RUSSIAN ACADEMY OF SCIENCES
INSTITUTE FOR INFORMATION TRANSMISSION PROBLEMS
(Kharkevich Institute)

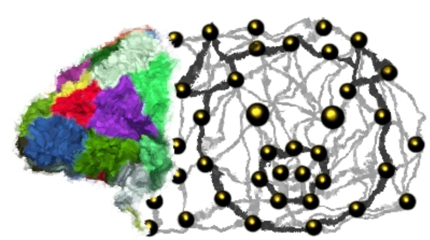
Skolkovo Tech
Skolkovo Institute of Science and Technology

HIGHER SCHOOL OF ECONOMICS
NATIONAL RESEARCH UNIVERSITY

Kernel Classification of Connectomes Based on Earth Mover's Distance between Graph Spectra

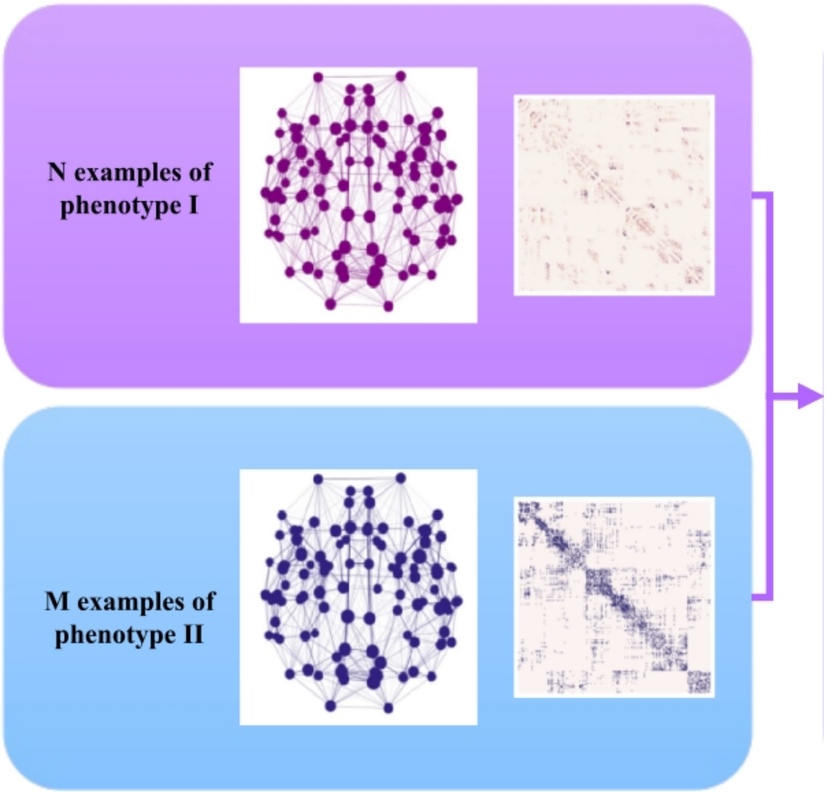
Yulia Dodonova, Mikhail Belyaev, Anna Tkachev,

Dmitry Petrov, Leonid Zhukov



MICCAI 2016 Athens GREECE
19TH INTERNATIONAL CONFERENCE ON MEDICAL IMAGE COMPUTING & COMPUTER ASSISTED INTERVENTION
October 17-21 2016
INTERCONTINENTAL ATHENAEUM ATHENS / GREECE

MRI aquisition → Network construction → Machine learning on networks



How to capture differences between the classes?

How to classify networks?

