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SCHOOL OF MEDICINE
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Performance metrics: Similarity or distance measures

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Similarity Measures in Hilbert space

Objectives

1) Understand correlations and other correlation-based similarity measures often used as validation metrics

2) Understand how to compute similarity measures for various data types.

Similarity measures

- Correlation based
- Statistical (goodness-of-fit)
- Information theoretic (mutual information/entropy)
- Geometric (kappa index)

Correlations

- Pearson correlation
- Rank correlation
- Partial correlation
- Multiple correlation
- Partial multiple correlation
- Canonical correlation

Pearson product moment correlation coefficient

Given paired measurements $(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n)$, the Pearson product-moment correlation coefficient (Fisher, 1915) is a measure of association given by

$$r_P = \frac{\sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n} (X_i - \bar{X})^2 \sum_{i=1}^{n} (Y_i - \bar{Y})^2}},$$

where $\bar{X}$ and $\bar{Y}$ are the sample mean of $X_1, X_2, \ldots, X_n$ and $Y_1, Y_2, \ldots, Y_n$ respectively.

Why correlation is inner product (vector multiplication)?

Scale and translation invariant

$$r_P(X, Y) = r_P(aX + b, cY + d)$$

Can be written as a matrix multiplication

$$r_P(X, Y) = Z^\top W$$

Question. Prove the above statements

Inference on correlation

$$H_0 : \rho = 0 \text{ vs. } H_1 : \rho \neq 0$$

Under normality,

$$T = \frac{r_P \sqrt{n-2}}{\sqrt{1 - {r_P}^2}}$$

T-statistic with n-2 degrees of freedom

This is most often used method in practice

How it is used in practice?

The threshold for statistical significance is set at a correlation magnitude of ± 0.2, which corresponds to a one-sided p-value of 0.0018. The significance level is determined using the *t-test for Pearson correlation*, where the test statistic is computed as

$$t = r \cdot \sqrt{\frac{n-2}{1-r^2}},$$

with t following a Student's t-distribution with $n-2$ degrees of freedom under the null hypothesis $H_0 : r = 0$ [23].

In general, fluid intelligence exhibits stronger correlations with the spectrogram than crystallized intelligence (Fig. 5 and 6), suggesting that dynamic brain activity is more relevant for problem-solving and reasoning abilities than

Chung et al. 2025, arXiv:2502.05814

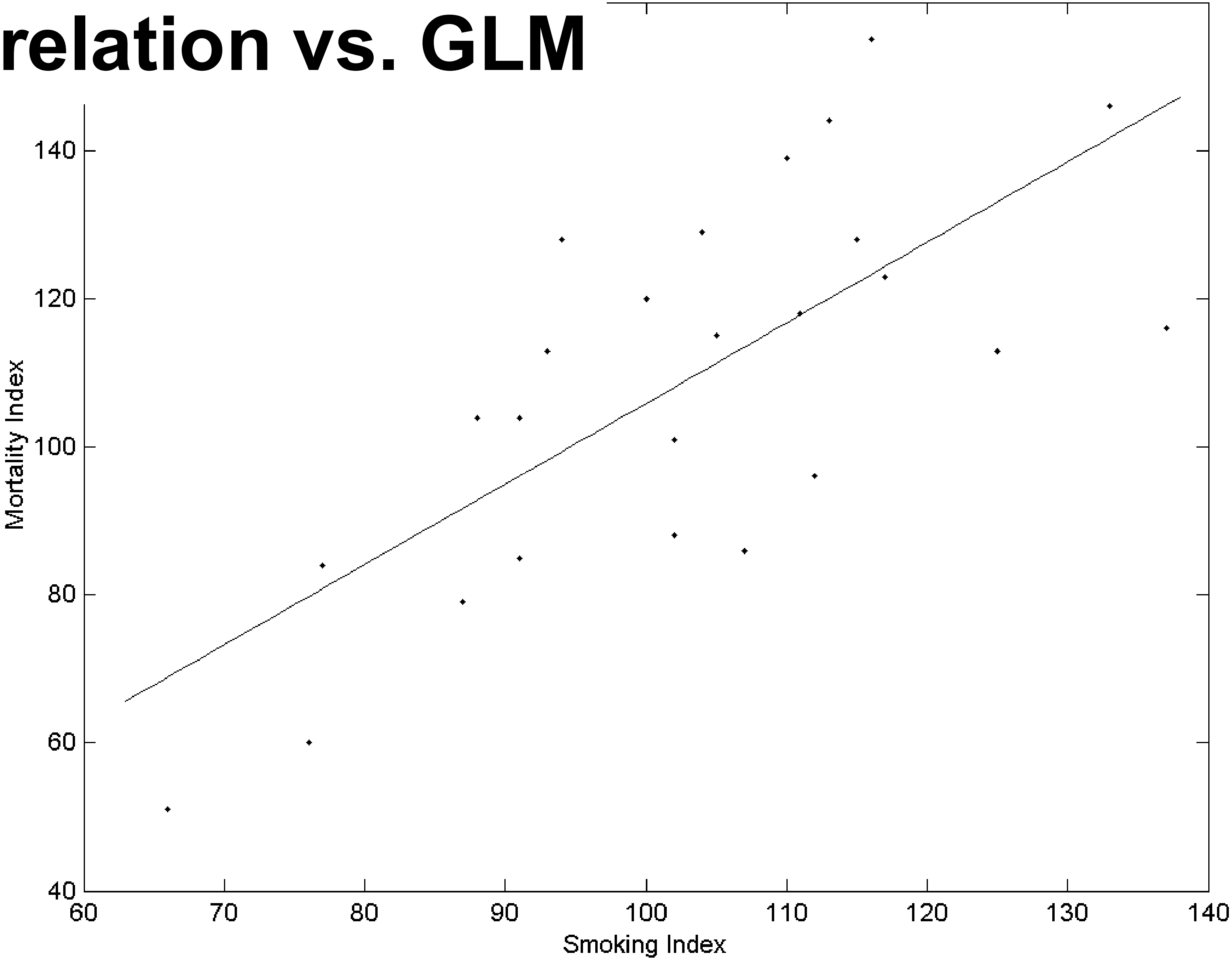
If we can not assume normality of data

Fisher transform: $$F(r_P) = \frac{1}{2}\ln\left(\frac{1+r_P}{1-r_P}\right)$$

$$Z = \sqrt{n-3}\left(F(r_P) - F(\rho)\right)$$: standard normal

Note: under the null hypothesis, this term vanishes.

Correlation vs. GLM



Are there any relationship between correlation analysis and GLM ?

Slope of regression vs. correlation

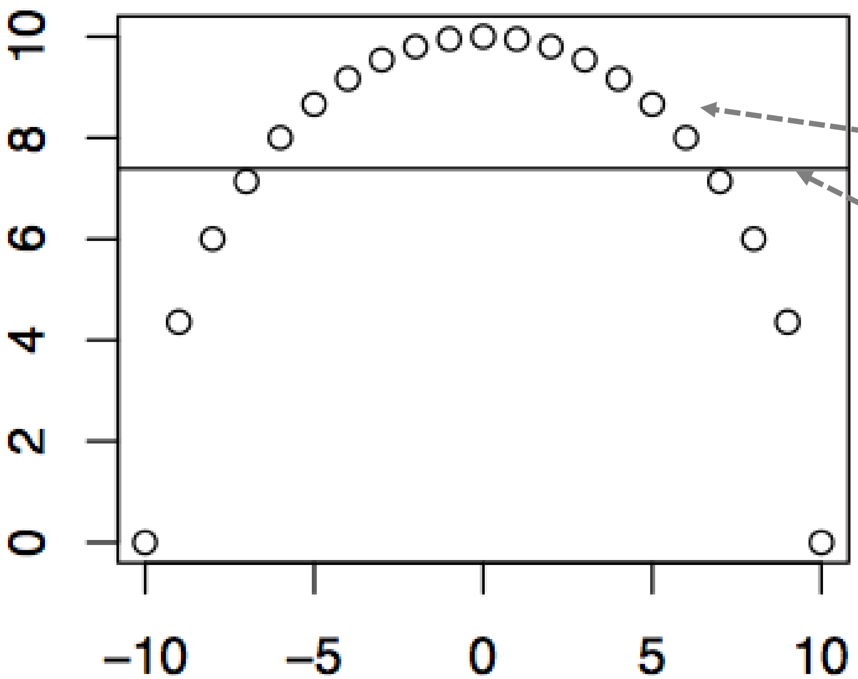
$$Y = \beta_0 + \beta_1 \square X$$

If (X,Y) are bivariate normal,

$$\beta_1 \cong \frac{\sigma_Y}{\sigma_X} r_P$$

Under normality, correlation analysis = linear regression

Limitation of correlations



Data $x_i^2 + y_i^2 = 10^2$

Linear regression fit

Slope=correlation=0

Correlation only measures linear dependency.
It does *not* measure nonlinear dependency.

Question: Mathematically show the correlation = 0

Using correlation, is it possible to measure nonlinear dependency?

