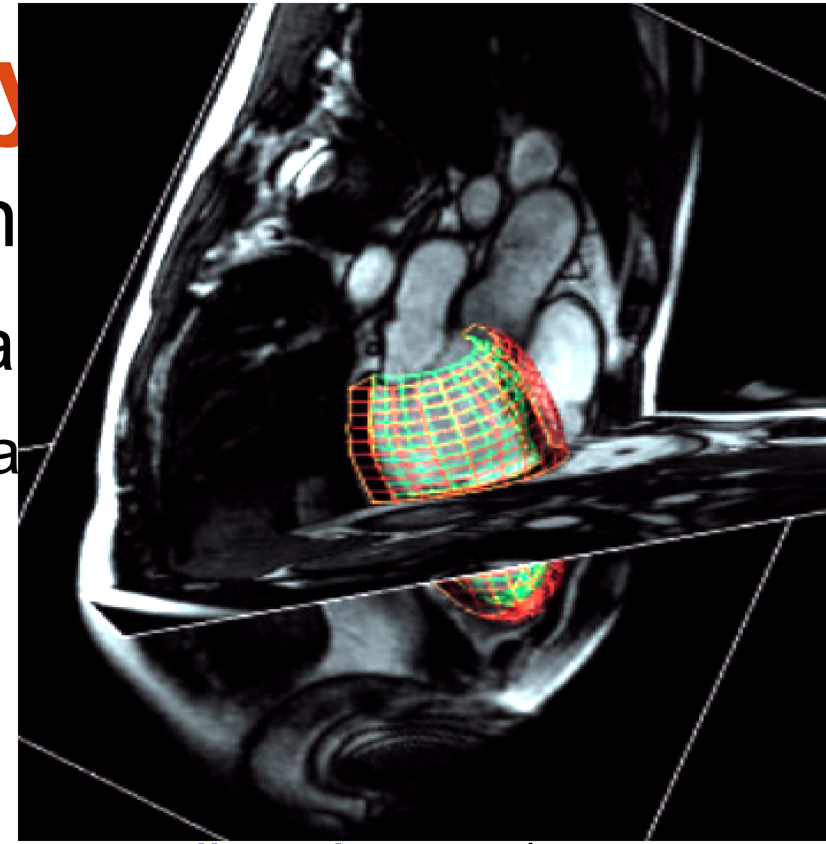


Analy

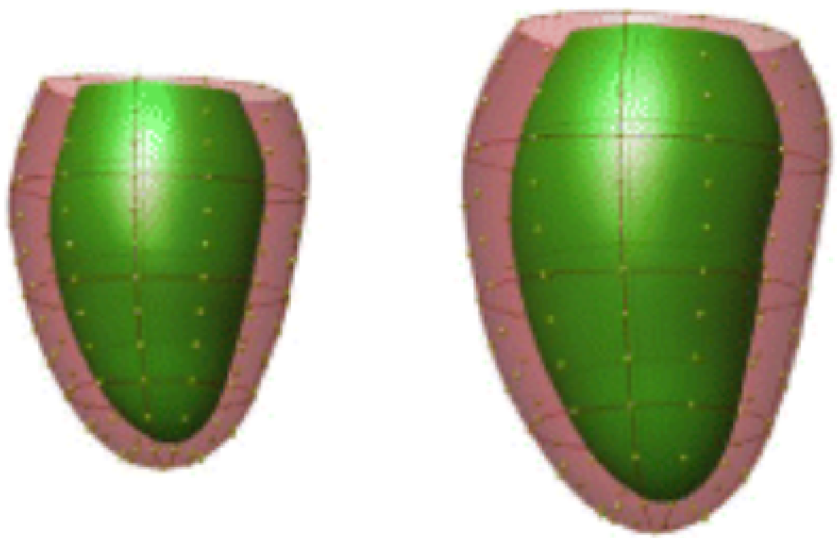
riation

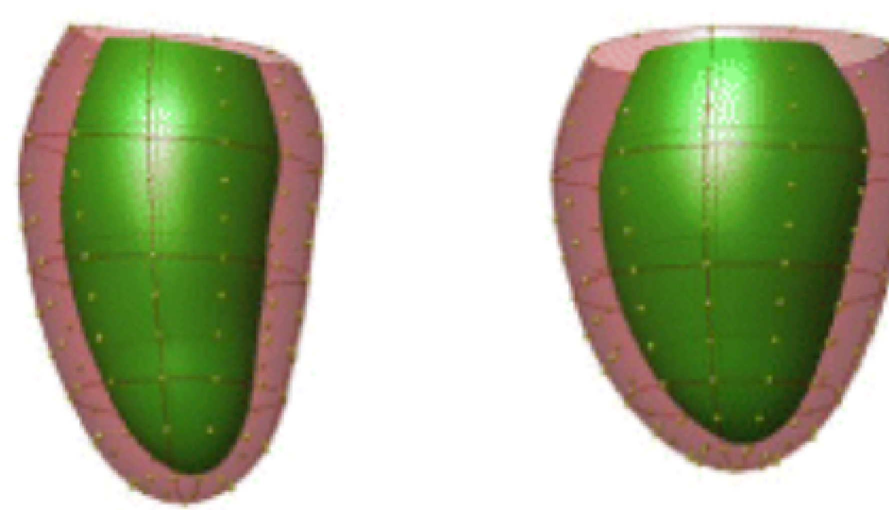
covaria

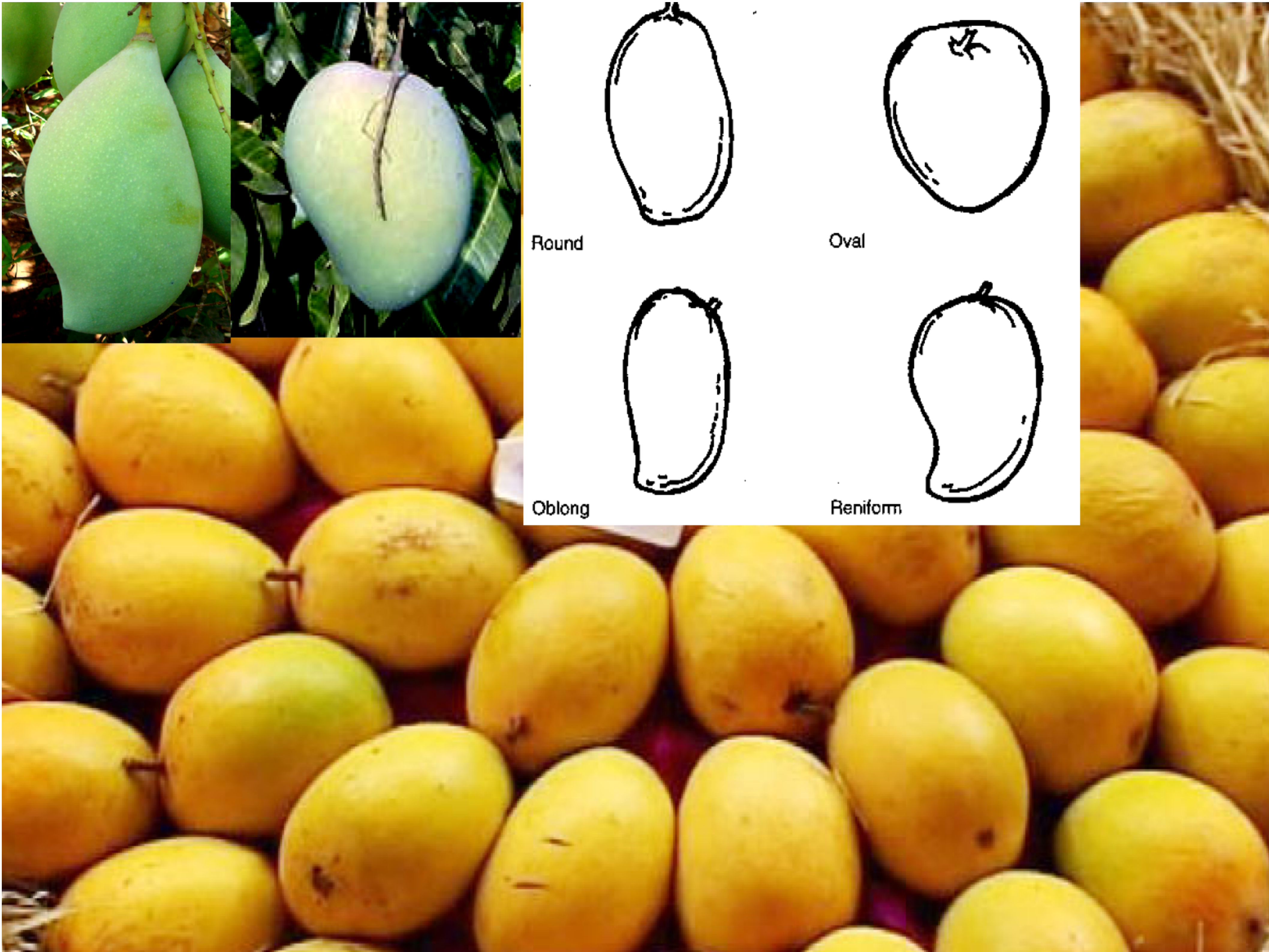
principa



- The Cardiac Atlas Project (http://www.cardiacatlas.org)
  http://openi.nlm.nih.gov/detailedresult.php?img=3150036_btr360f4&req=4
- Left: Mode 1. Right: Mode 2.






Round
Oval
Oblong
Reniform

Shape Analysis

- Medical applications of learning statistical shape models

  (1) Scientific study to understand variability

  (2) Hypothesis testing to test for shape differences in a specific disorder / disease

  (3) Classification of a patient based on shape

  - e.g., autism spectrum disorder

  (4) Shape priors for segmentation