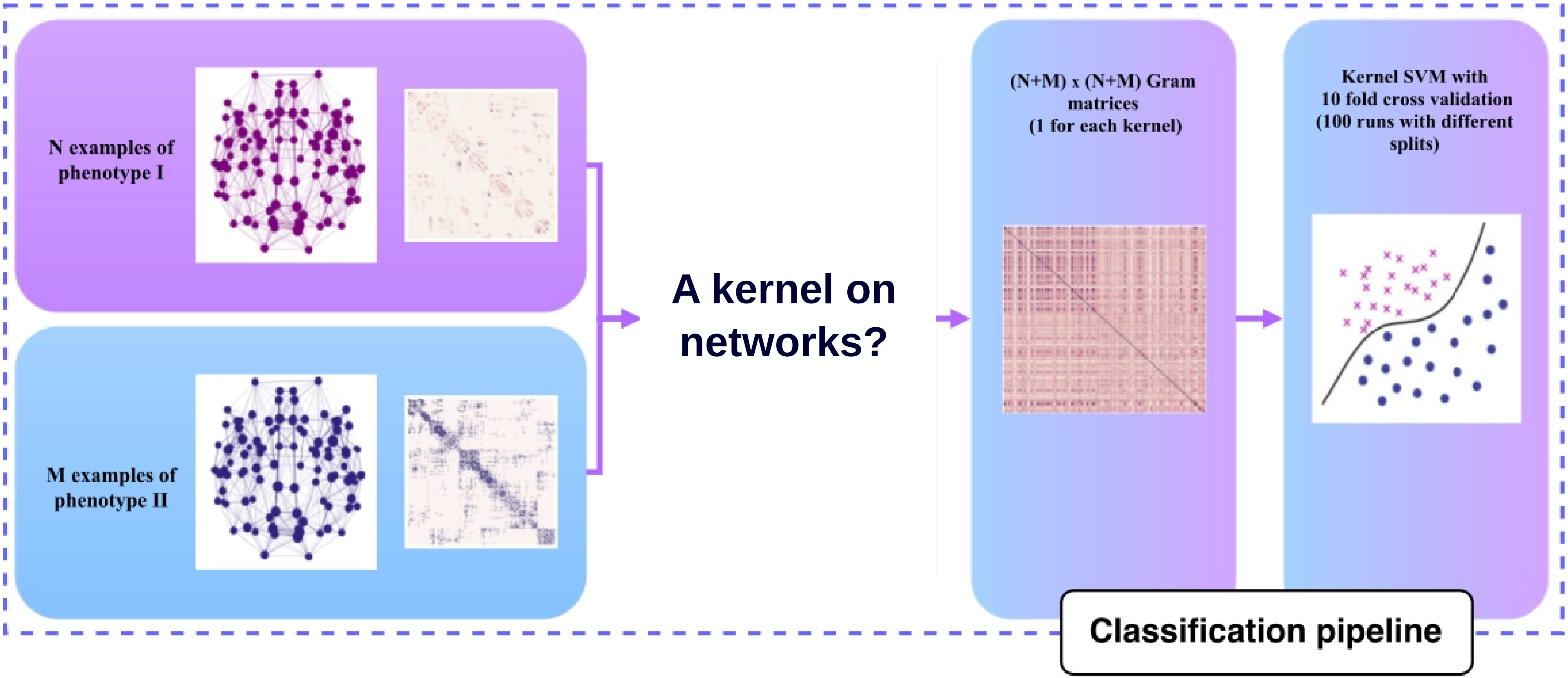
- Graph embedding methods

  - describe a network via a vector

- Kernel classifiers

  - define a positive semi-definite function on graphs
    and feed it to the SVM (support vector machines)

Kernel approach



A kernel on networks?

Provided we have a distance between the two networks G_1 and G_2, we can compute a kernel by:

$$K(G, G') = e^{-\alpha\omega(G, G')}$$

How to compute a distance between two connectomes?

Idea

Use spectral distributions

of the normalized graph Laplacians

to capture differences

in the structure of connectomes

What is a normalized Laplacian?