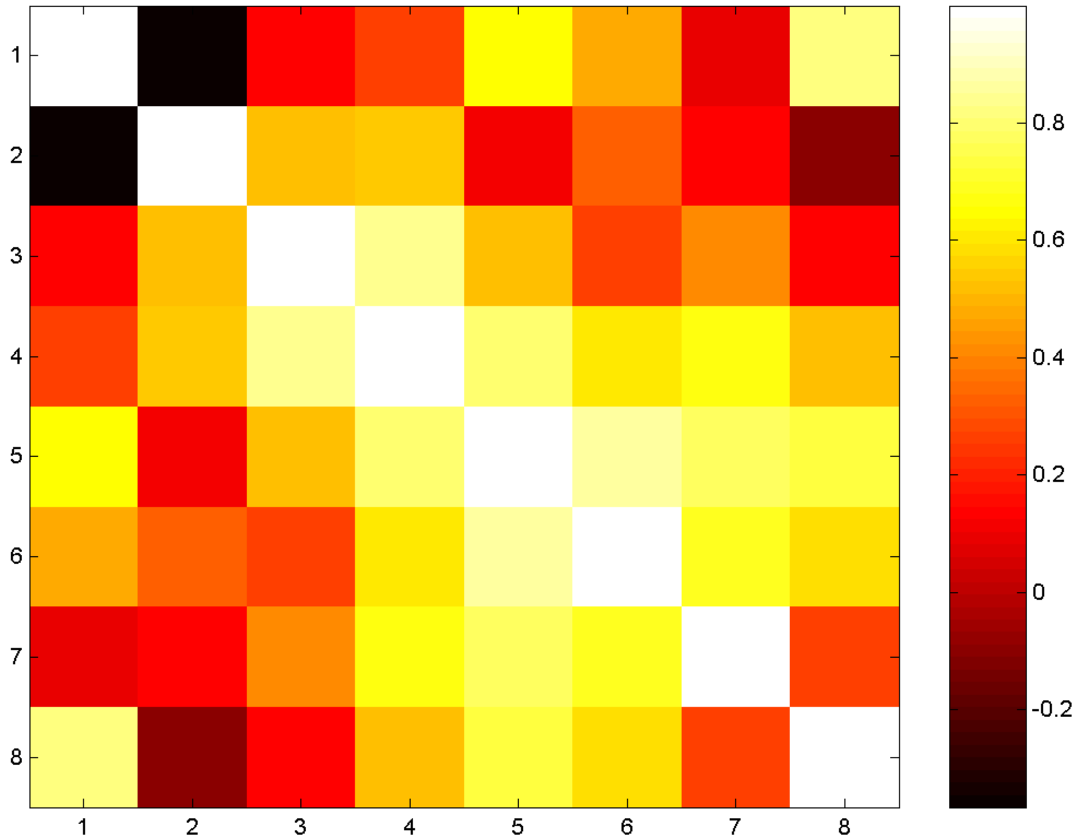
$$Y = f(X)$$

$$f(X) = \sum_i c_i X^i$$

$$\rho(X^i, Y^j)$$

Correlation mapping technique

CT intensity values for 8 regions of interests (ROI) in <u>mouse breast cancer study</u>



Regions denoted by numbers

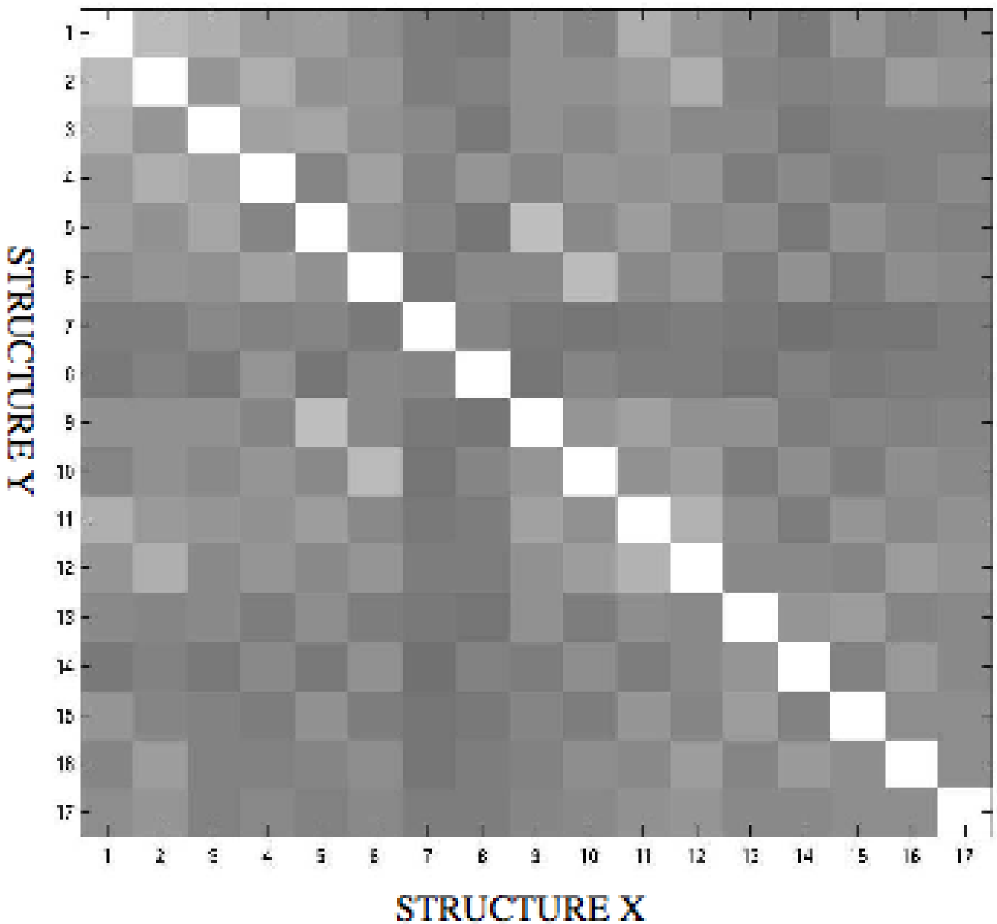
Sorted correlation map can be used to display the pairwise correlation

Not very illustrative visualization

→ Dendrogram (TDA)

Correlation mapping technique
(anatomical connectivity analysis)

1 = Left Lateral Ventricle
2 = Right Lateral Ventricle
3 = Left Caudate
4 = Right Caudate
5 = Left Putamen
6 = Right Putamen
7 = Left Accumbens
8 = Right Accumbens
9 = Left Pallidum
10 = Right Pallidum
11 = Left Thalamus
12 = Right Thalamus
13 = Left Amygdala
14 = Right Amygdala
15 = Left Hippocampus
16 = Right Hippocampus
17 = Brain Stem



James Gee

Example

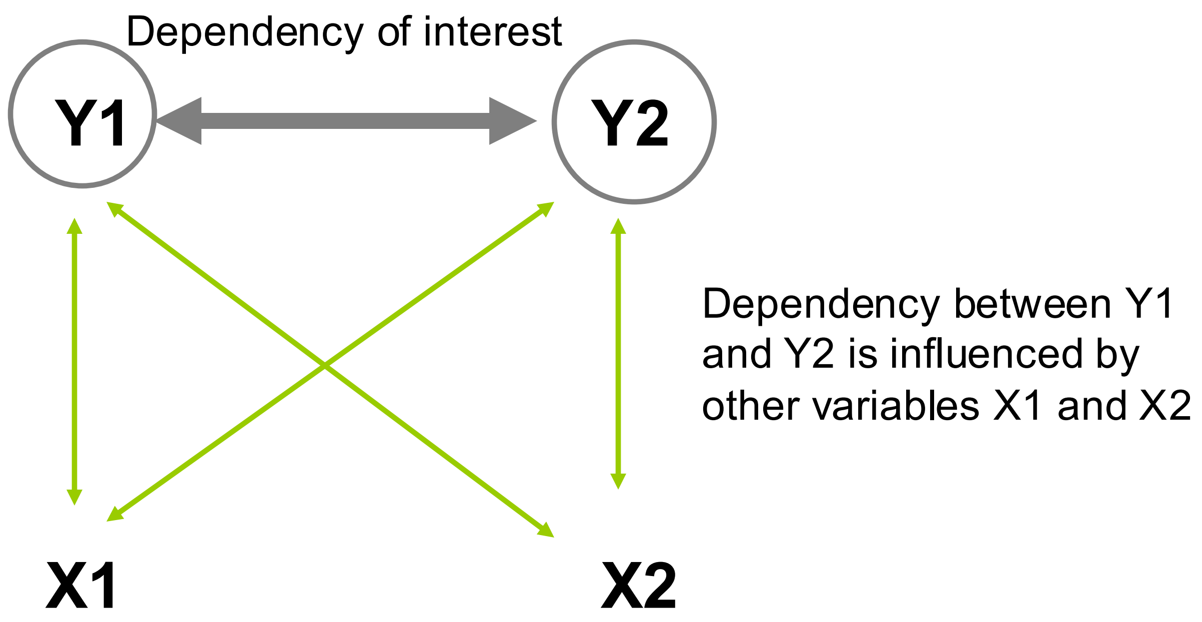
Interested in knowing the relation between
Y1 = brain cortical thickness
Y2 = behavioral measure

Biological facts:
•Cortical thickness is related to age (X1)
•Cortical thickness is related to brain size (X2)

We need:
Corr(Y1,Y2) while accounting for *confounding nuisance covariates* X1 and X2

Partial correlation

Measure of dependency while removing the effect of other variables.



$$Y = (Y_1, Y_2), X = (X_1, X_2)$$

Covariance matrix: $\mathbb{V}(Y,X)' = \begin{pmatrix} \Sigma_{YY} & \Sigma_{YX} \\ \Sigma_{XY} & \Sigma_{XX} \end{pmatrix}$

Partial covariance of Y given X:

