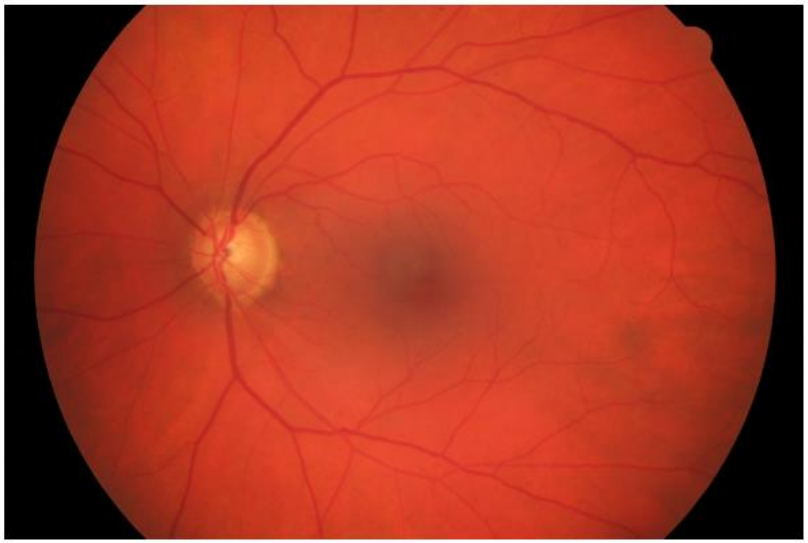

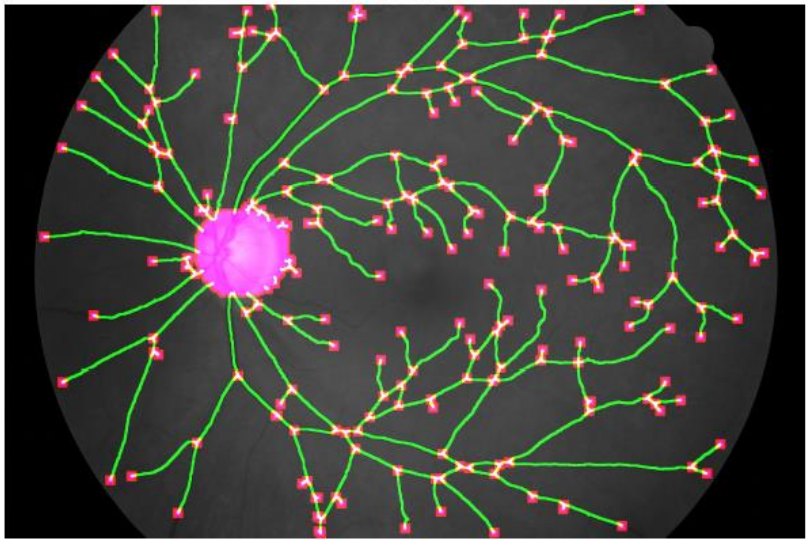

Networks tools for outlier detection and image classification

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Campus d'Excel·lència Internacional

Dynamical Methods in Data-based Exploration of Complex Systems
Dresden, Germany, October 2019

GOBIERNO DE ESPAÑA MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

BE-OPTICAL *Advanced Biomedical Optical Imaging and Data Analysis*

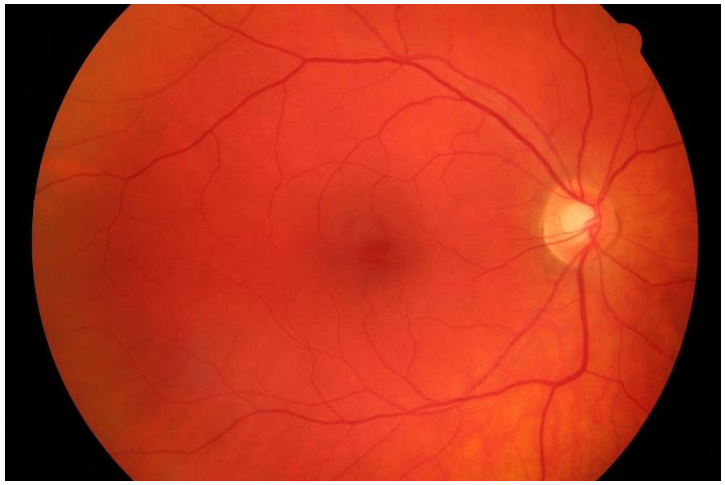
ICREA

Goal: use complex networks tools and machine learning algorithms to classify ophthalmic images

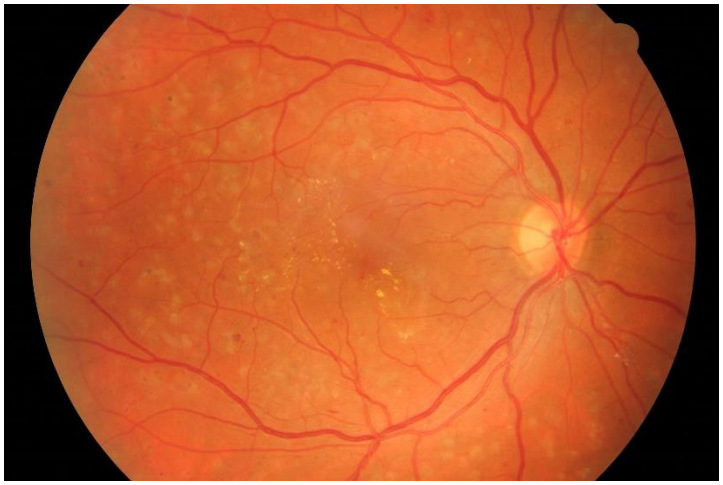
- Early diagnosis of eye deceases (glaucoma, diabetes) & follow up of treatments
- Person identification
- Signatures of other deceases (eg alterations in the brain arterial system)

Examples

Healthy



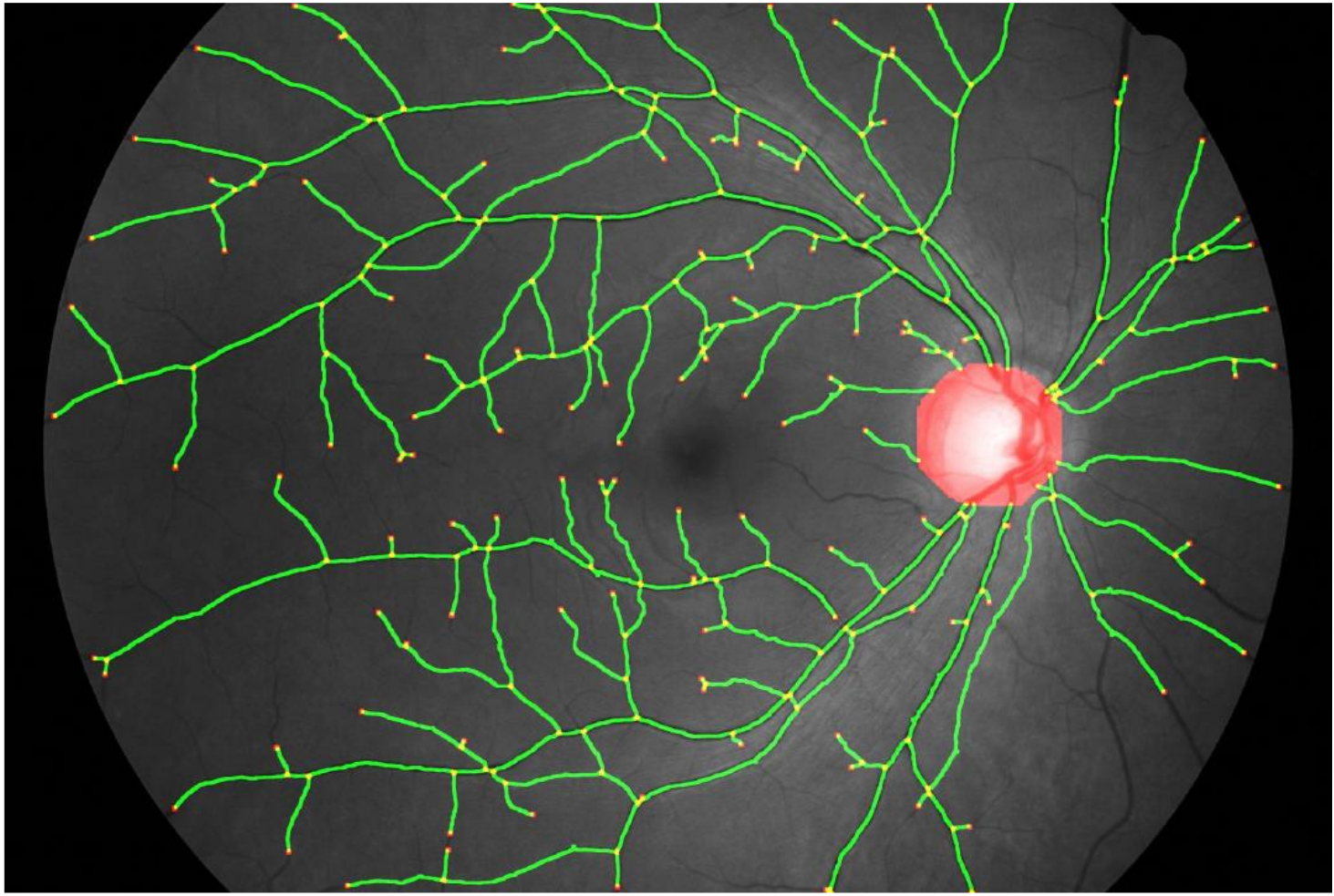
Diabetic



Steps

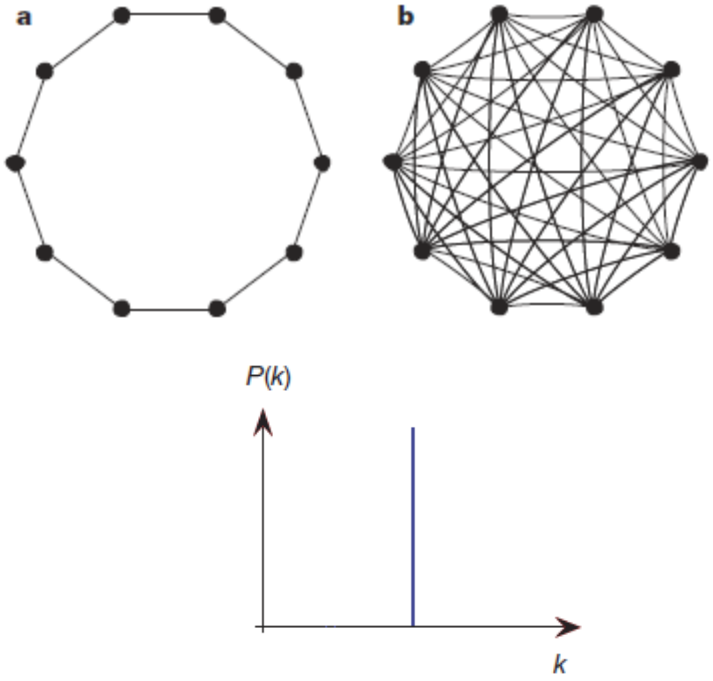
- Extract network
- Compare with other networks
- Use machine learning algorithms

$\Rightarrow$ Image classified

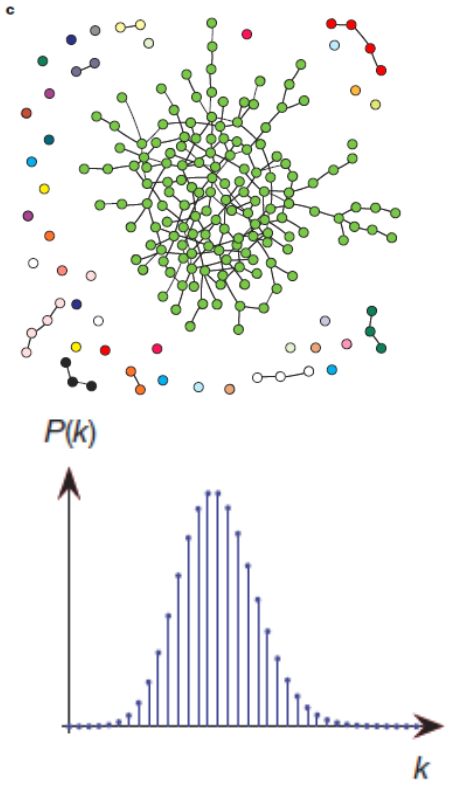


How to compare networks with different number of nodes? The degree distribution?