Let A be a graph adjacency matrix

D is a diagonal matrix of weighted node degrees:

$$d_i = \sum_j a_{ij}$$

Graph Laplacian is:

$$L = D - A$$

Normalized graph Laplacian is:

$$\mathcal{L} = D^{-1/2} L D^{-1/2}$$

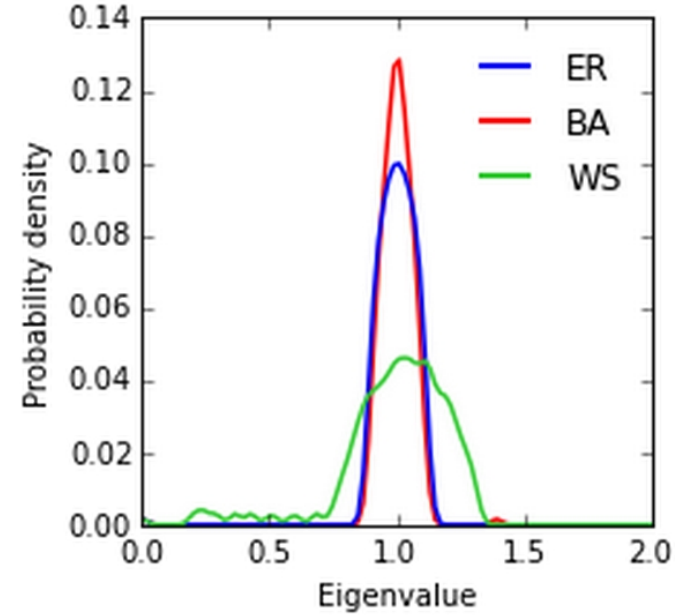
Why its spectra are so special?

The eigenvalues are in range from 0 to 2:

- can compare networks with different sizes

- no need to normalize networks

The shape of the eigenvalue distribution, its symmetry and the multiplicity of particular values capture information about graph structure