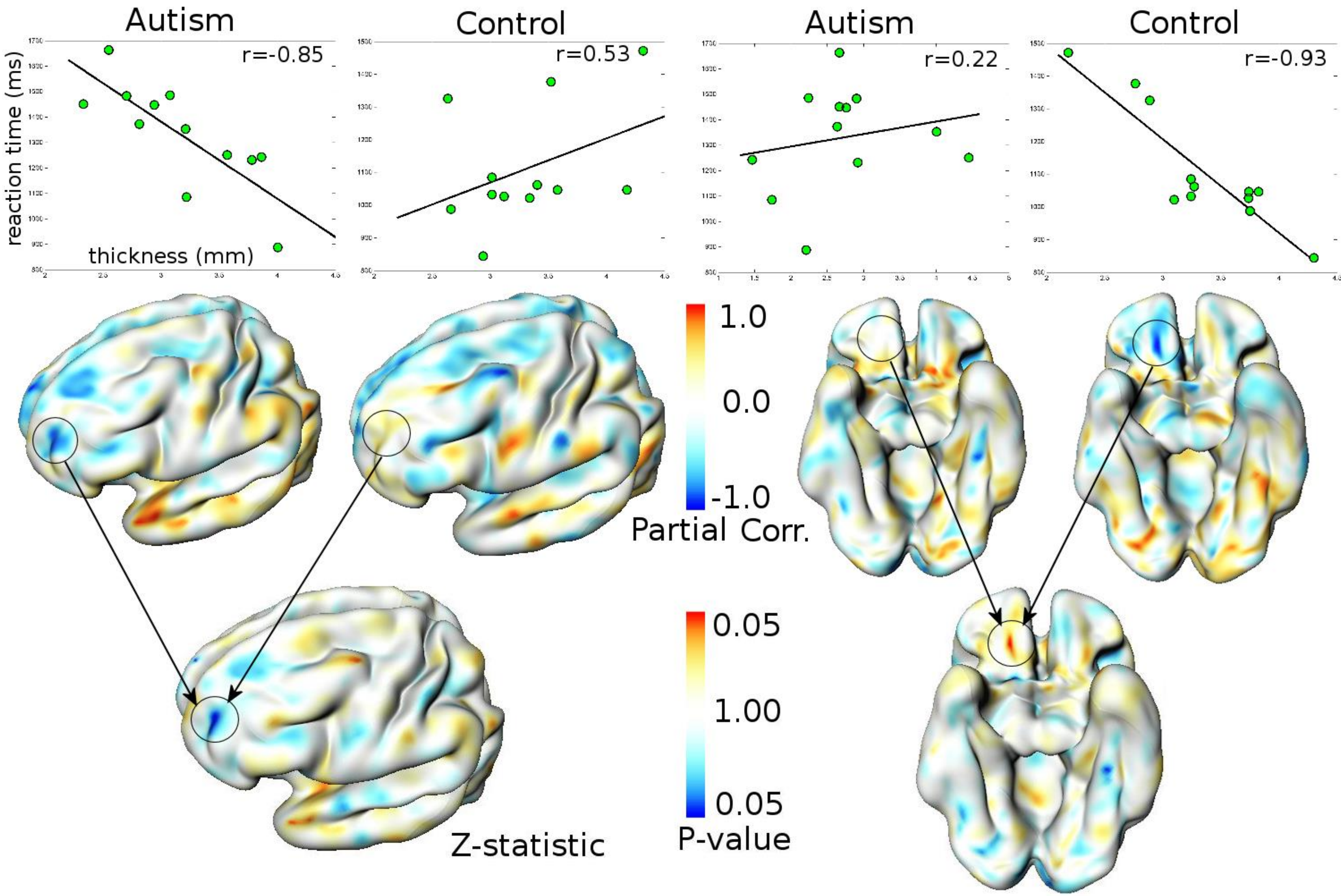
$$\Sigma_{YY} - \Sigma_{YX}\Sigma_{XX}^{-1}\Sigma_{XY} = (\sigma_{ij})$$

Under normality,
this is equivalent to the conditional covariance:

Cov(Y|X)

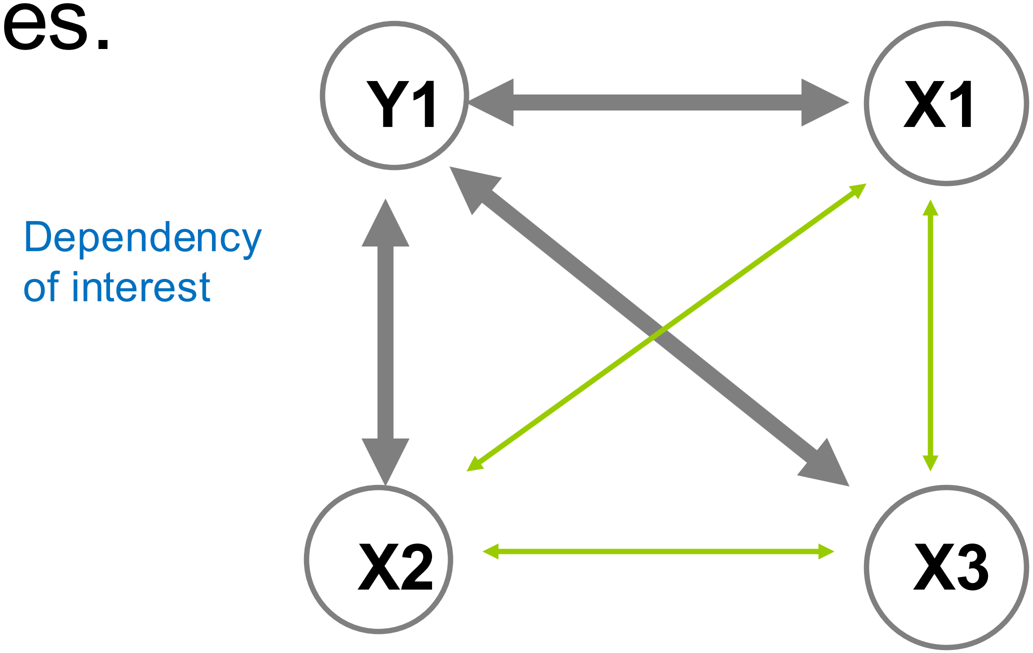
Exercise: prove the above claim

Correlation of emotion recognition response time and cortical thickness while accounting for age and brain size



Multiple correlation

Measure of dependency between one variable and remaining multiple variables.



Example. correlating a reference fMRI time series (amygdala) to fMRI time series in other regions simultaneously

Definition of multiple correlation

Given X_1,X_2,X_3, consider weighted average $w_1X_1 + w_2X_2 + w_3X_3$

The multiple correlation is defined as

$$\rho = \max_{w_1, w_2, w_3} corr(Y, w_1X_1 + w_2X_2 + w_3X_3)$$

The maximum of all possible linear combinations of correlations

How to compute multiple correlations?

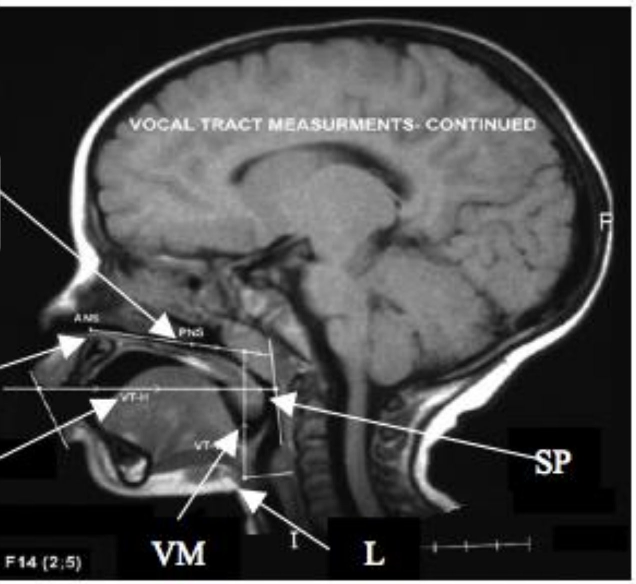
Least squares estimation

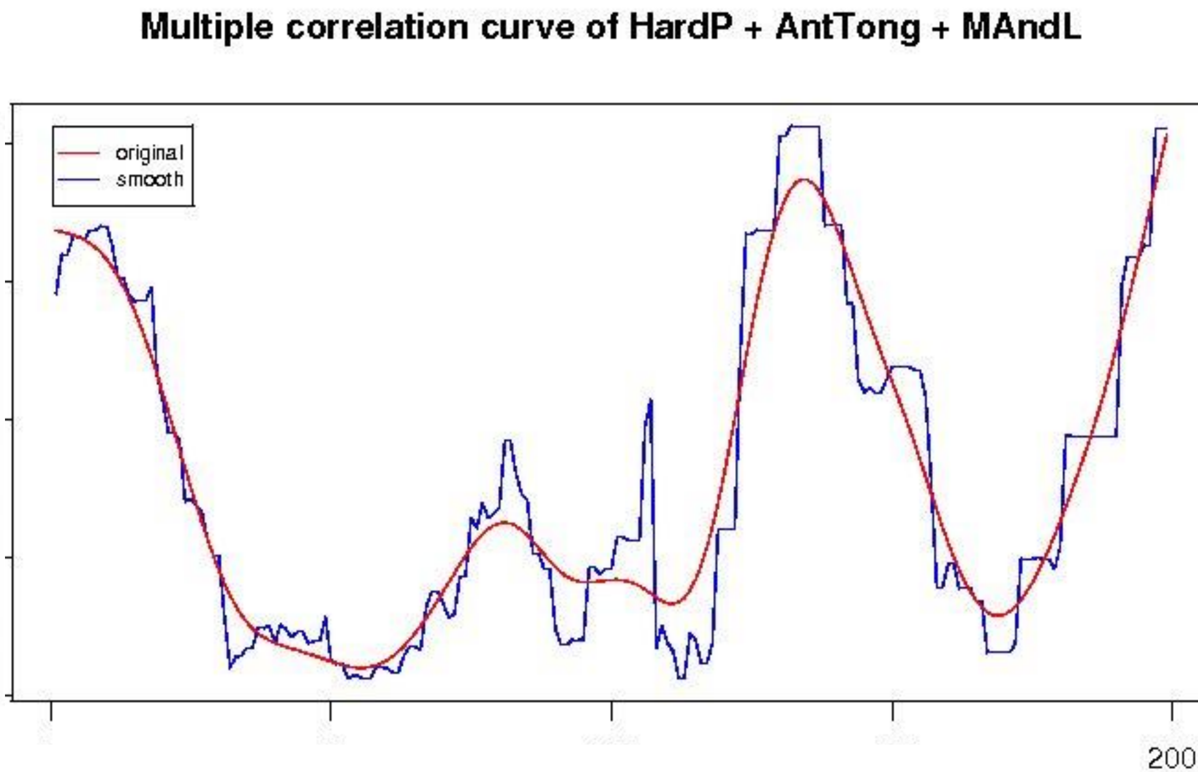
Multiple correlation can be obtained from multiple linear regression analysis