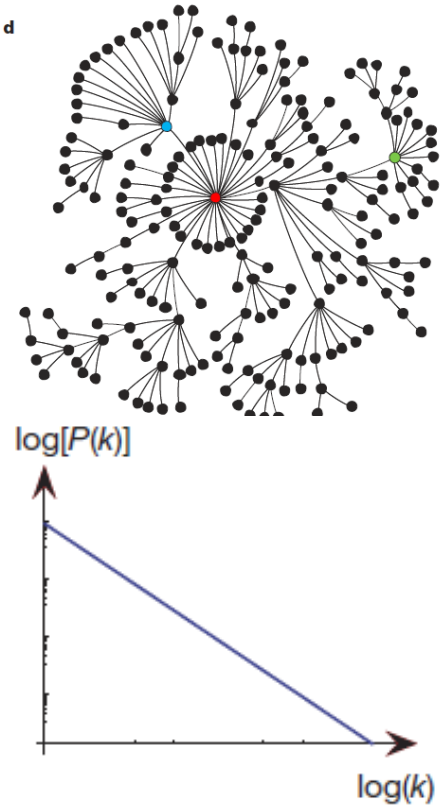
Regular



Random



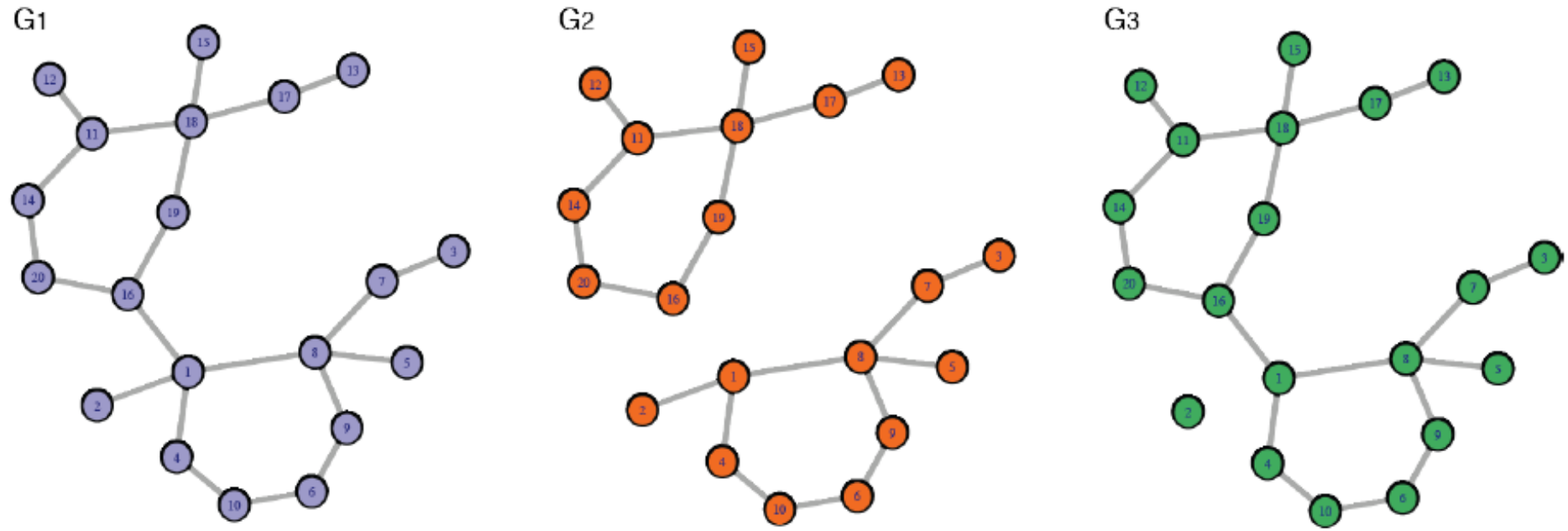
Scale-free



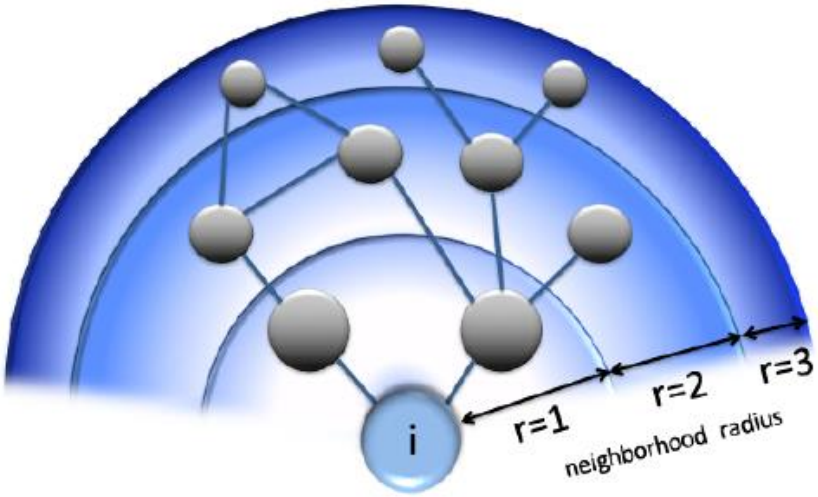
Strogatz, Nature 2001

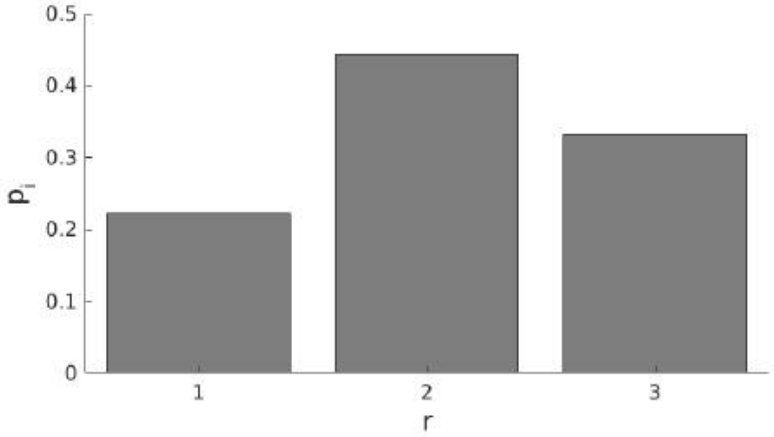
To detect structural differences between networks we need a precise measure to compare them.

- Degree distribution (centrality, assortativity, etc.) provide *partial* information.
- Main problem: not all the links have the same importance.



Node Distance Distribution (NDD) of node i: fraction of nodes that are connected (shortest path) to i at distance j.





- A network with N nodes:

  NDDs = vector of N pdfs $\{p_1, p_2, \ldots, p_N\}$

- If two networks have the same set of NDDs $\Rightarrow$ they have the same diameter, average path length, etc.

Adapted from A. Viol et al. Entropy 2019

How to summarize the information contained in the node distance distributions?

The *Network Node Dispersion (NND*) of a graph G quantifies the heterogeneity of the node distance distributions $\{p_1, p_2, \ldots, p_N\}$

average NDD: $\mu = \langle p_i \rangle_i$

Kullback distance between p_i and μ: $J(p_i, \mu) = \sum_r p_i(r) \log\left(\frac{p_i(r)}{\mu(r)}\right)$

$$NND(G) = \frac{\langle J(p_i, \mu) \rangle_i}{\log(d+1)}$$

d = diameter

Dissimilarity measure

$$D(G,G') = w_1\sqrt{\frac{\mathcal{J}(\mu_G,\mu_{G'})}{\log 2}} + w_2\left|\sqrt{\mathrm{NND}(G)} - \sqrt{\mathrm{NND}(G')}\right|$$

$w_1=w_2=0.5$

compares the averaged connectivity

compares the heterogeneity of the connectivity distances

- Extensive numerical experiments demonstrate that isomorphic graphs return ***D=0.***
- Computationally efficient.
- Can be used to compare networks with different number of nodes.

T. A. Schieber et al, Nat. Comm. 8, 13928 (2017)

First example of application: classification of EEG signals

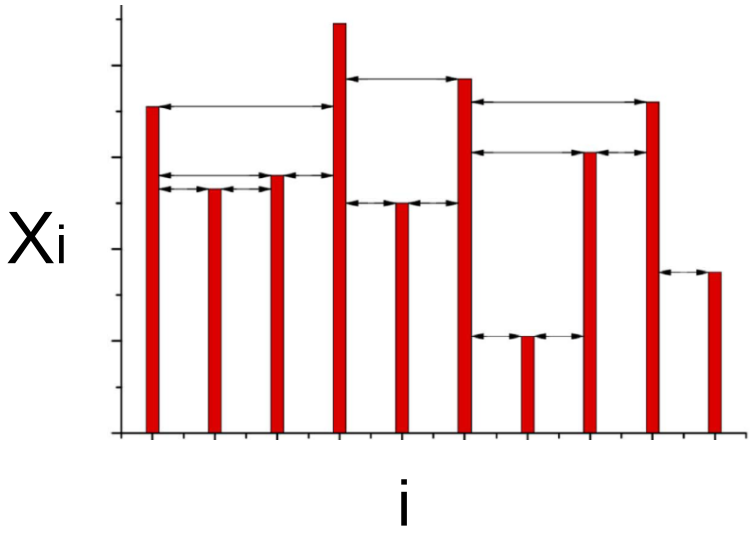
Data and methodology

- EEG data (*)
  - 64 electrodes placed on the subject's scalp sampled at 256 Hz during 1s
  - 107 subjects: 39 control and 68 alcoholic

- Each time series is transformed into a network using the horizontal visibility rule.

* *https://archive.ics.uci.edu/ml/datasets/eeg+database*

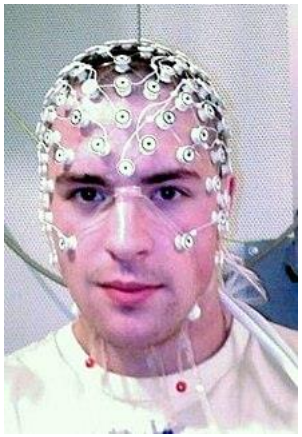
Horizontal visibility graph

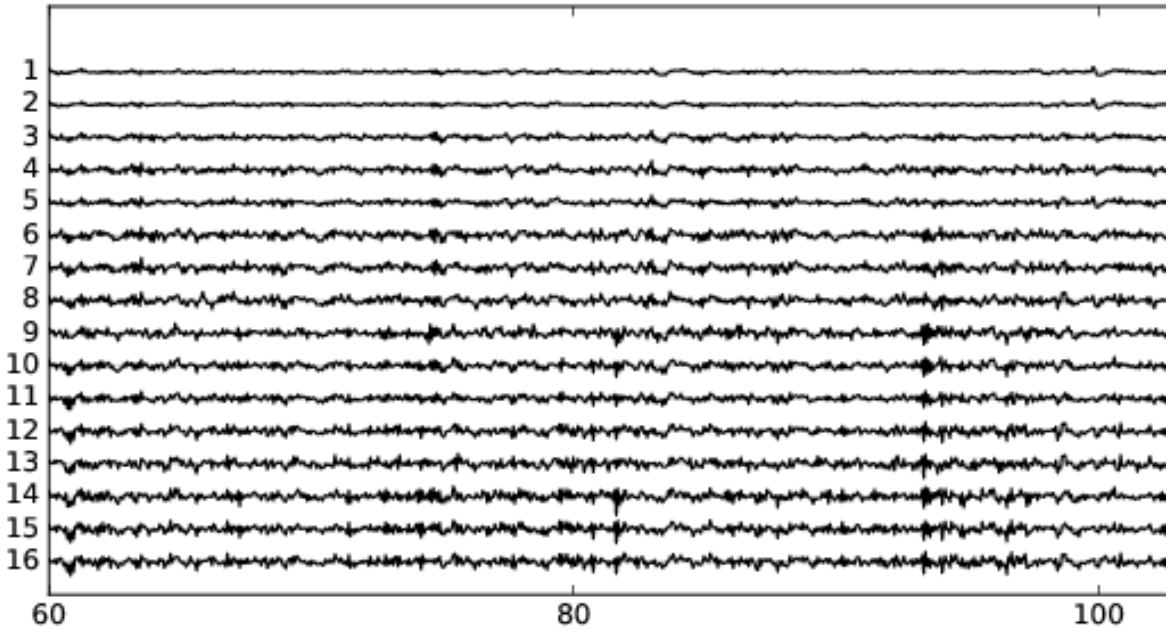


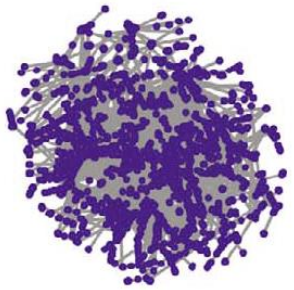
- Data points i and j are connected if there is “visibility” between them.
- We obtain an unweighted and undirected graph.
- Parameter free!

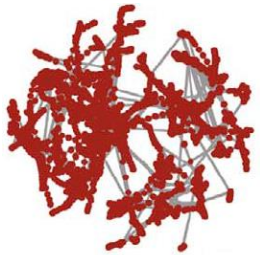
Luque et al PRE (2009); Gomez Ravetti et al, PLoS ONE (2014)

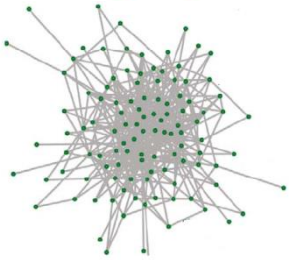
For each subject dataset has 64 channels ⇒ 64 networks











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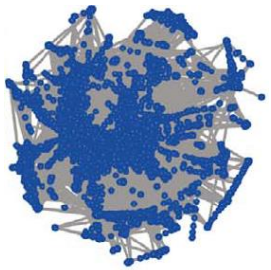
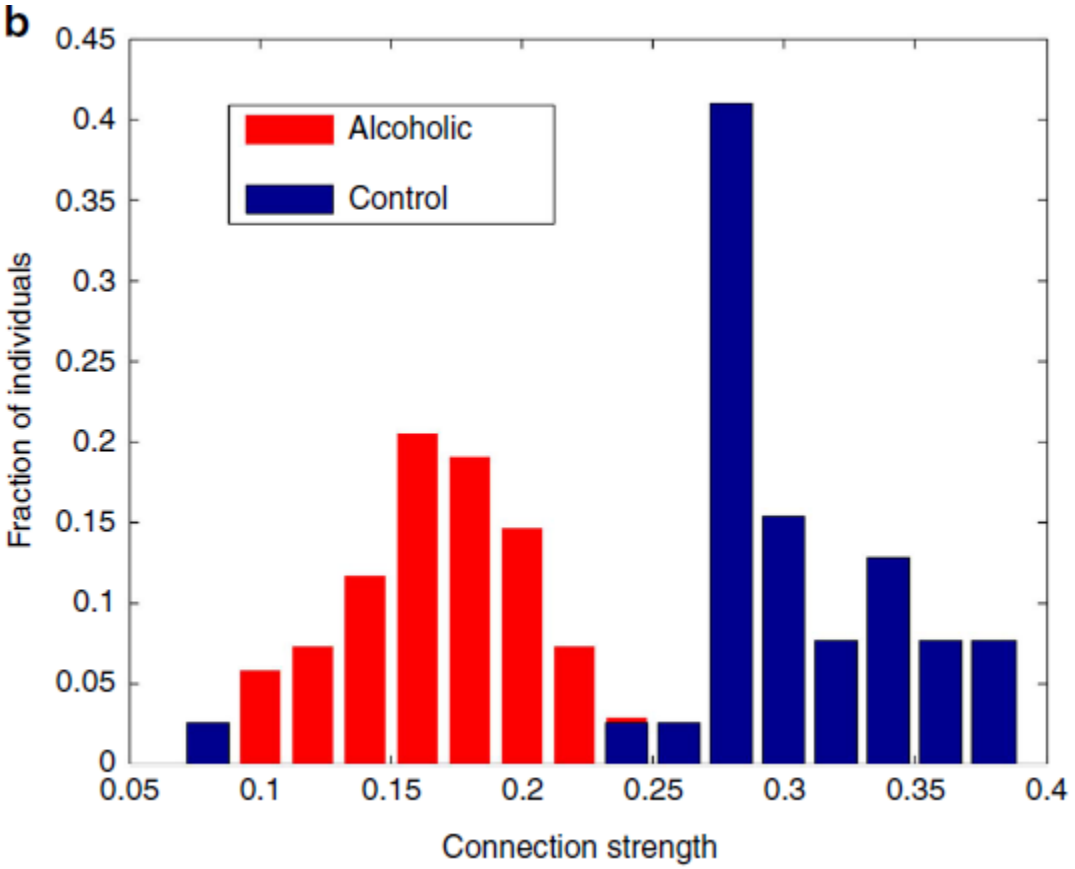