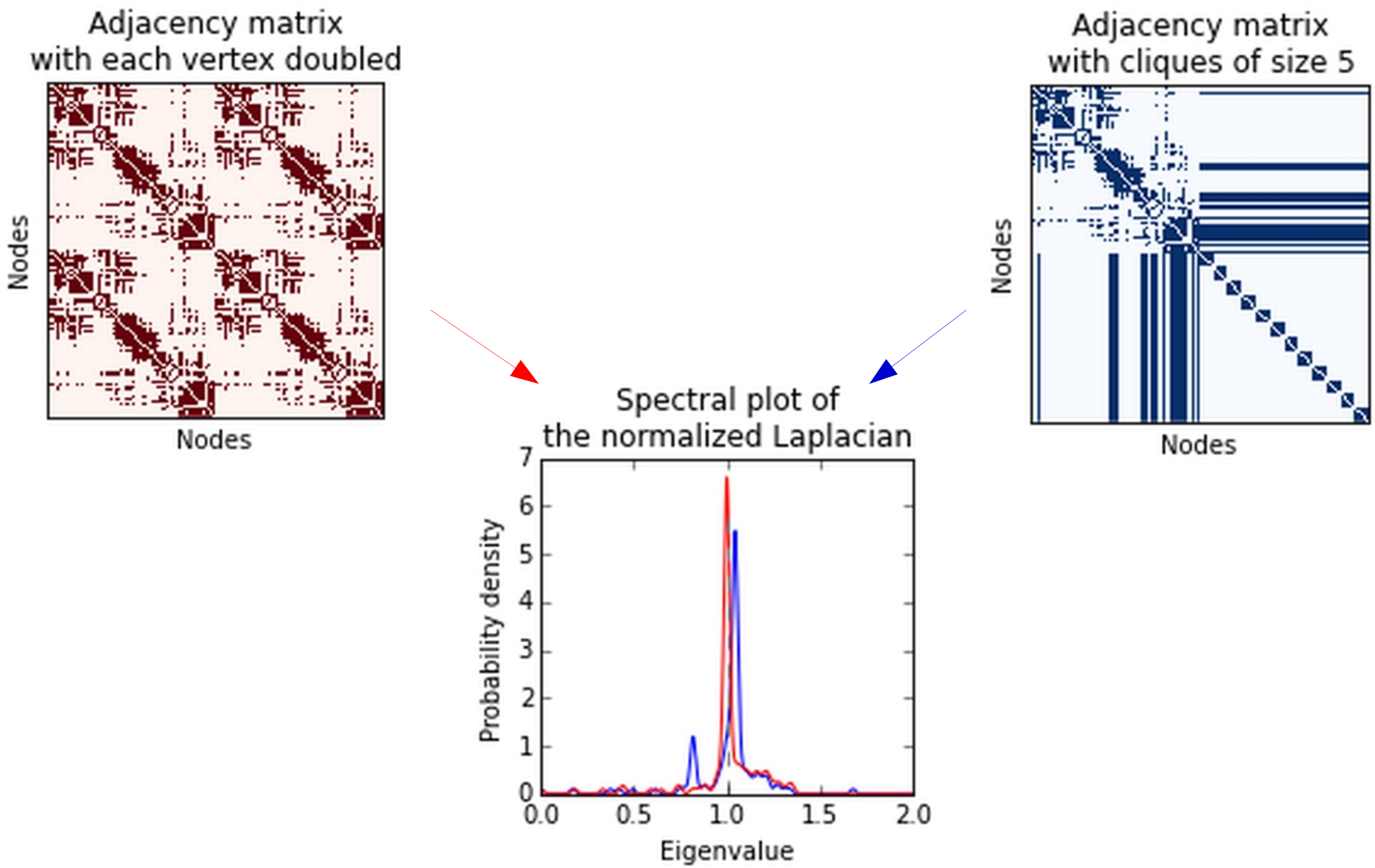


Spectral distributions of random graphs (Erdös-Rényi, Barabási-Albert, Watts-Strogatz)

Chung F. (1997) Spectral Graph Theory

Banerjee A., Jost J. (2008) Spectral plot properties: towards a qualitative classification of networks. Networks and heterogeneous media, 3, 2, 395–411

Graph structure in spectral distributions



de Lange S.C., de Reus M.A., van den Heuvel M.P. (2014) The Laplacian spectrum of neural networks. Frontiers in Computational Neuroscience, 1–12

Distance between spectral distributions?