$$Y = w_1 X_1 + w_2 X_2 + w_3 X_3 + \varepsilon$$

Exercise: Show that LSE gives the maximum correlation

Coordinated growth of vocal tract and other anatomy





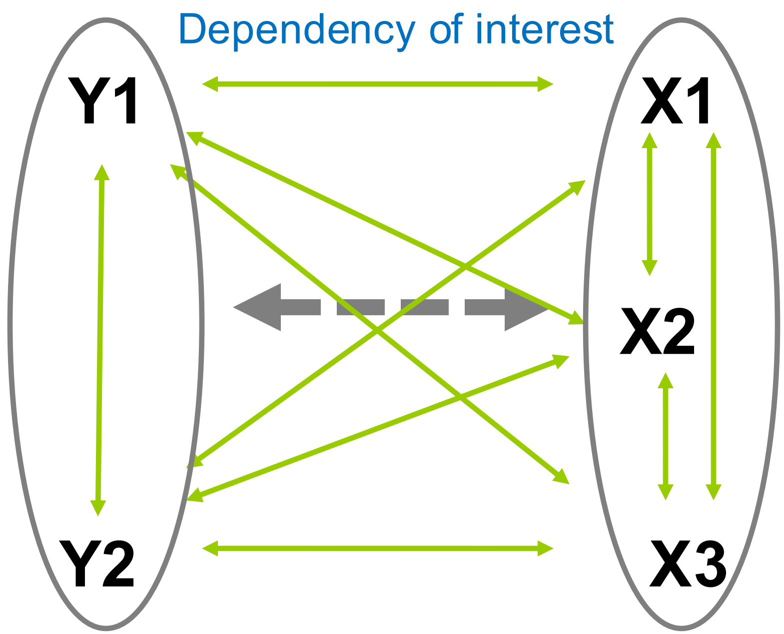
Question.

How anatomical parts develop together longitudinally?
How variables dynamically change together?

Shubing Wang

Canonical correlation

Measure of similarity/dependency between two vectors of unequal size



Applications. network modeling, anatomical and functional connectivity in brain. Distance between two graphs of unequal size

Canonical correlation

$$X = w_1 X_1 + w_2 X_2 + w_3 X_3$$

$$Y = v_1 Y_1 + v_2 Y_2$$

$$\rho = \max_{w,v} corr(X, Y)$$

$$\Sigma_{xx}{}^{-1}\Sigma_{xy}\Sigma_{yy}{}^{-1}\Sigma_{yx} w = \rho^2 w$$

$$\Sigma_{yy}{}^{-1}\Sigma_{yx}\Sigma_{xx}{}^{-1}\Sigma_{xy} v = \rho^2 v$$

→ Eigenvalues are identical. The principal engienvalue is the canonical correlation

Need to solve the eigenequations simultaneously.

Project. Can you develop sparse canonical correlations?

Application to anatomical shape analysis

Ventricle surface in brain

Surface coordinates are taken as a vector data $x=(x_1,x_2,\ldots x_n)$.

The vector data is canonically correlated with the surface coordinates of other anatomical objects.

Games Gee

Canonical correlation map showing pairwise correlation

1 = Left Lateral Ventricle
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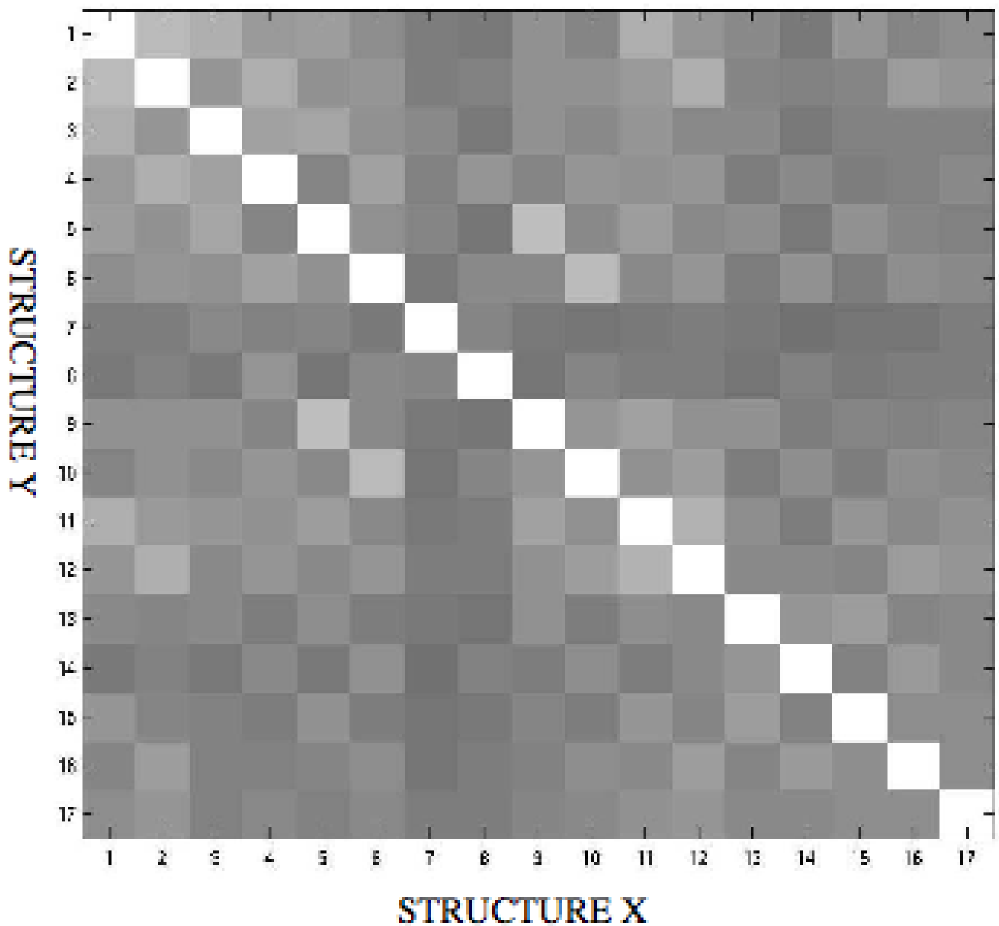


Rao et al. 2008 Medical Image Analysis

Set theoretic similarity measures

Often used validation metric on mostly on image segmentation and clustering

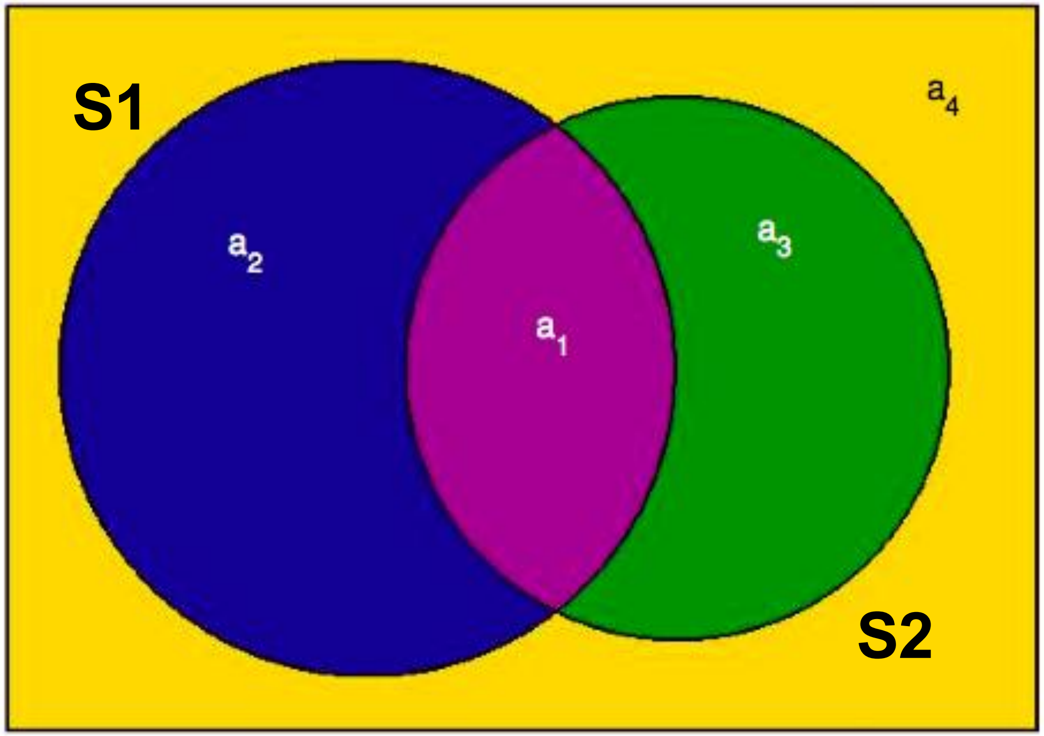
Kappa index measures the proportion of areal overlap:

$$\kappa(S_1, S_2) = 2\frac{|S_1 \cap S_2|}{|S_1| + |S_2|}$$

manual segmentation

gold standard

Range of Kappa index

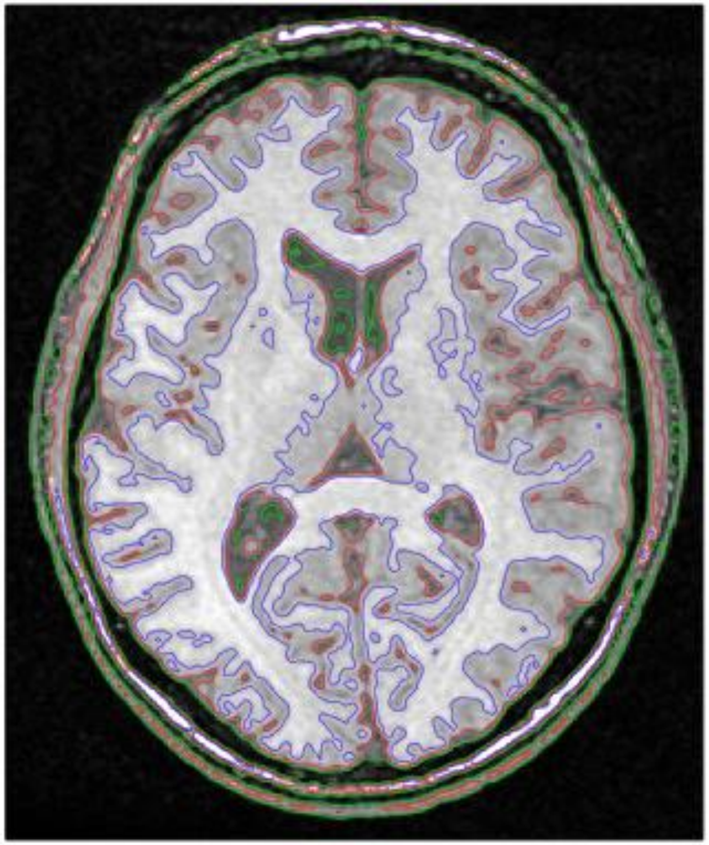


Minimum is obtained when there is no intersection:
a_1=0, k(S1,S2) =0

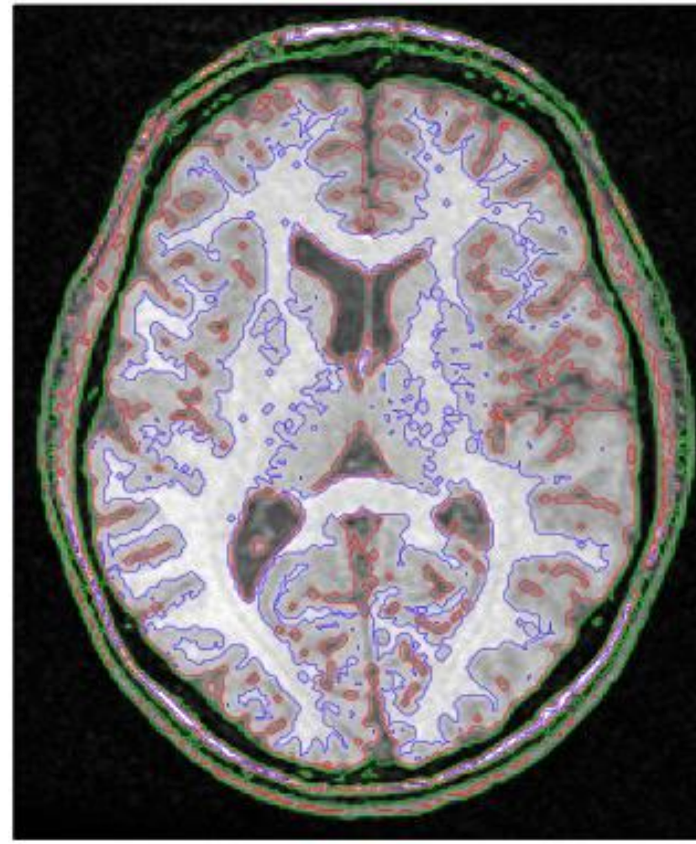
Maximum is obtained when every points intersect:
a_1=a_2=a_3, k(S1,S2)=1

$$\kappa(S_1, S_2) = \frac{2a_1}{2a_1 + a_2 + a_3}$$

Comparing different segmentation techniques



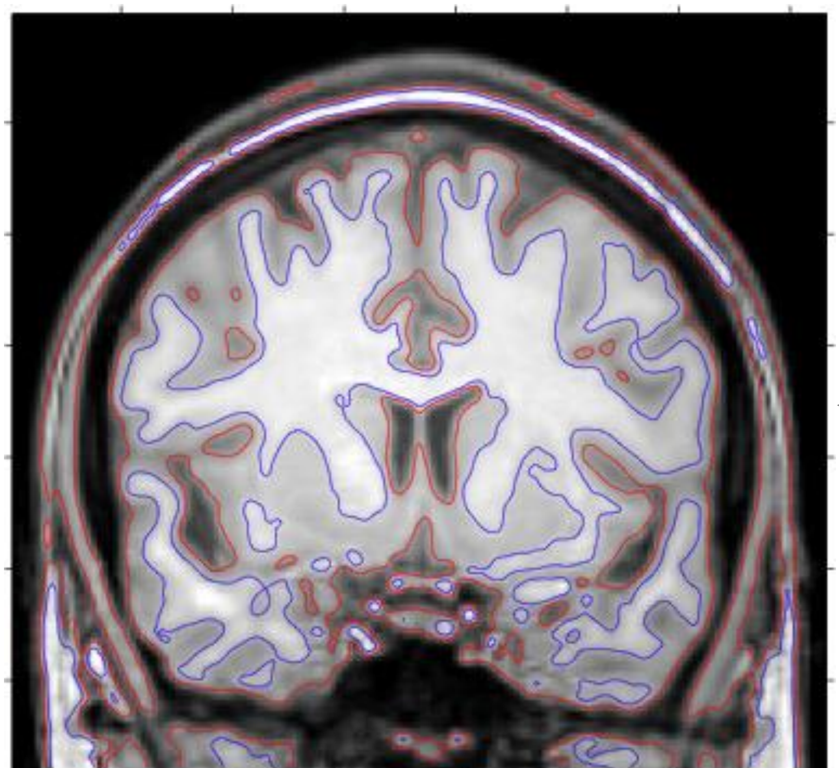
Thin plate spline (TPS) segmentation



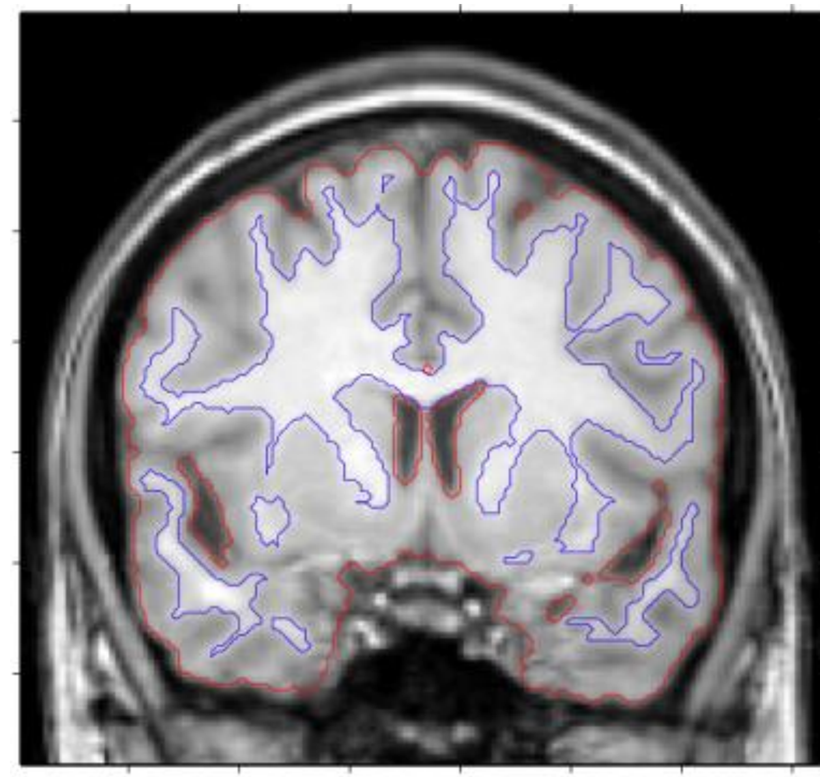
Neural network segmentation

X. Xie (in collaboration with Grace Wahba)

Automatic vs. manual (gold standard)



TPS segmentation



manual segmentation

Correlation vs. Kappa index

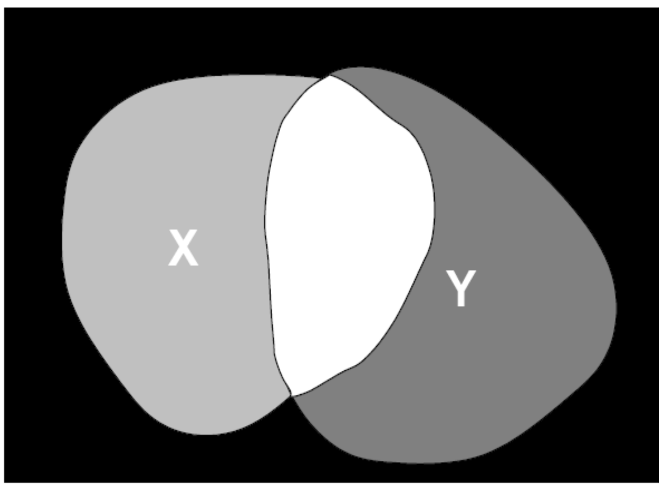
	subject no.	Corr. Coef.		Kappa Index	
		GM	WM	GM	WM
TPS vs Manual	1	0.660	0.827	0.836	0.872
	2	0.702	0.757	0.841	0.827
	3	0.654	0.787	0.811	0.850
	4	0.410	0.678	0.723	0.770
	5	0.612	0.791	0.776	0.838
mean (sd)		0.608(0.115)	0.768(0.056)	0.798(0.049)	0.831(0.038)
SPM vs Manual	1	0.675	0.846	0.883	0.866
	2	0.686	0.839	0.887	0.880
	3	0.637	0.810	0.863	0.842
	4	0.091	0.672	0.679	0.753
	5	0.450	0.803	0.825	0.824
mean (sd)		0.518(0.250)	0.794(0.071)	0.827(0.087)	0.833(0.050)
TPS vs SPM	1	0.806	0.883	0.848	0.900
	2	0.626	0.759	0.794	0.824
	3	0.734	0.822	0.808	0.861
	4	0.426	0.767	0.730	0.793
	5	0.645	0.800	0.785	0.836
mean (sd)		0.647(0.143)	0.806(0.050)	0.793(0.043)	0.843(0.040)

Pearson correlation is *not* a good measure for binary output.
Question. So should Kappa index be used over correlation?