- The connection strength between two brain regions is: **1-*D*(G,G')**

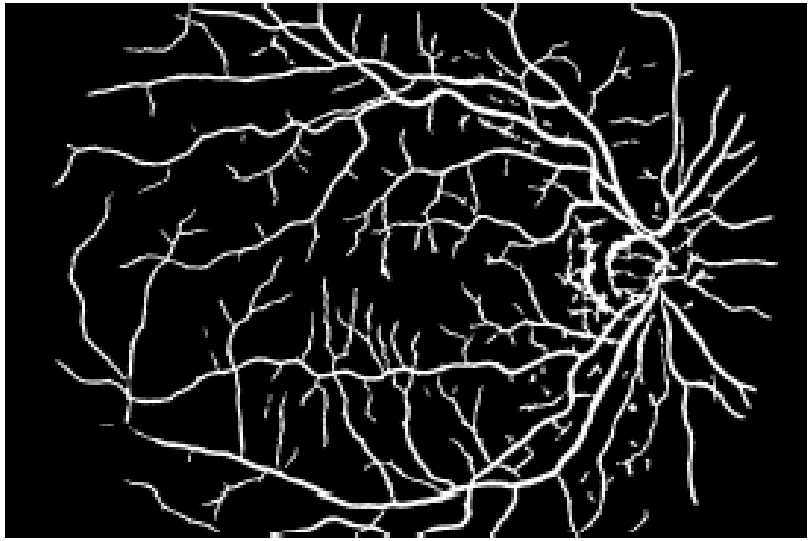
We identified two brain regions (called ‘nd’ and ‘y’), where the connection strength between these regions is higher in control than in alcoholic subjects.



T. A. Schieber et al, Nat. Comm. 8, 13928 (2017)

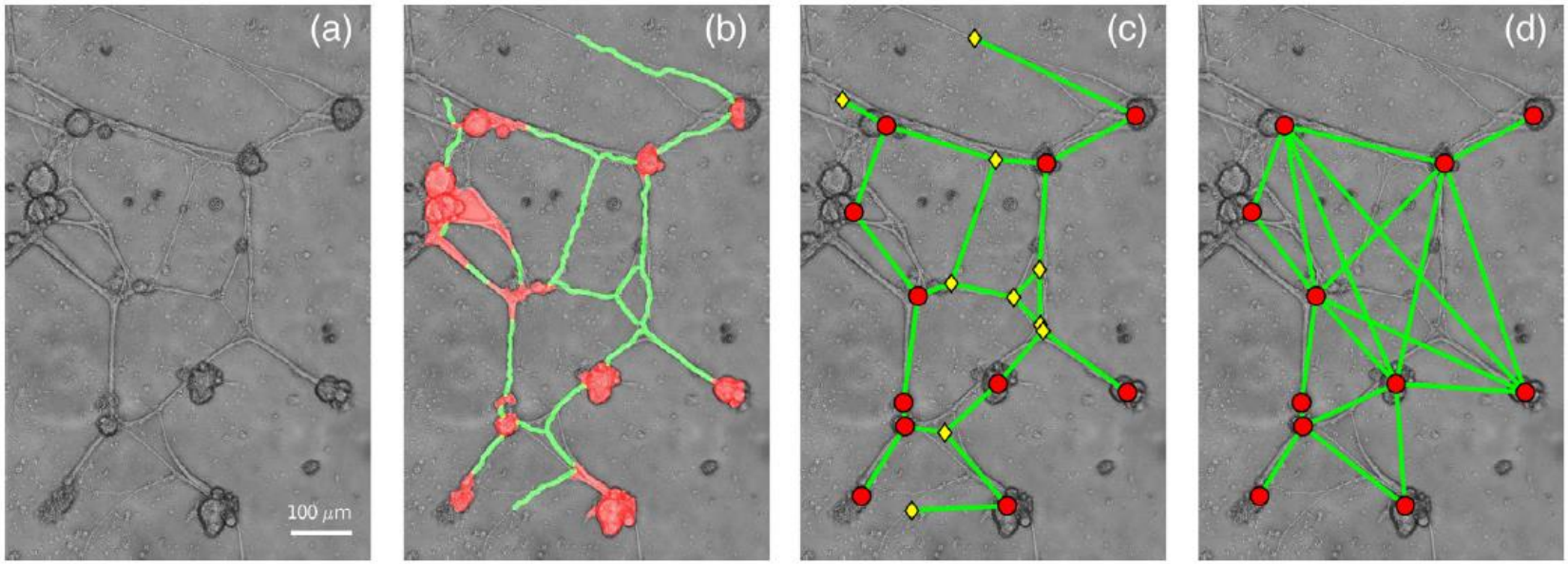
Second application: classification of retina images

Segmentation



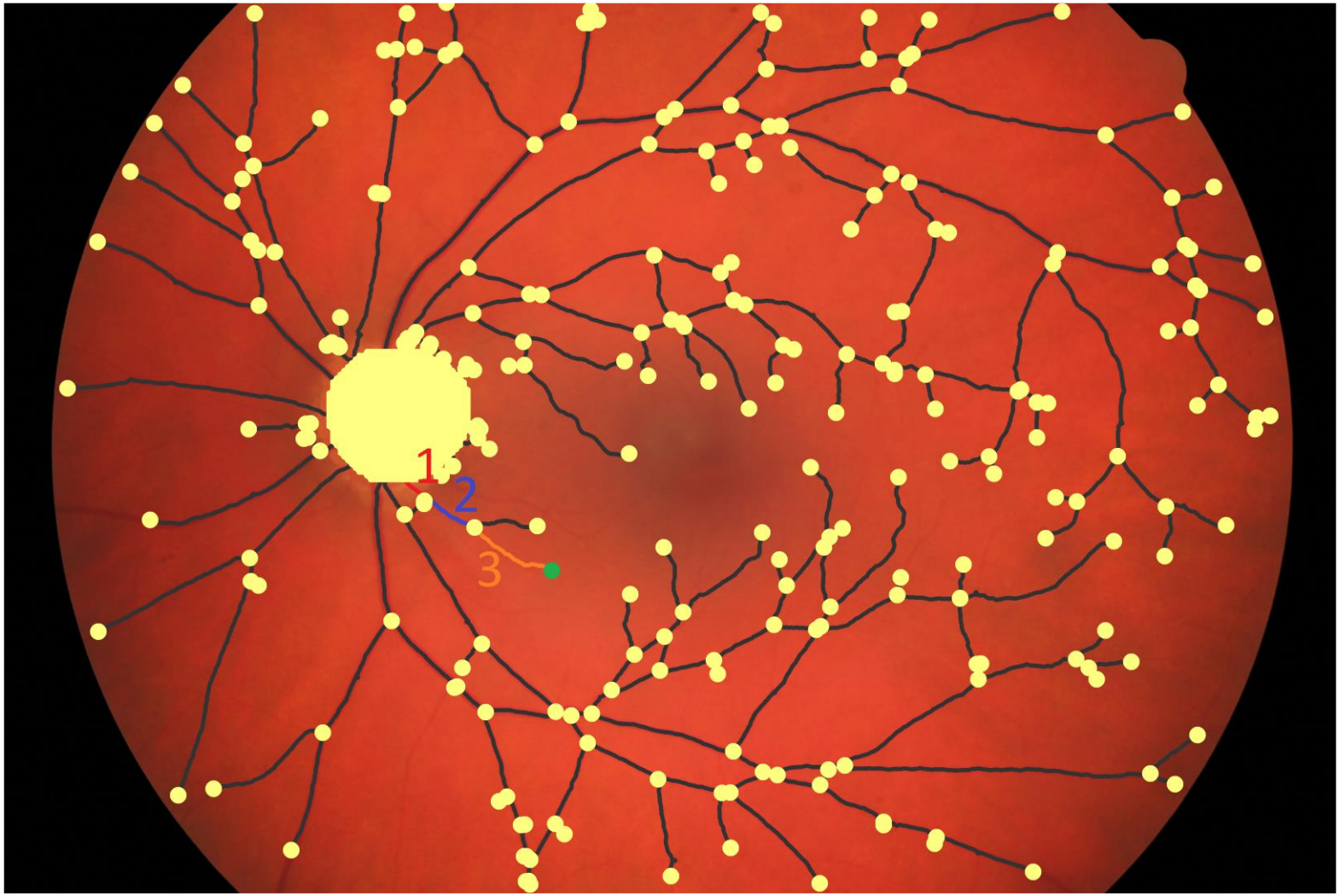
Problem: arteries and veins networks collapse.

Unsupervised segmentation algorithm adapted from an algorithm developed for segmenting images of cultured neuronal networks.



Santos-Sierra D, Sendiña-Nadal I, Leyva I, et al. *Graph-based unsupervised segmentation algorithm for cultured neuronal networks' structure characterization and modeling*. Cytometry Part A. 87, 513 (2015).

Identification of nodes and links.
Then, analysis of the connectivity paths to the central node (optical nerve)

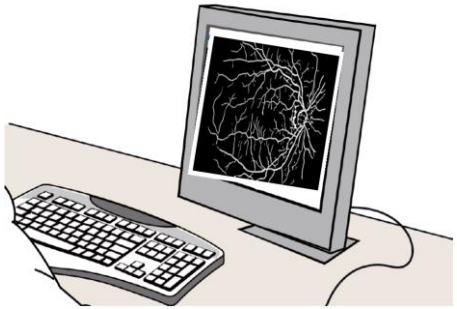


Data (1/2)

- High-resolution public database with
  - 15 healthy subjects
  - 15 glaucoma
  - 15 diabetic retinopathy

- For every subject there is
  - fundus photography
  - manual segmentation of the vessels done by an expert.

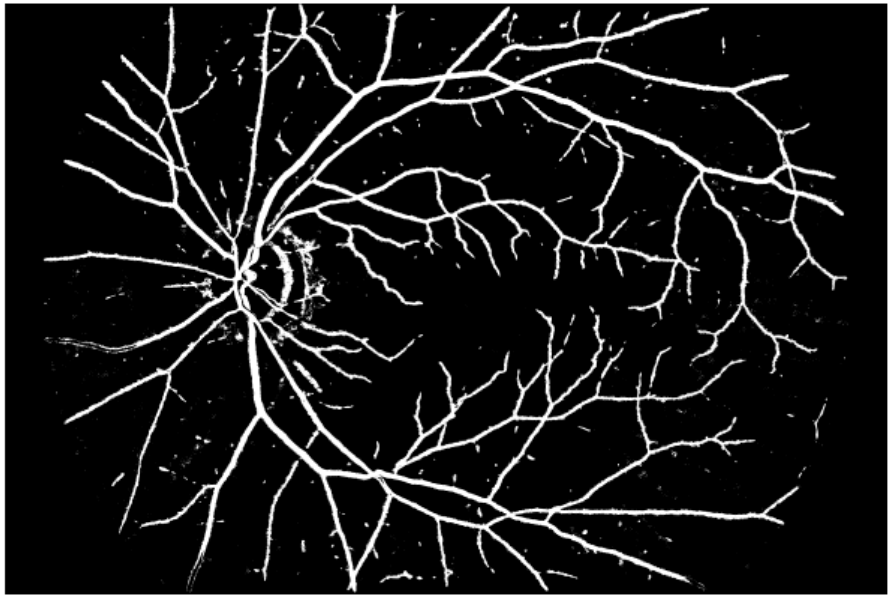
- From each fundus photography ⇒ automated segmentation.



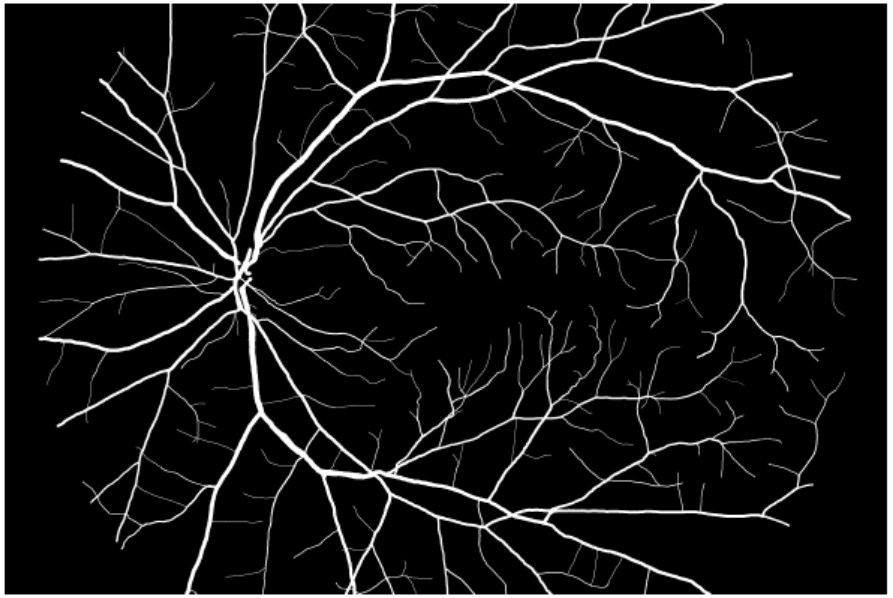
https://www5.cs.fau.de/research/data/fundus-images/

Comparison

Automated



Manual



Data (2/2)

- For both segmentations (manual and automated) we analyzed
  - raw segmented image (i.e., a binary image that includes all the pixels that correspond to vessels);
  - skeletonized image (i.e., a binary image where the width of each vessel segment is reduced to one pixel, without changing the length, location and orientation of the segment).

- We also analyzed two larger databases but with lower resolution. Best results obtained for high-resolution images.