Other set theoretic similarity measures

Willams’ index (Bouix et al., 2005)

Housdorff distance

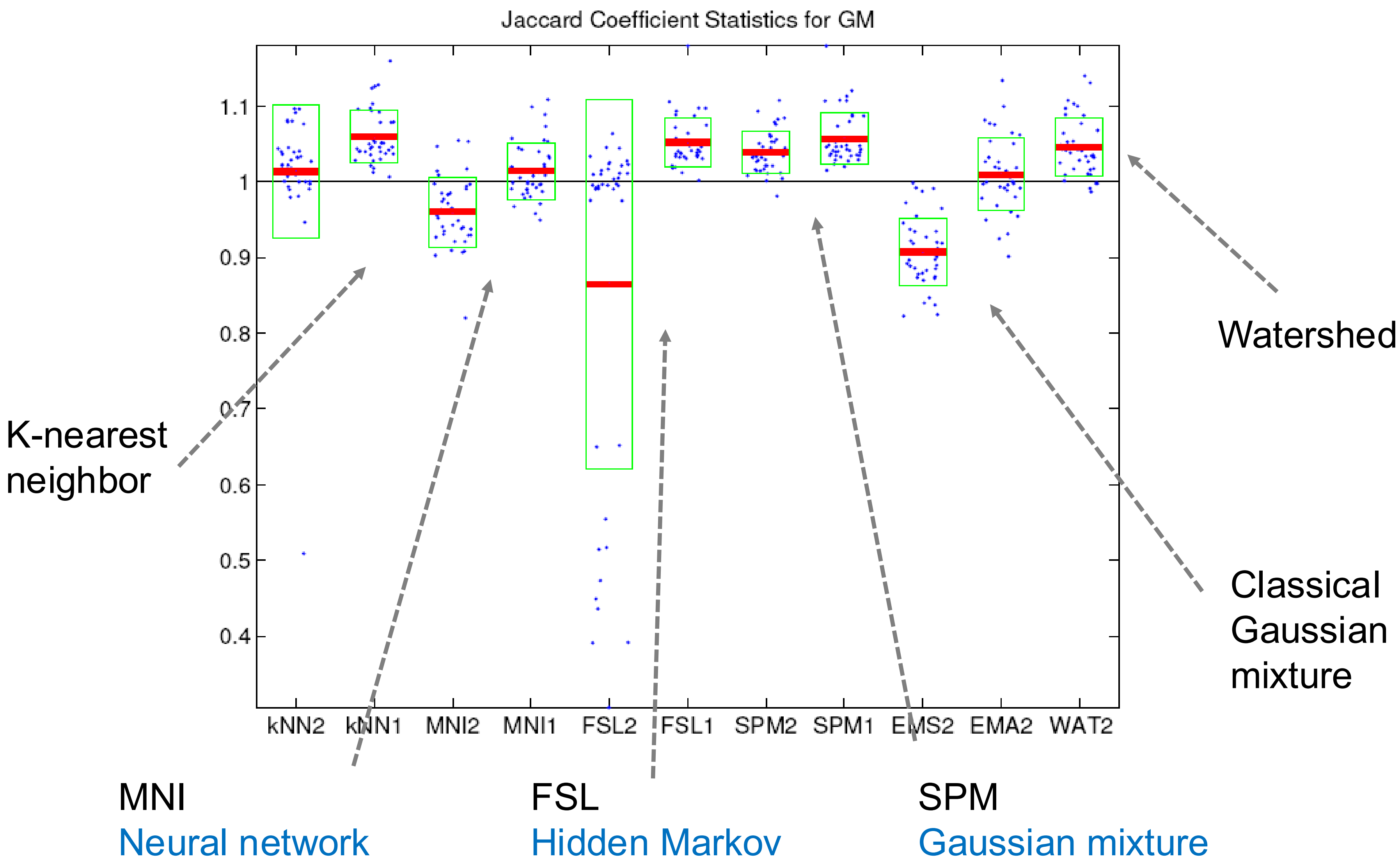


Jaccard $$\frac{|X \cap Y|}{|X \cup Y|}$$

Simple matching: $$\frac{|X \cap Y| + |\overline{X} \cap \overline{Y}|}{n}$$

Volume similarity: $$1 - \frac{||X| - |Y||}{|X| + |Y|}$$

Performance analysis of brain image segmentation algorithms before deep learning

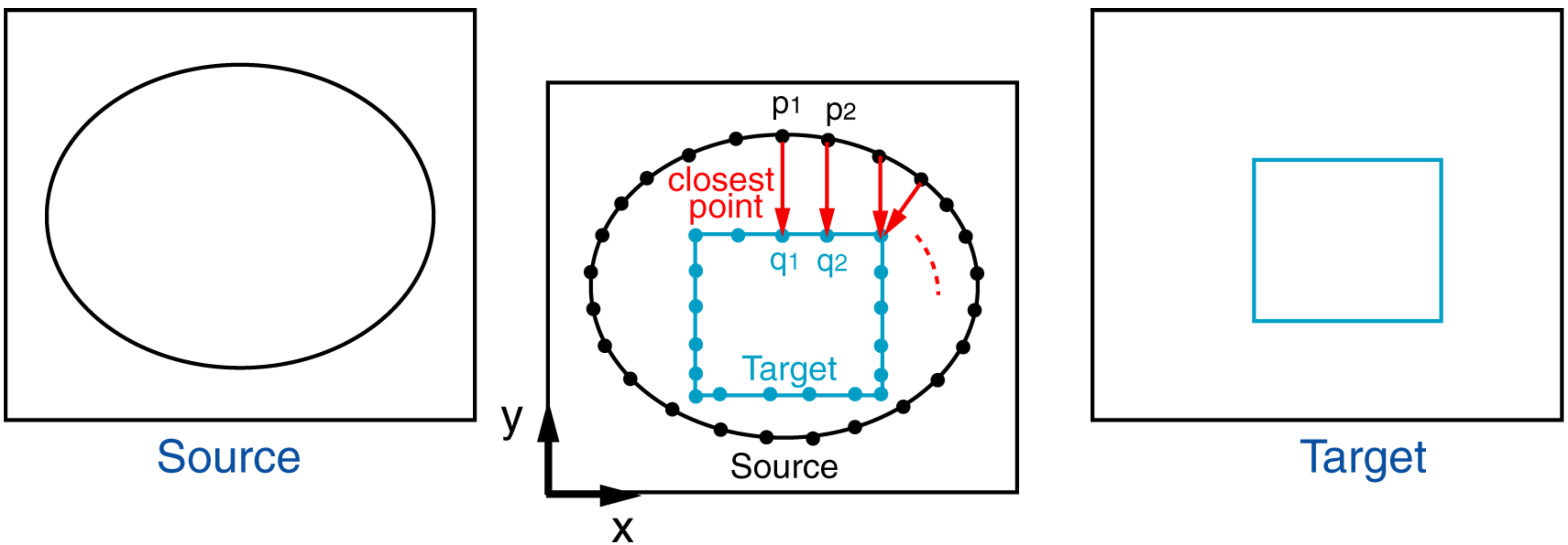


Geometric similarity measures

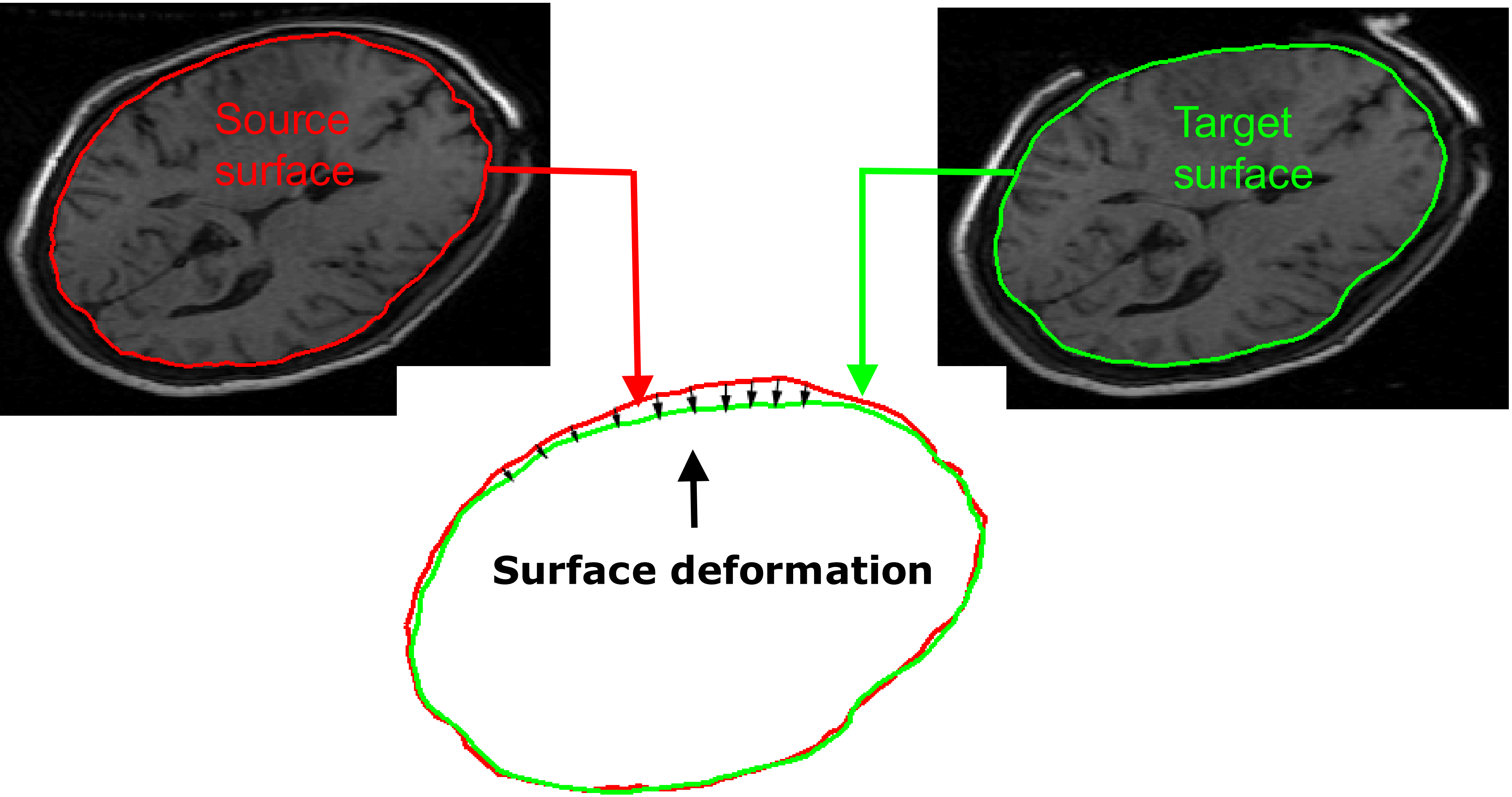
Measure of surface/curve similarity

$$e(X_1, X_2) = \int \min_{p' \in A'} \left\| X_1(p') - X_2(p) \right\|^2 dA \Big/ \int \left\| X_2(p) \right\|^2 dA$$

Staib (1996)



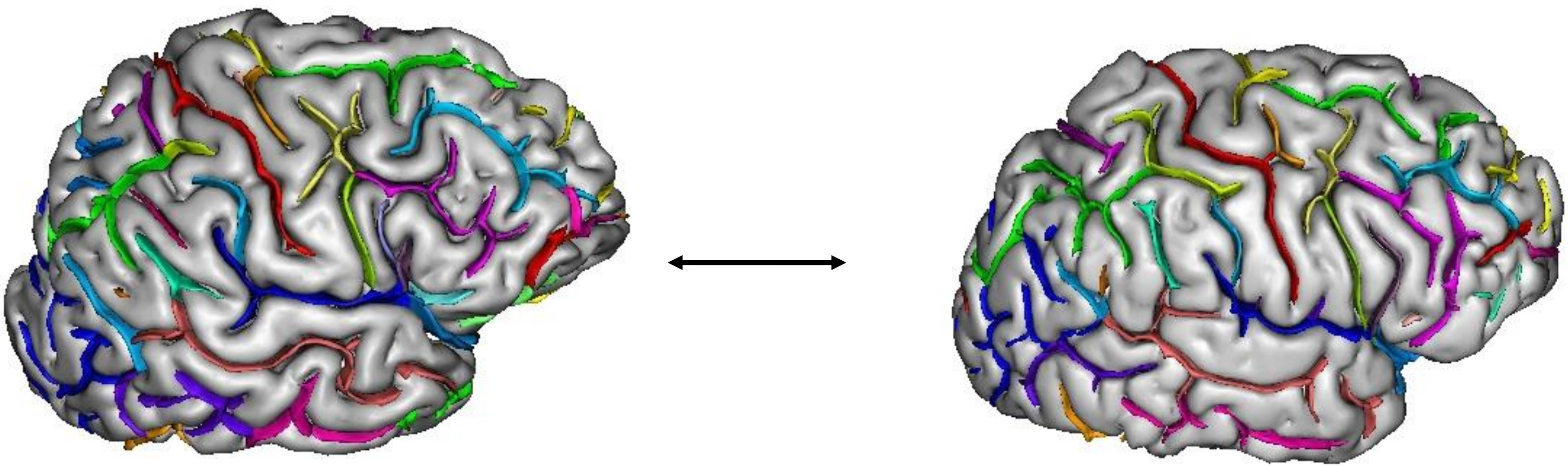
Application of geometric similarity measures



Deformable surface modeling: surface-to-surface registration

→ Diffomorphic image registration (state-of-art): ANTS, SPM

Application of surface similarity measure

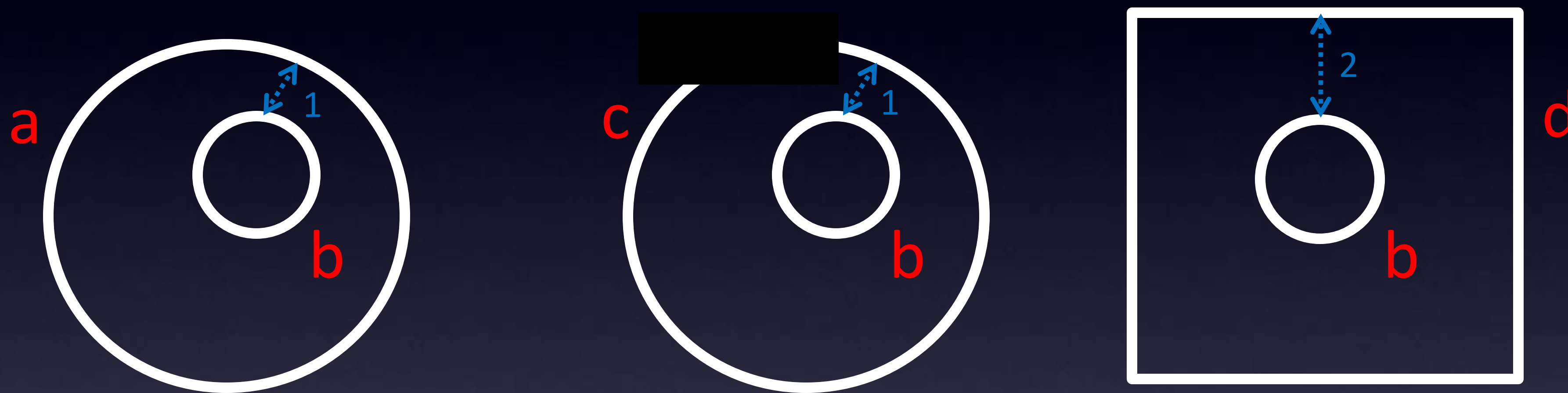


Sulcal pattern matching and brain shape analysis

BrainVisa (J.-F. Mangin) output

Project: design topological similarity measure

What is the difference between similarity measure vs distance?



$$d_{geo}(a,b) = 1 \qquad d_{geo}(c,b) = 1 \qquad d_{geo}(d,b) = 2$$

$$d_{top}(a,b) = 0 \qquad d_{top}(c,b) = 1 \qquad d_{top}(d,b) = 0$$

Information theoretic similarity measures

- Entropy: thermodynamic concept of measuring the amount of chaos in a system
- Shannon (Bell lab, 1948) introduced it as the measure of complexity in information
- Kullback (Kullback & Leibler, 1951) used it in defining the distance between two random variables and distributions

Kullback-Leibler divergence

For probability density *f* and *g*, the Kullback-Leibler divergence (KL distance) is defined as

$$H(f,g) = \mathbb{E}_f \ln \frac{f(X)}{g(X)} = \int \log \frac{f(x)}{g(x)} f(x) \, .dx$$

$$H(f,g) \geq 0$$

Equality is obtained when $H(f,f) = 0$

Smaller *H* → more similar

H is called *relative entropy.*

Kullback-Leibler divergence

Question: Is H symmetric?