Weights of the links

$$w_{i,j} = (L_{i,j})^l (W_{i,j})^a$$

length and width (in # of pixels) of the segment that connects nodes i and j

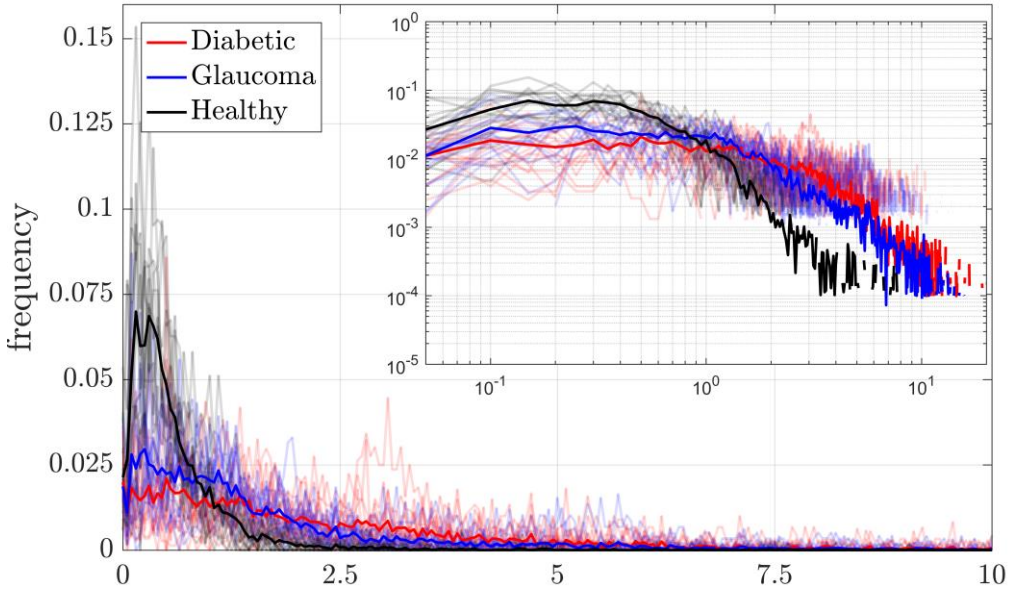
- For diabetic retinopathy (DR) length/area (l = 1, a = -2) provide the best differentiation between groups (DR produces neovascularization, which perhaps affects the vessels' flow capacity).

- For glaucoma patients, the volume performed the best (glaucoma is linked to an increase of the intraocular pressure, which perhaps modifies the volume of the vessels).

Methodology (1/2)

From each image we calculate

- Fractal dimension (raw and skeletonized segmented images)
- Distribution of distances to the central node
- Distribution of average weights along the path to central node
- Distribution of weighted degrees



distribution of average weights
(l=1, a=-2)

Methodology (2/2)

- We use the Jensen-Shannon (JS) divergence to compare distributions (image i with all other images)
- For each image i we obtain a vector

$$\{d_{i1}, d_{i2}, \ldots d_{iN}\} \text{ (N = number of images)}$$

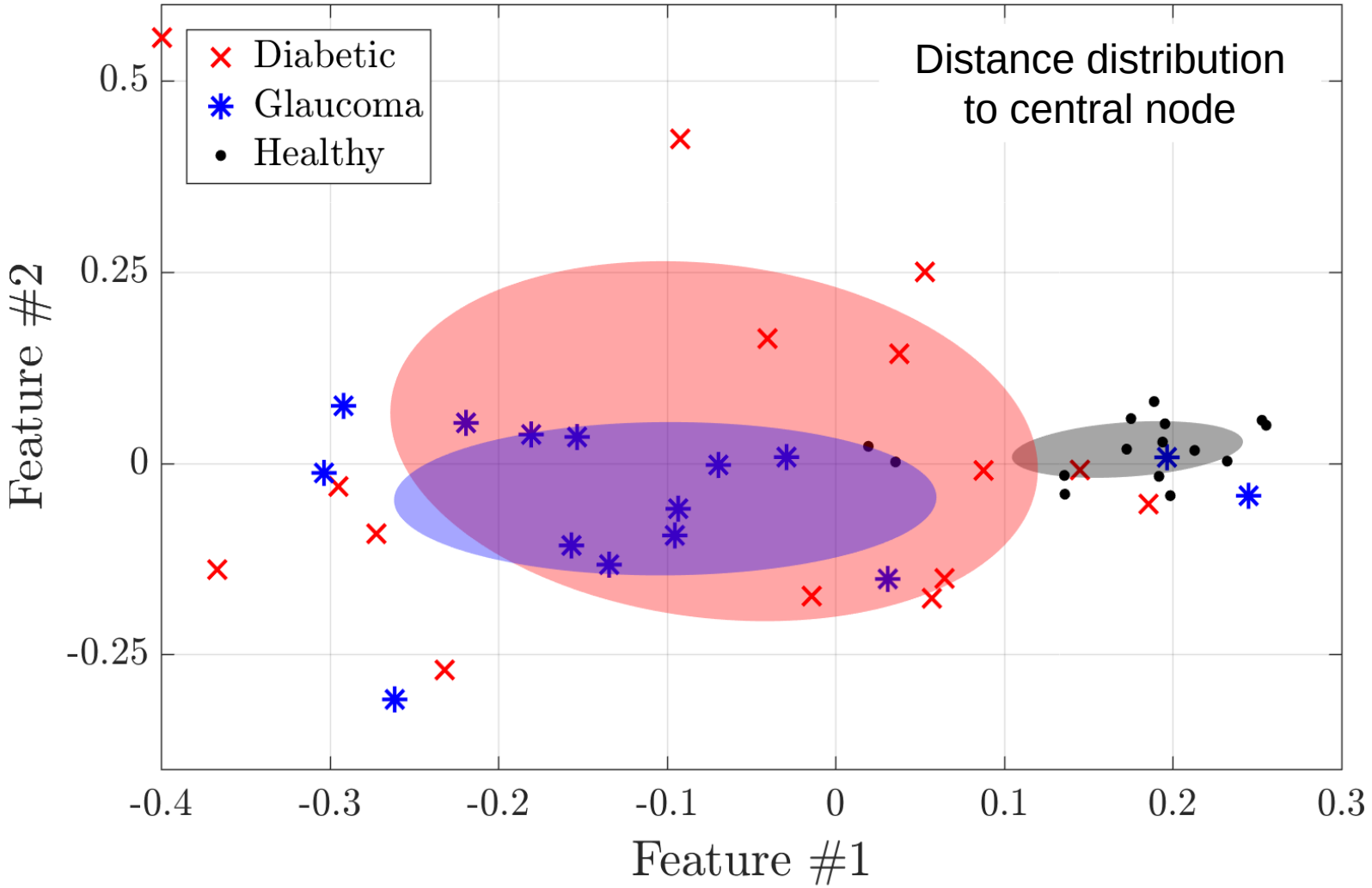
whose elements are the distances between the distributions extracted from image i and image j (j in 1…N).

- This vector of N “features” characterizes image i.

- We apply a nonlinear dimensionality reduction algorithm (*IsoMap*) to obtain only 2 features for each image.

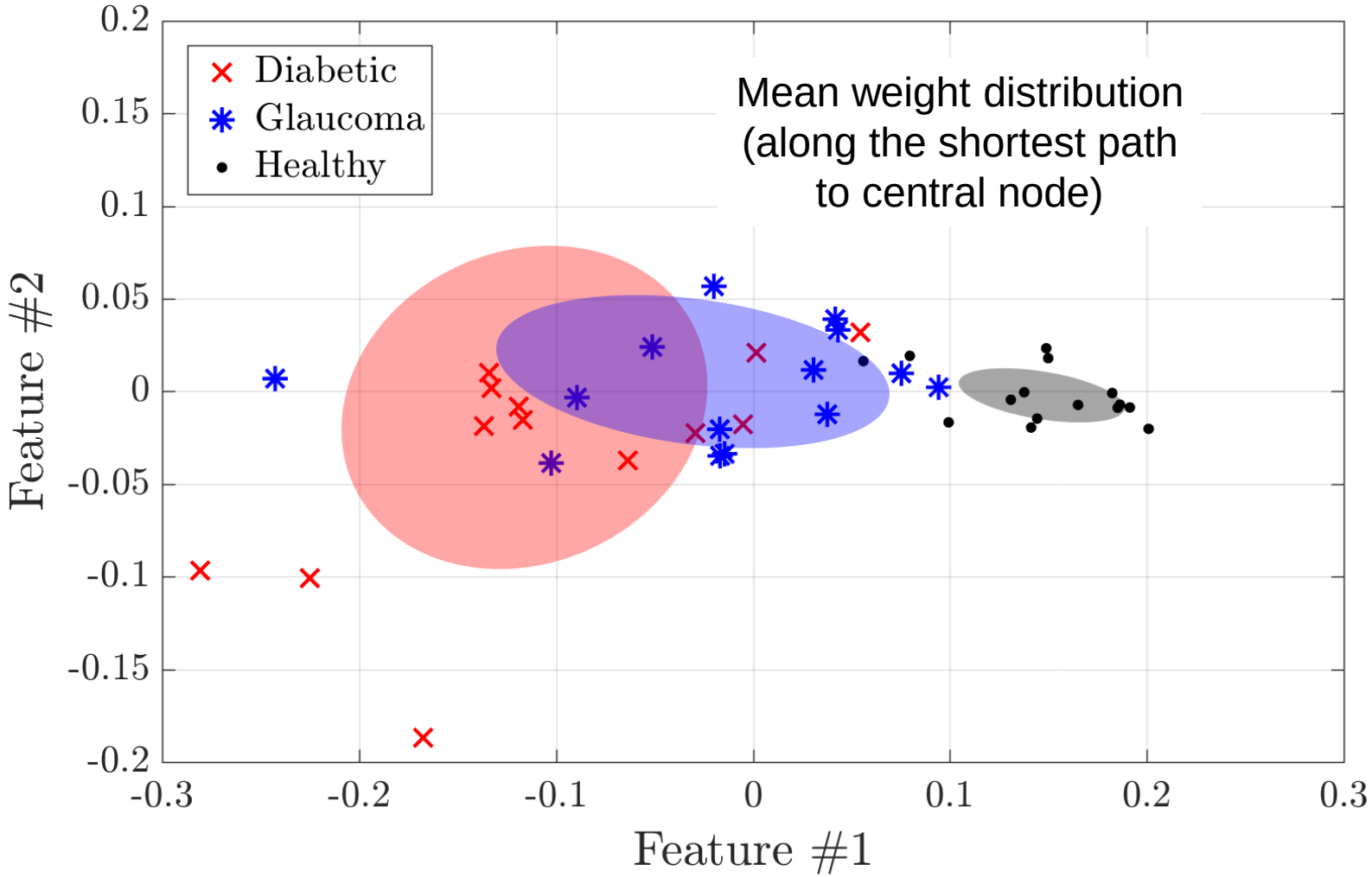
J. B. Tenenbaum et al, A global geometric framework for nonlinear dimensionality reduction. Science 290, 2319 (2000).

Performance of network features in manual segmentation:



P. Amil et al, Network-based features for retinal fundus vessel structure analysis, PLoS ONE 14 e0220132 (2019).

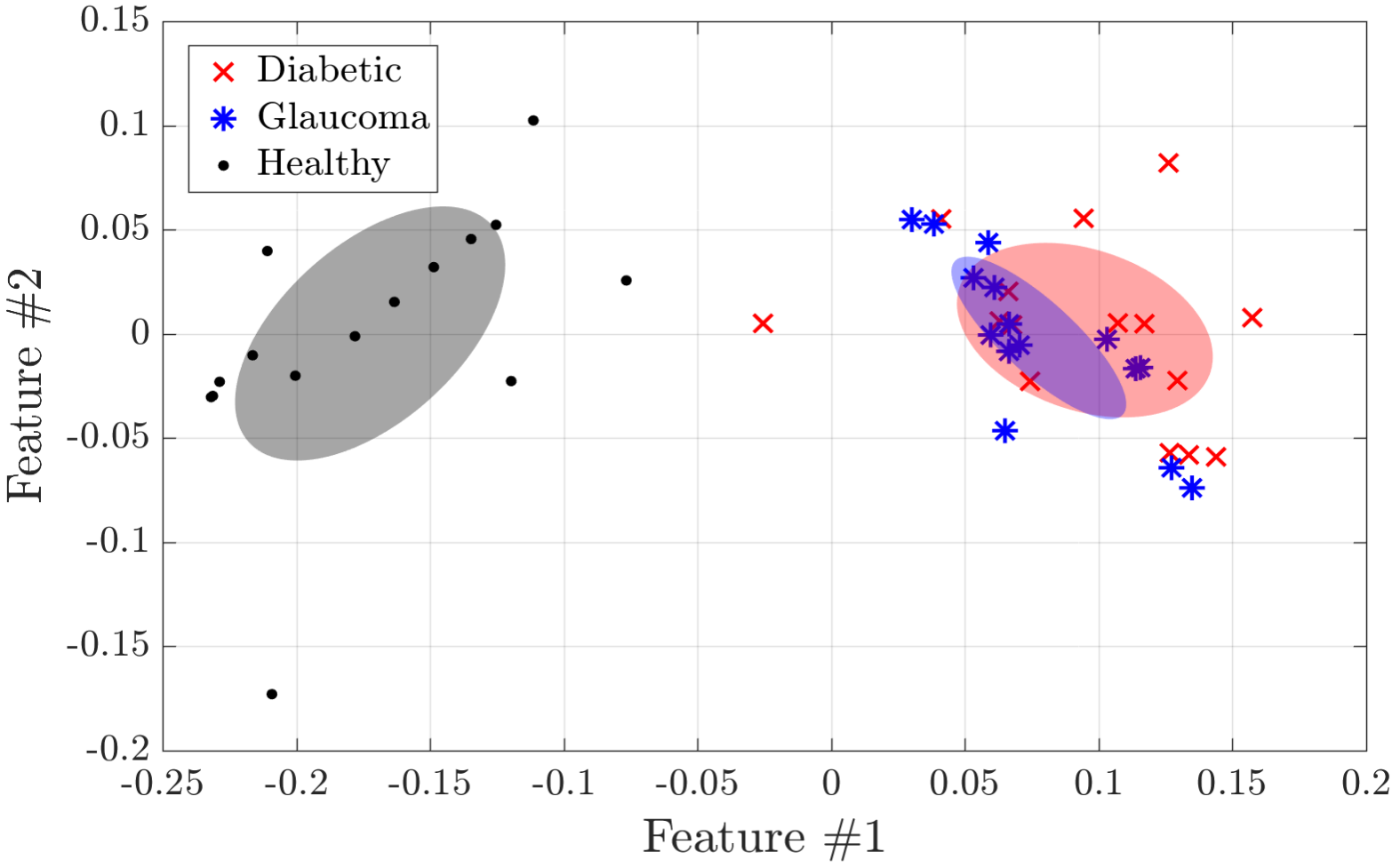
Performance of network features in manual segmentation:



P. Amil et al, Network-based features for retinal fundus vessel structure analysis, PLoS ONE 14 e0220132 (2019).

Manual segmentation: distribution of weighted degrees

$$s_i = \sum_j w_{i,j}$$

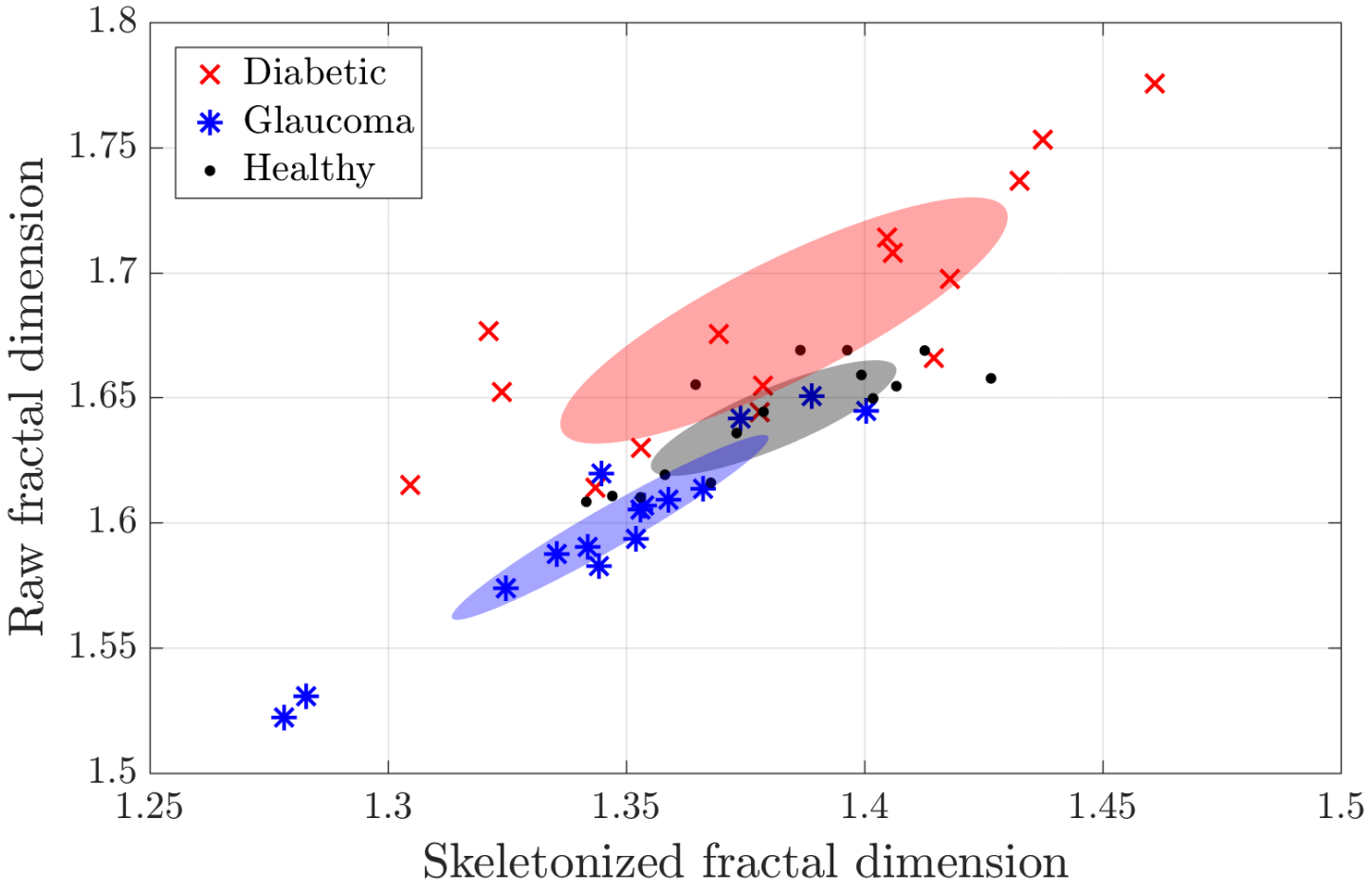


P. Amil et al, Network-based features for retinal fundus vessel structure analysis, PLoS ONE 14 e0220132 (2019).

In the automated segmentation:

Fractal dimension analysis separates the three groups

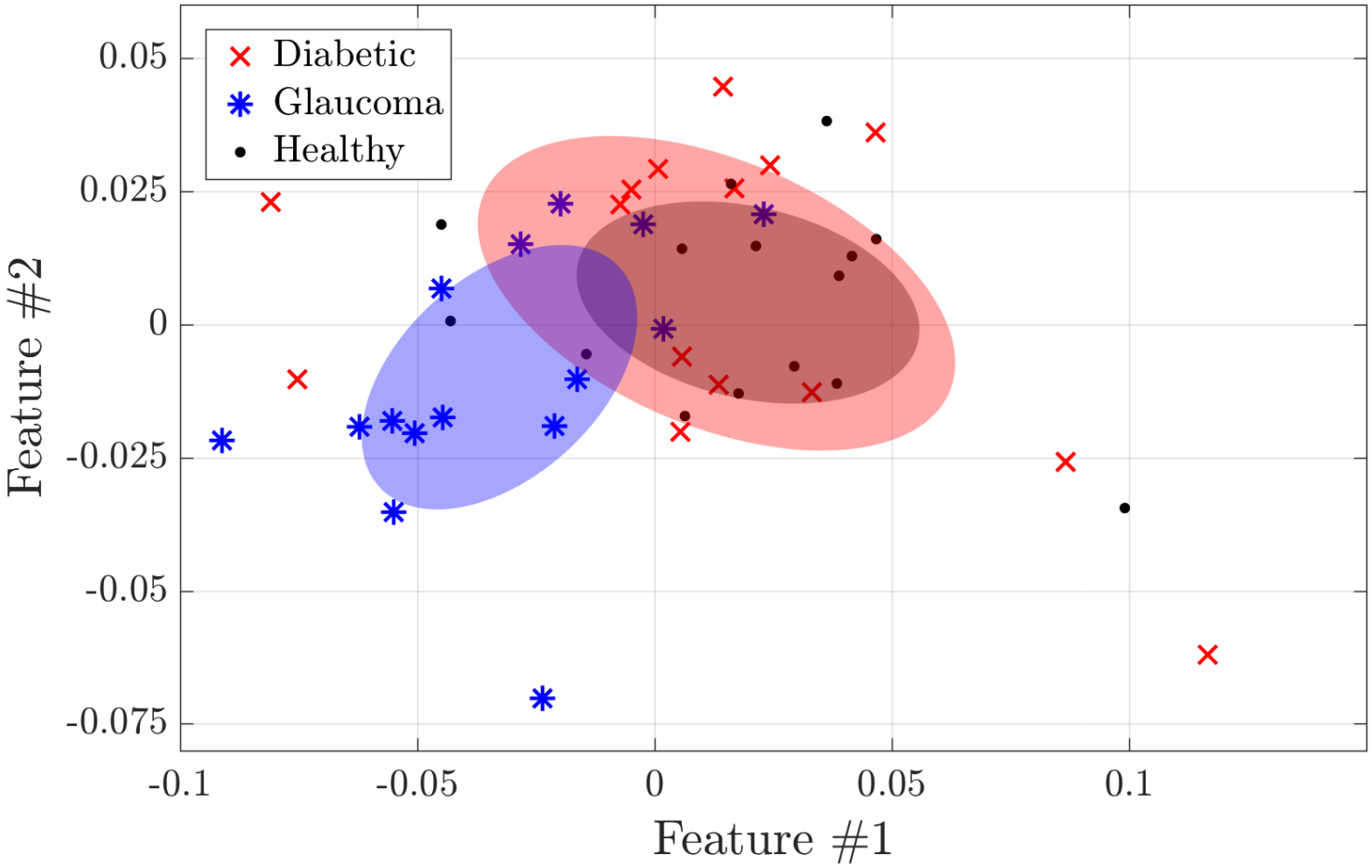
$$D = \lim_{\varepsilon \to 0} \frac{\log(N(\varepsilon))}{\log(1/\varepsilon)}$$



P. Amil et al, Network-based features for retinal fundus vessel structure analysis, PLoS ONE 14 e0220132 (2019).

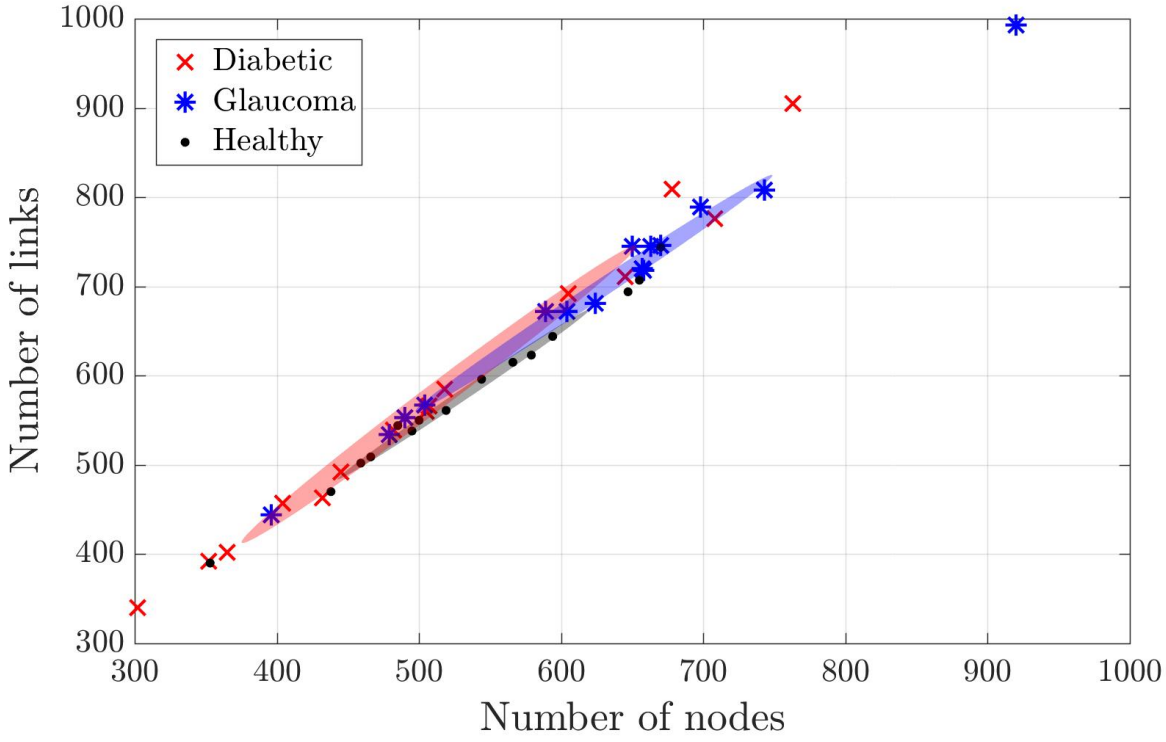
In the automated segmentation:

Mean weight distribution (along the shortest path to central node) identifies glaucoma



P. Amil et al, Network-based features for retinal fundus vessel structure analysis, PLoS ONE 14 e0220132 (2019).

Simple network features do not differentiate



P. Amil et al, Network-based features for retinal fundus vessel structure analysis, PLoS ONE 14 e0220132 (2019).

Summary I

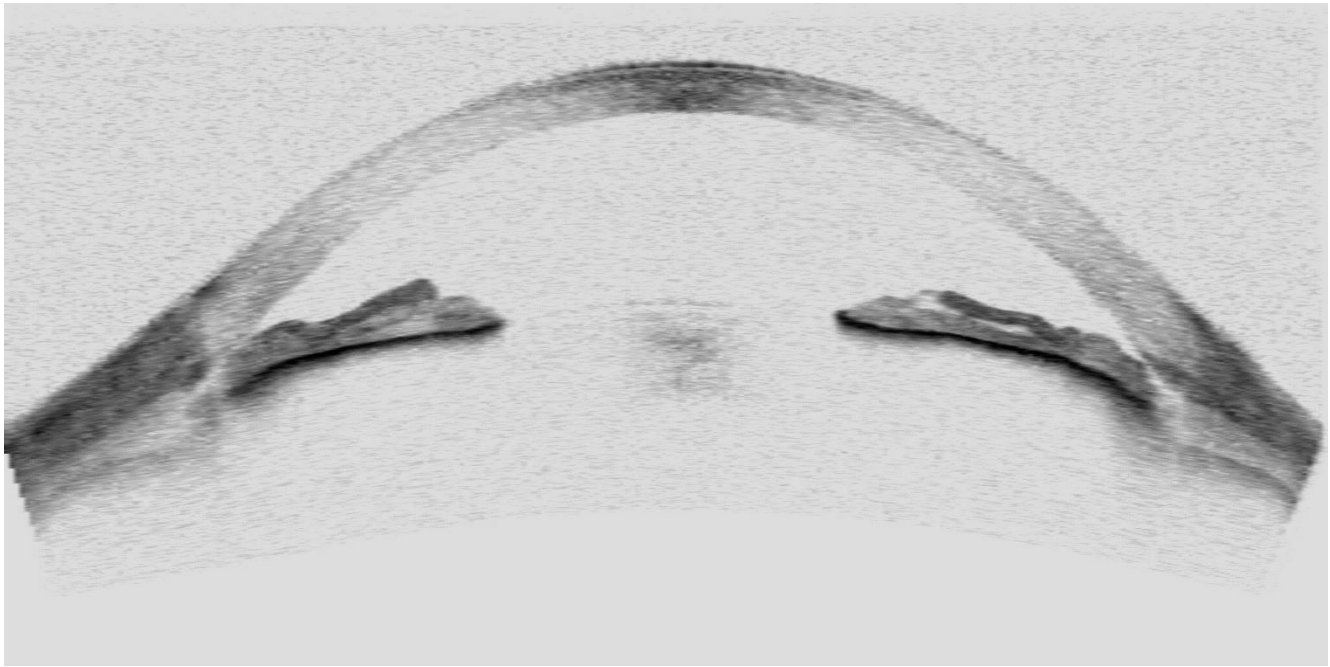
A measure for comparing graphs (unlabeled nodes, undirected links) was used for

- EEG classification: two brain regions were identified that have different connection strength in control and in alcoholic subjects.

- Retina fundus image classification: perfect classification of healthy and non-healthy patients was obtained using high resolution images and manual segmentation.

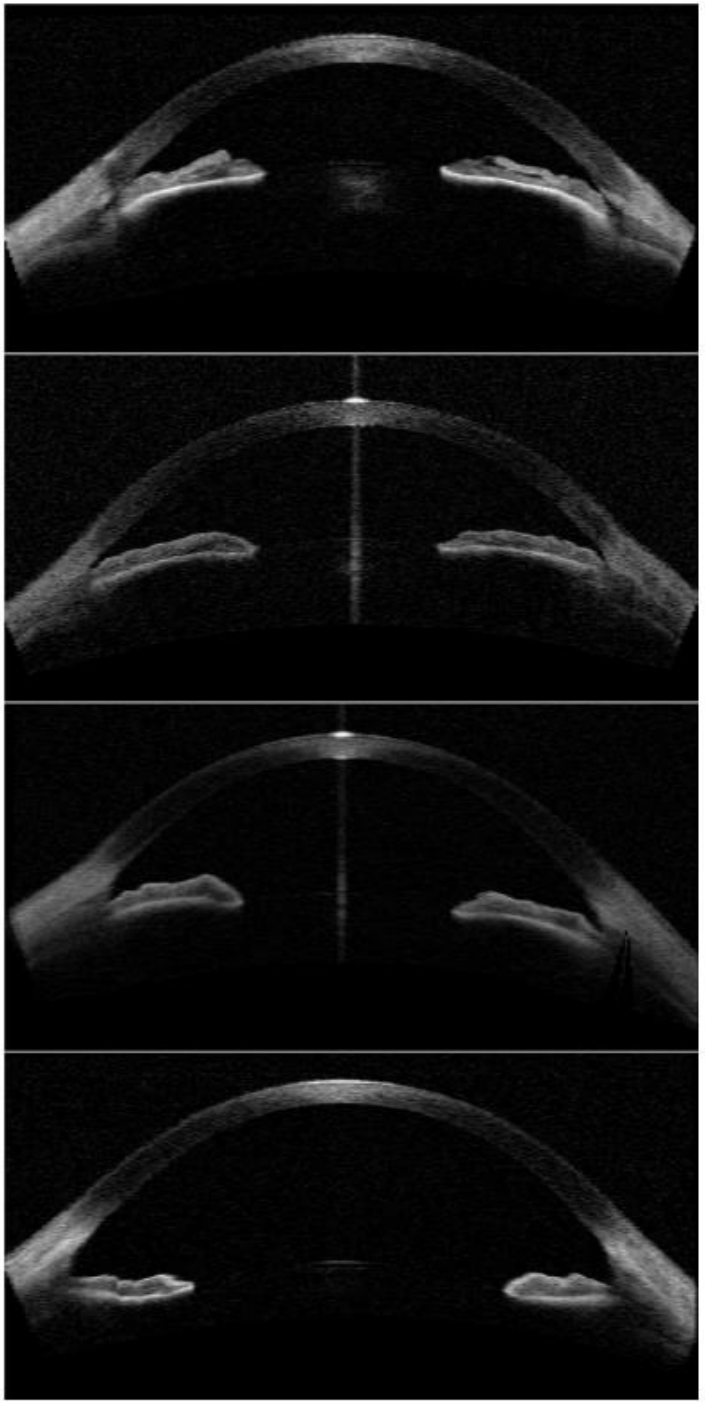
Unsupervised ordering of optical coherence tomography (OCT) images

- Used for diagnosis of glaucoma.
- More than 1000 images from patients of Instituto de Microcirugia Ocular (IMO, Barcelona).



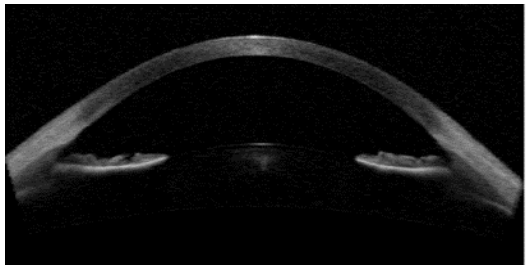
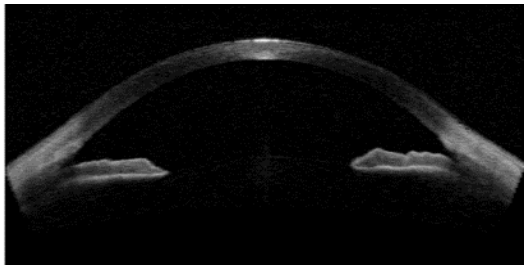
Classified into 4 categories by two ophthalmologists and a trained PhD student

- Closed
- Narrow
- Open
- Wide open

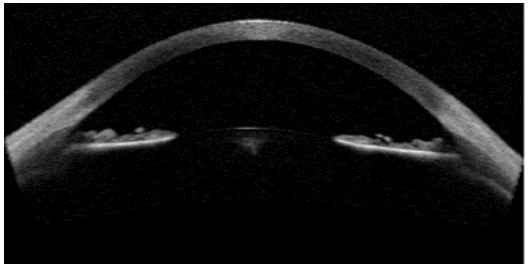
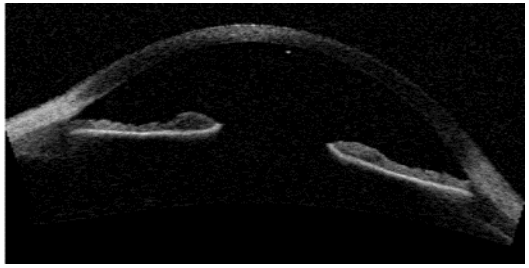


P. Amil et al., "*Unsupervised feature extraction of anterior chamber OCT images for ordering and classification*", Sci. Rep. 9, 1157 (2019).

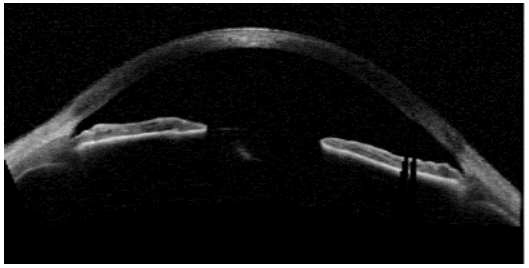
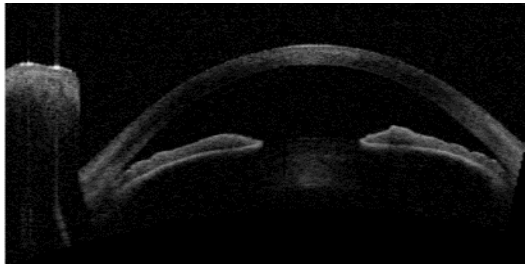
Using an appropriated distance (aligned Hellinger), by comparing pairs of images we extract features that can be used to order the images in a plane.

Small distance

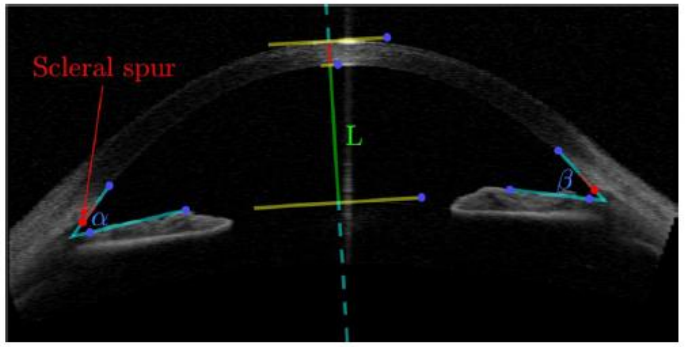
Medium distance

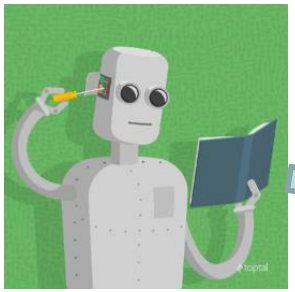



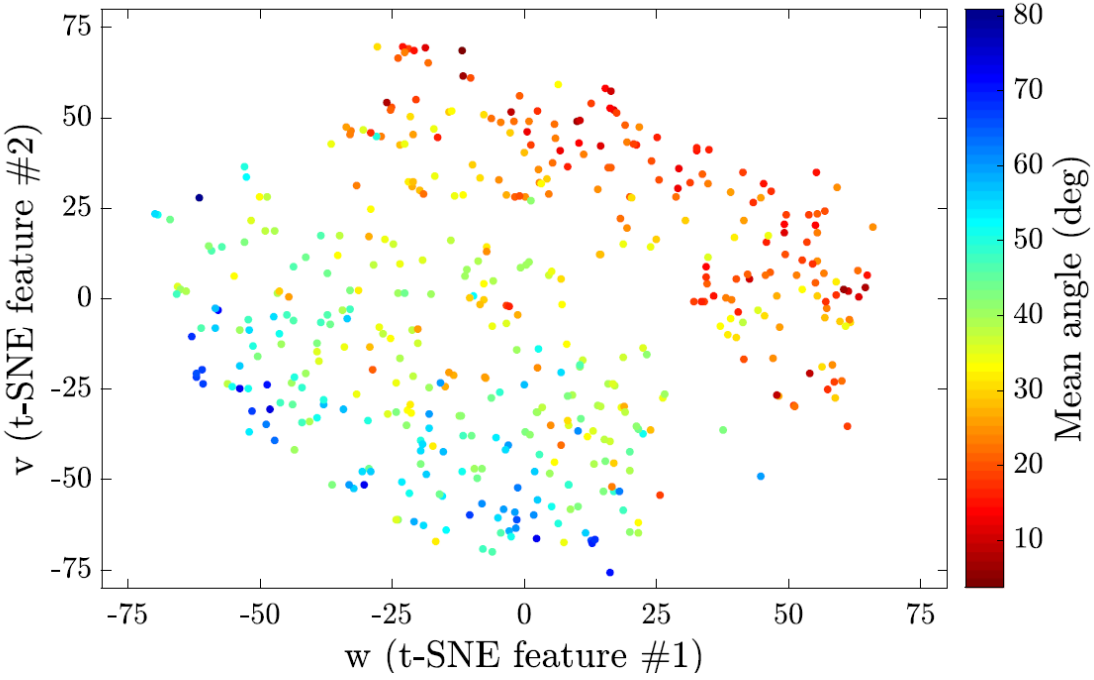
Large distance

P. Amil et al., “*Unsupervised feature extraction of anterior chamber OCT images for ordering and classification*”, Sci. Rep. 9, 1157 (2019).

Correlation between unsupervised features and the “manual” feature from expert annotation.

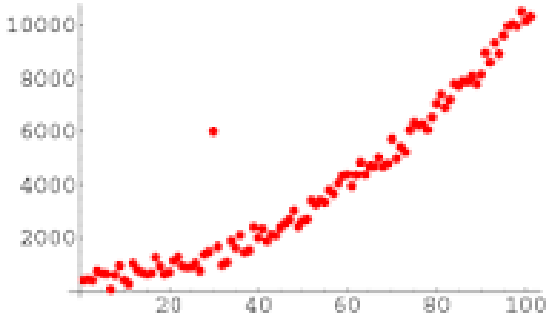






Can we improve this correlation if images with artifacts (outliers) are removed from the training set?

What is an outlier?



Practical definition: improved performance of machine learning algorithms when outliers are removed from the training set.

Two “network-based” & “distance based” outlier detection methods

- network percolation (fragmentation)

- manifold learning

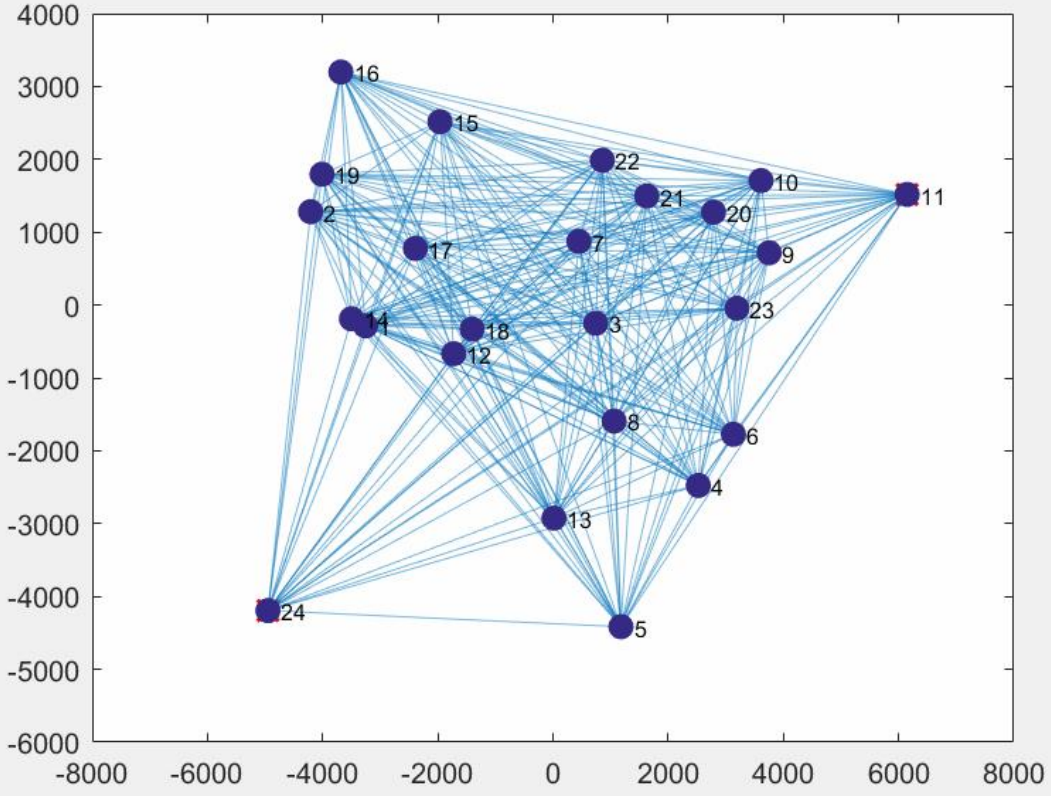
Vector of features that describe an item of a dataset