$$H(f,g) = H(g,h)?$$

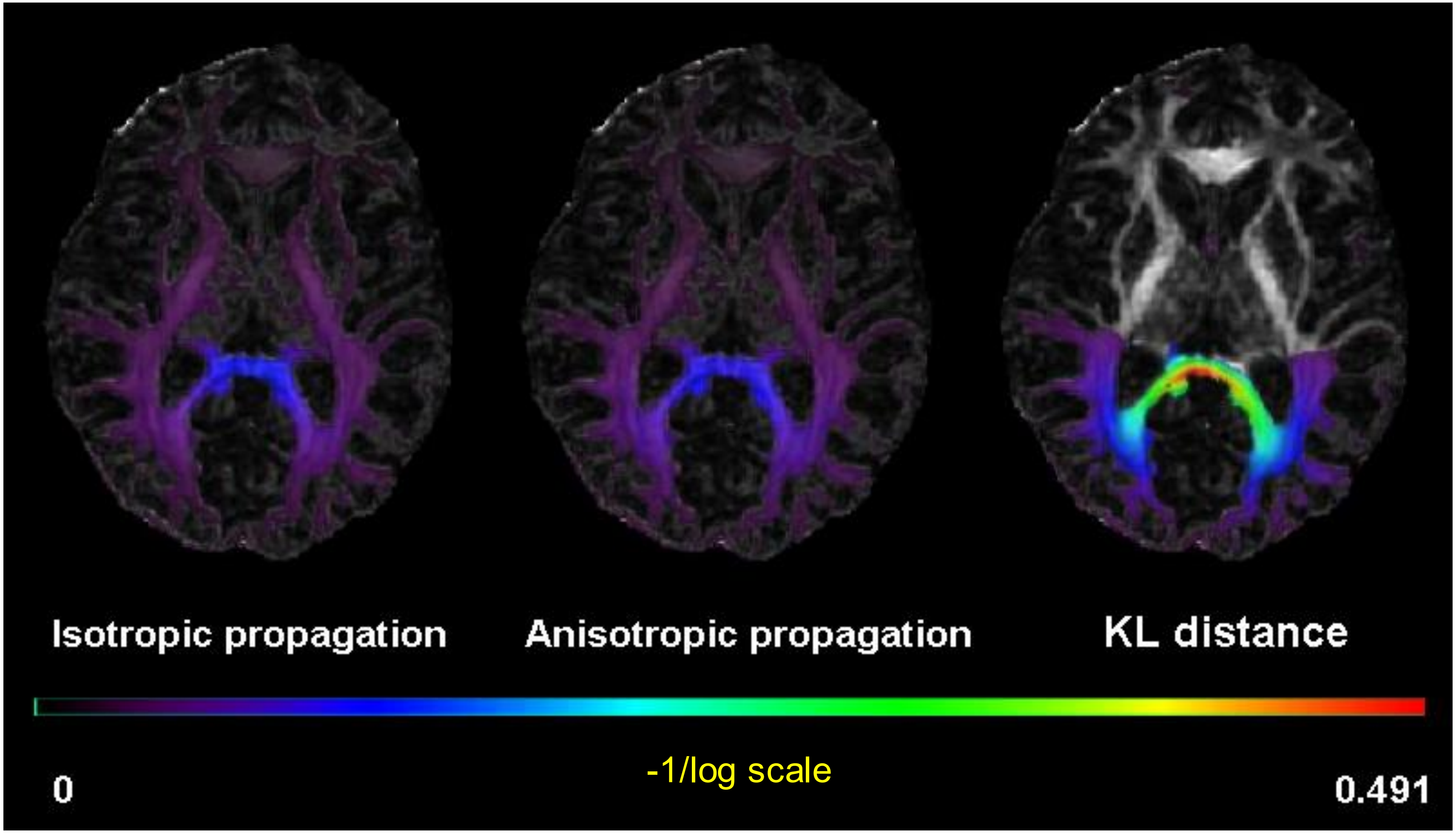
Computing KL-distance

In practice, we estimate the distribution of a random variable via the empirical distribution (histogram).

Discretization:

$$\int \ln \frac{f(x)}{g(x)} f(x)\, dx = \sum_i \ln \frac{f(x_i)}{g(x_i)} f(x_i)$$

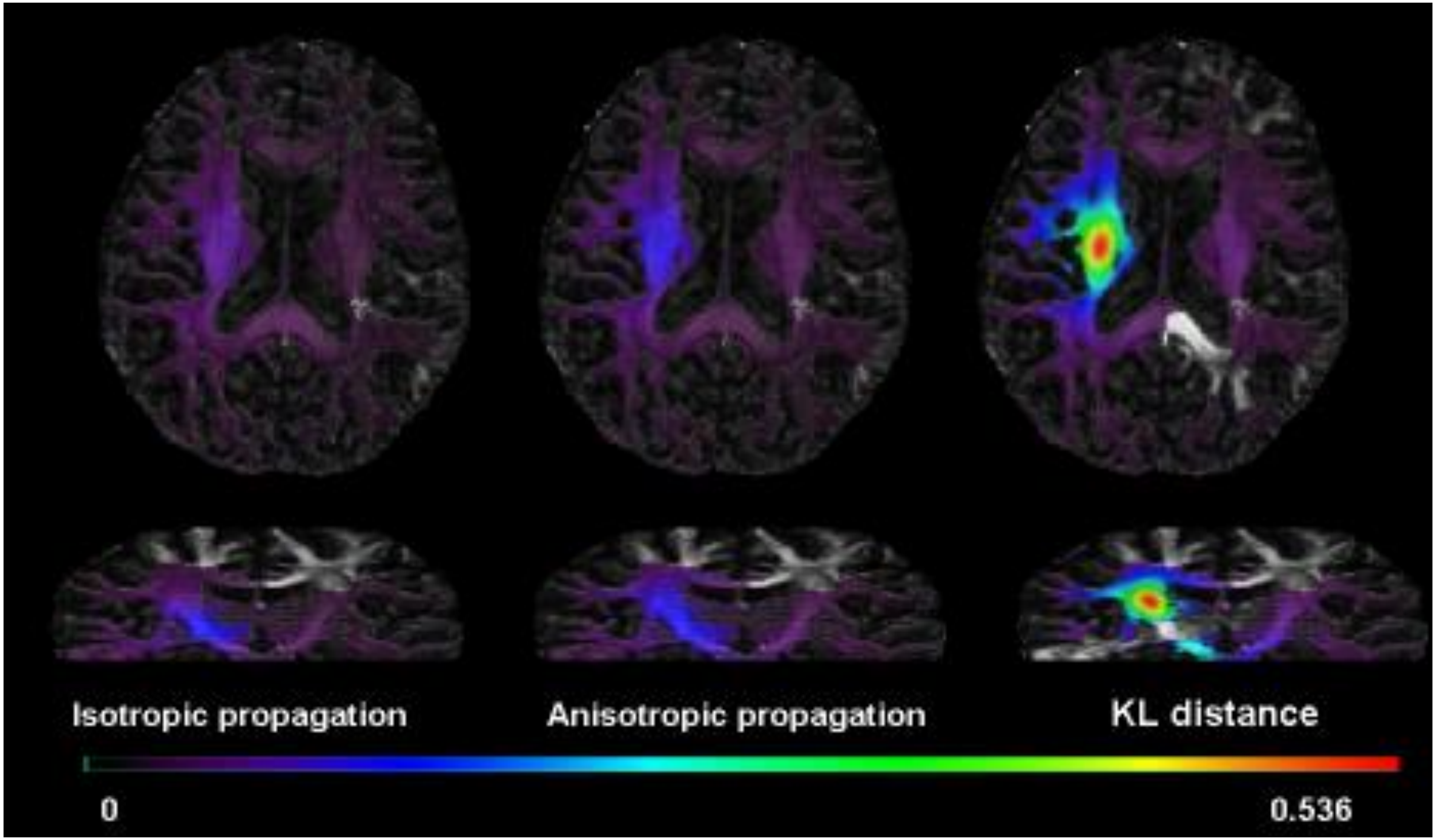
DTI connectivity via KL-distance



KL-distance is computed within a small window around each voxel

J.E. Lee

KL-distance in DTI

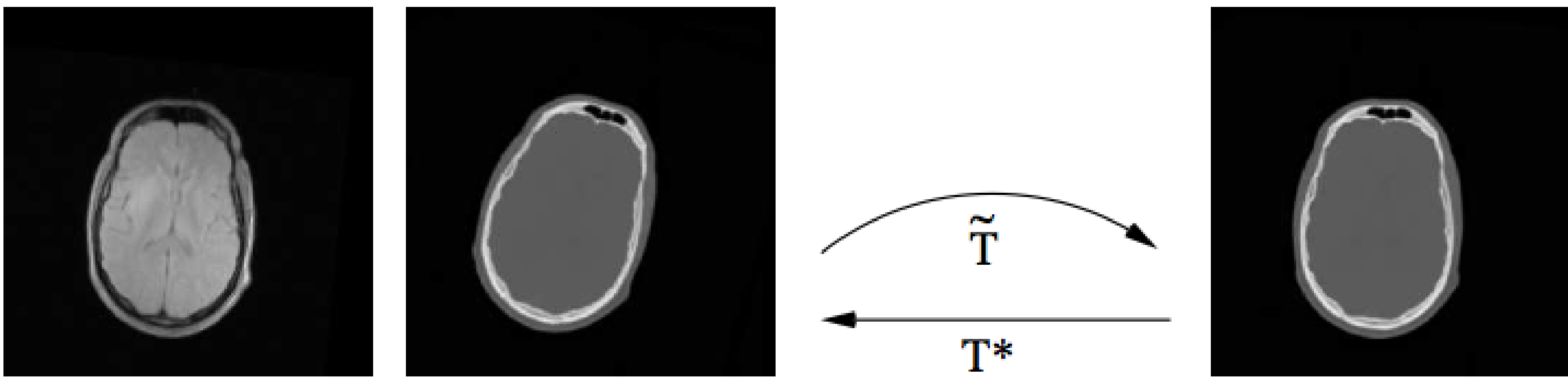


Null model Alternate model

Significance of connectivity can be also tested.

Other use of KL-distance

Registration cost function for locally varying image intensity histogram



MRI CT

Mutual information

Let f be the joint density of f_1 and f_2. The mutual information of f_1 and f_2 is defined as

$$I(f_1, f_2) = H(f, f_1 f_2)$$

Mutual information

If $f=f_1 f_2$, two random variables are independent. If random variables are independent, $I(f_1,f_2)=0$.

If two random variables are independent, $corr(f_1,f_2)=0$. So mutual information behaves like correlation.

Questions

1) Prove that Pearson correlation is scale and translation invariant

2) Suppose there are two groups of data and resulting Pearson correlations.

$$\begin{array}{ccc} x_1, x_2, \cdots, x_m & & y_1, y_2, \cdots, y_n \\ \downarrow & & \downarrow \\ \rho_1 & \longleftarrow \text{Permutation test} \longrightarrow & \rho_2 \end{array}$$

Perform the permutation test. Compare the result against the parametric approach (Fisher transform + standard normal).