$$V_i = \{v_1^i \dots v_m^i\}$$

Distance between any two items

$$D_{ij} = \left(\sum_k \left| v_k^i - v_k^j \right|^p \right)^{1/p}$$

First method: Outlier detection using percolation

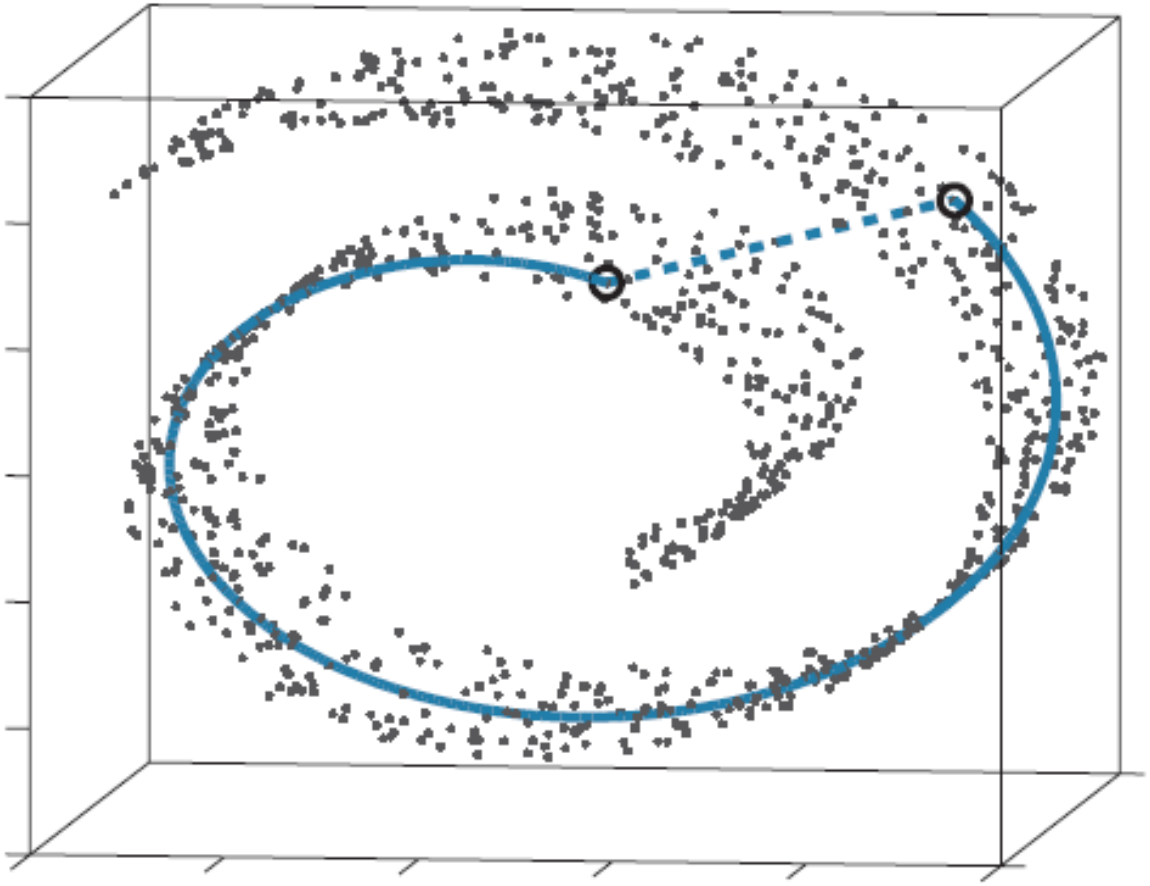


Outlier score = order in which elements disconnect from the giant component.

Parameter free.

Second method: manifold learning

- *Main idea: how well or how poorly an element fits in the learned manifold*.



Distance in the high dimensional space (dash) and distance in the learned (lower dimensional) manifold (solid).

Tenenbaum et al., A global geometric framework for nonlinear dimensionality reduction. Science 290, 2319-2323 (2000)

Steps

- Apply *IsoMap* to the distance matrix $\mathbf{D_{ij}}$ to obtain
  - a new set of features
  - a new distance matrix in the geodesic space, $\mathbf{D^G_{ij}}$
- With the new features, recalculate the distance matrix $\mathbf{D'_{ij}}$
- For each element, calculate correlation between $\mathbf{D^G_{ij}}$ and $\mathbf{D'_{ij}}$
- $AL_i = 1 - \rho_i{}^2$
- Two parameters (integers):
  - Dimension of reduced space
  - # of geodesic neighbors

Note: other methods detect outliers by analyzing the features returned by Isomap

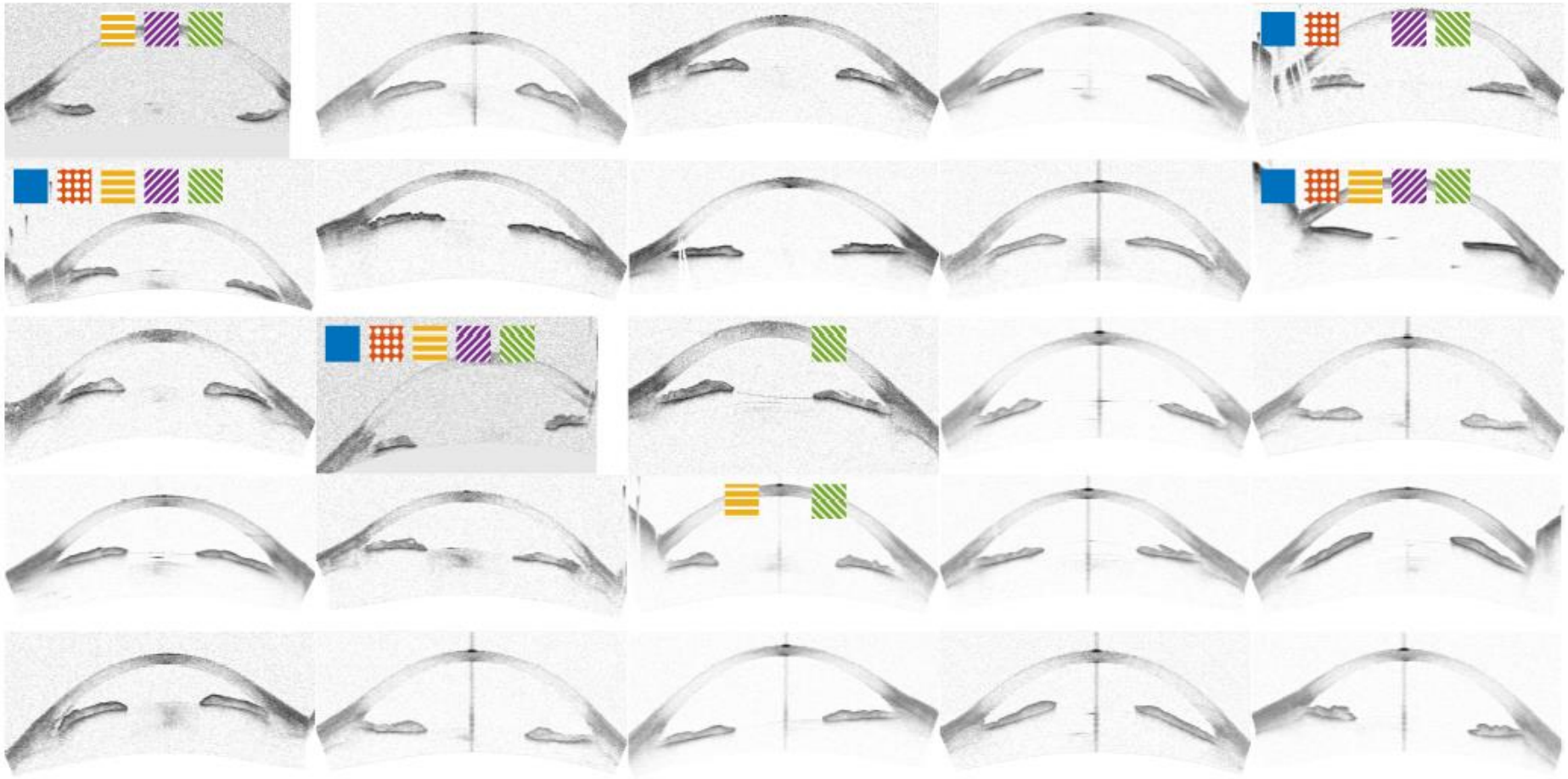
Comparison with other methods

- d2CM – Distance to center of mass. This method simple computes a “mean point” (center of mass) and computes the distance of each other point to this center of mass.
- Ramaswamy. A distance-based method that assigns an anomaly level to each point equal to its distance to its kth nearest neighbor.
- OCSVM - One Class Support Vector Machine. This method uses the inner product between the elements in the database to estimate a function that is positive in a subset of the input space where elements are likely to be found, and negative otherwise.

Ramaswamy et al., Efficient algorithms for mining outliers from large data sets. ACM Sigmod Record (Vol. 29, No. 2, pp. 427-438, 2000).

Schölkopf et al., Estimating the support of a high-dimensional distribution. Neural computation13, 1443-1471, 2001.

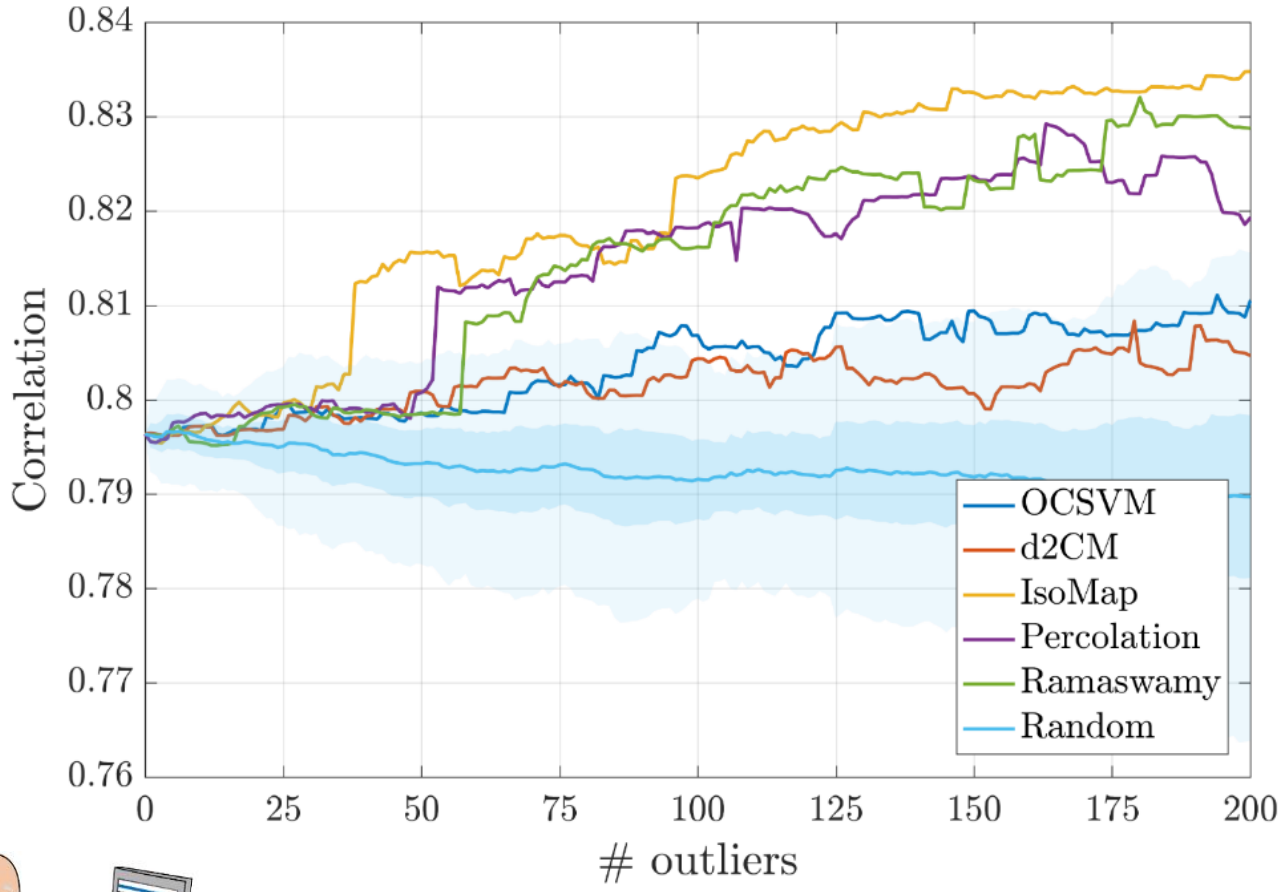
Results with OCT images (1/2)

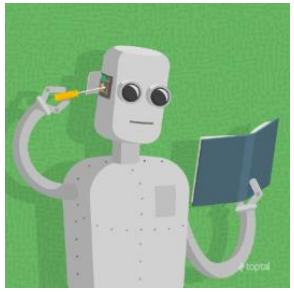


All except the first one were randomly sampled. Marked images correspond to top 15% outlier score for OCSVM (Blue), distance to center of mass (Orange), IsoMap (Yellow), Percolation (Purple), and Ramaswamy (Green)

Results with OCT images (2/2)

Correlation between unsupervised features and the “manual” feature (mean angle) obtained from expert annotation.





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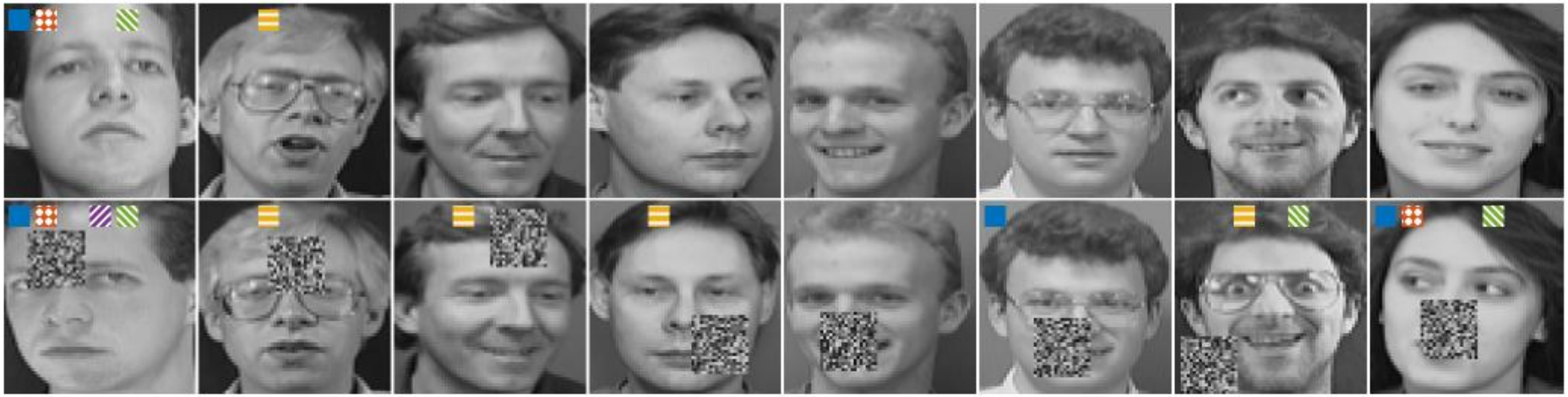
⇔

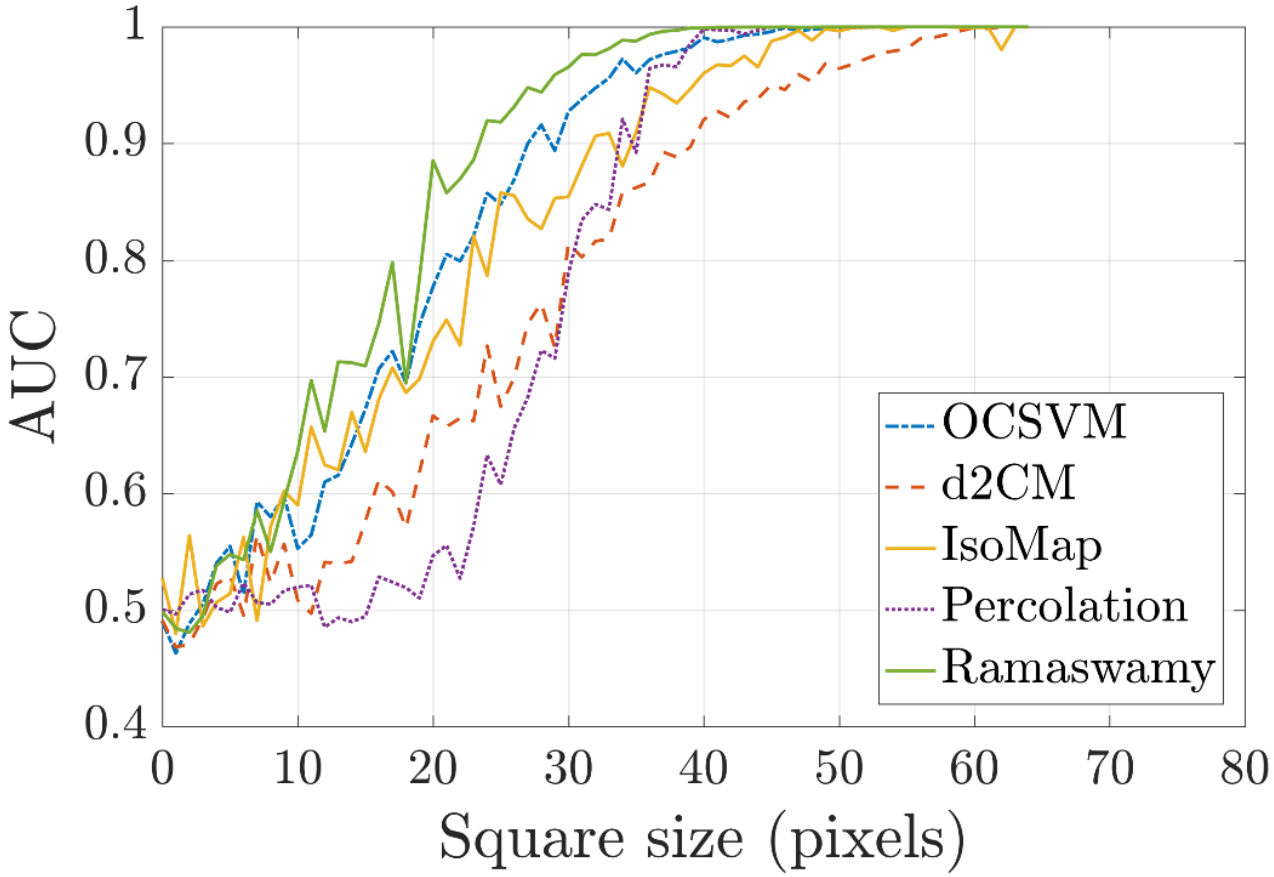
Can these methods work with other images?

- Freely available face database
- Added to some random images a square with gray-scale pixels whose color distribution is the same as that of the image.
- Measure success with the area under the ROC curve.



http://www.cl.cam.ac.uk/research/dtg/attarchive/facedatabase.html

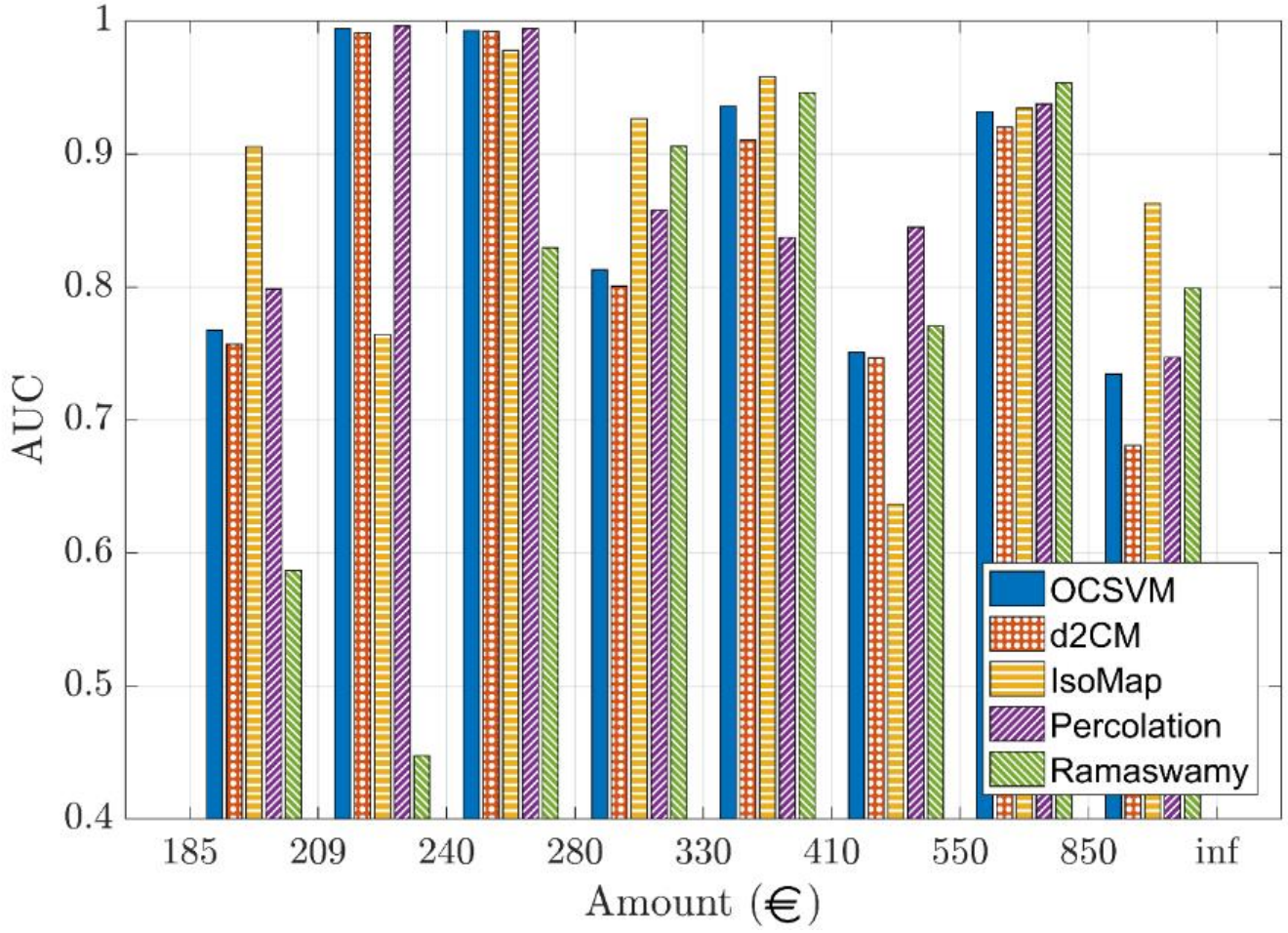
Results from the face database



(similar results obtained with the area under the “precision-recall” curve)

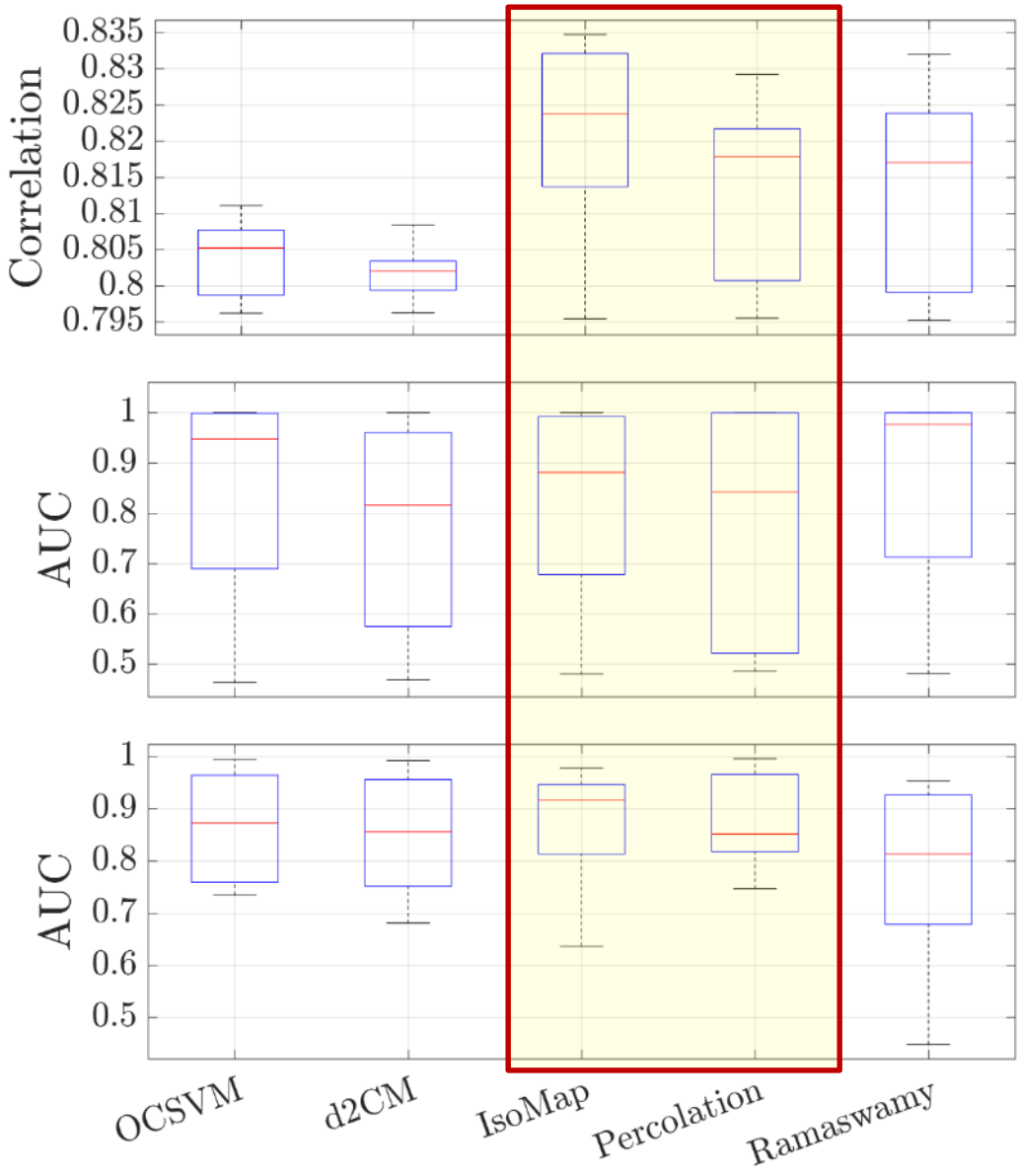
How about other types of elements?

Results from freely available credit card transactions (some identified as frauds)



https://www.kaggle.com/mlg-ulb/creditcardfraud

Summary of results



OCT database

Face database

Credit card database

Summary II

- The performance of the outlier detection methods depends on the data; it is in general competitive with other methods used in the literature.
- The percolation method is parameter free, which makes it perfect for blind outlier finding.
- The *IsoMap* method has 2 parameters that, when set properly, can outperform other methods, but the performance is very sensitive to the parameters.
- Both methods are suitable for high dimensional, not too large databases (execution time grows linearly with the dimension of the data and at least as NxN with the size of the database).

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Thank you for your attention !

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- P. Amil et al., "*Unsupervised feature extraction of anterior chamber OCT images for ordering and classification*", Sci. Rep. 9, 1157 (2019).
- P. Amil et al., "*Network-based methods for retinal fundus image analysis and classification*", PLoS ONE 14 e0220132 (2019).
- P. Amil et al., "*Outlier mining methods based on network structure analysis*", submitted (2019).

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