Could use measures from information theory

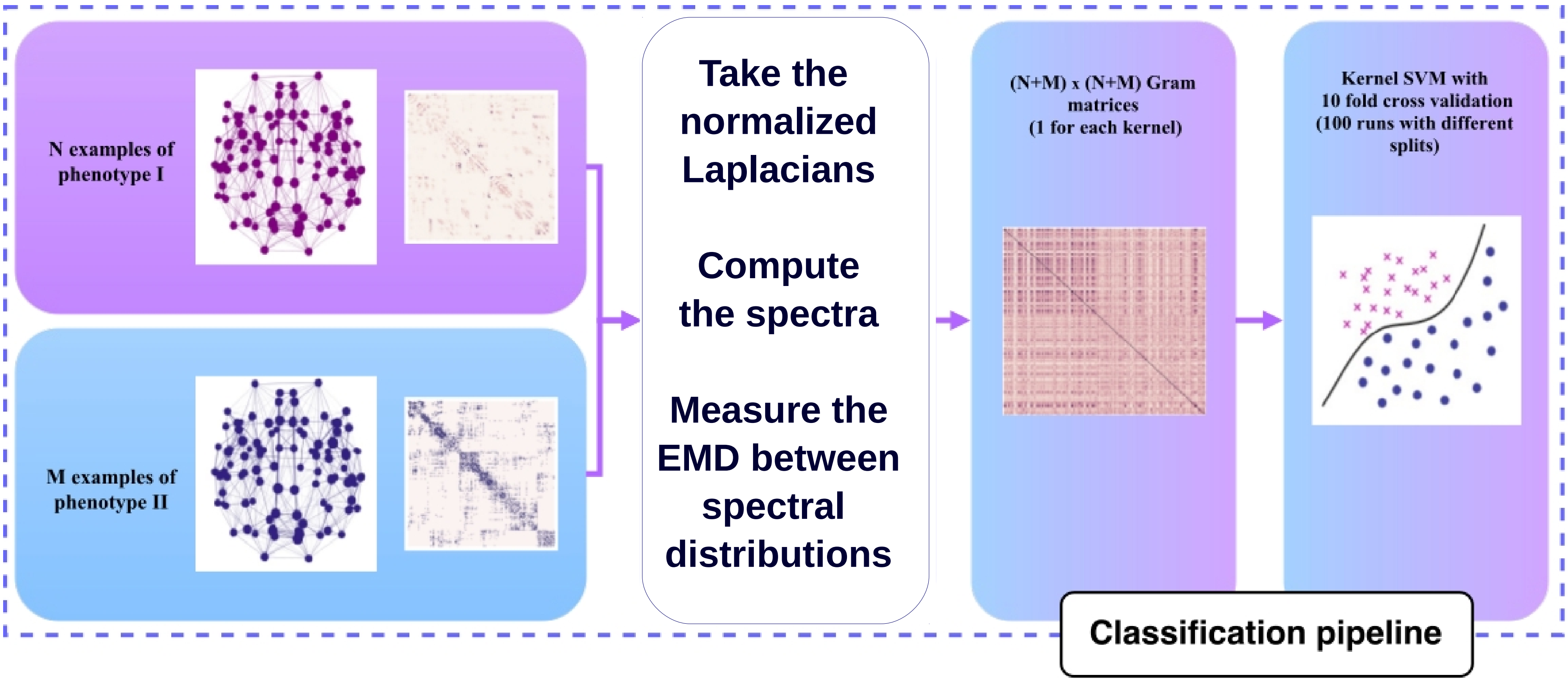
- need density reconstruction

An idea behind the earth mover's distance (EMD):

If each distribution is represented by some amount of dirt, EMD is the minimum cost required to move the dirt of one distribution to produce the other. The cost is the amount of dirt moved times the distance by which it is moved.

Rubner, Y. , Tomasi, C., Guibas, L. J.: The earth movers distance as a metric for image retrieval, International Journal of Computer Vision, 40, 2000 (2000)

Pipeline


N examples of phenotype I
M examples of phenotype II
Take the normalized Laplacians
Compute the spectra
Measure the EMD between spectral distributions
(N+M) x (N+M) Gram matrices
(1 for each kernel)
Kernel SVM with
10 fold cross validation
(100 runs with different splits)
Classification pipeline

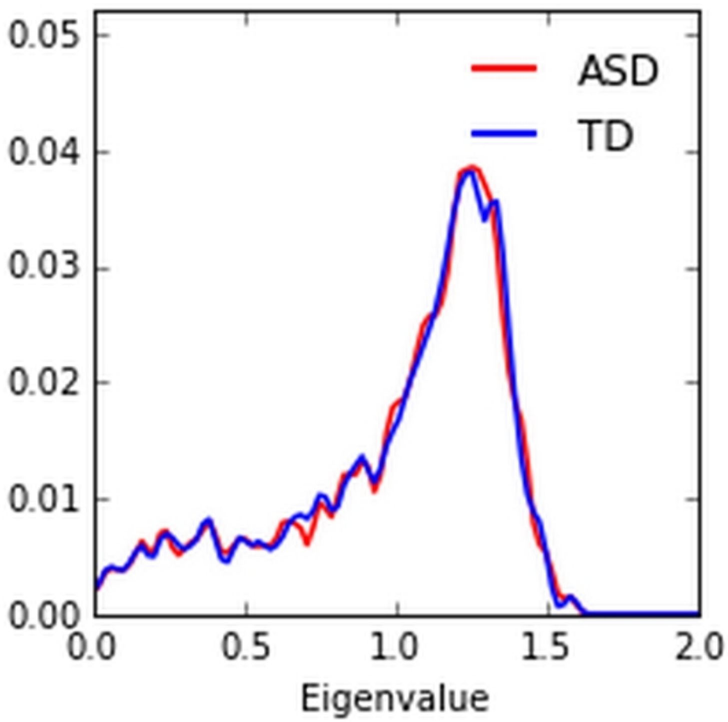
Example dataset: UCLA Autism

- structural connectomes
- 94 subjects
- 51 ASD subjects (age 13 ± 2.8 years),
  43 TD subjects (age 13.1 ± 2.4 years)
- 264x264 matrices
  deterministic tractography (FACT)

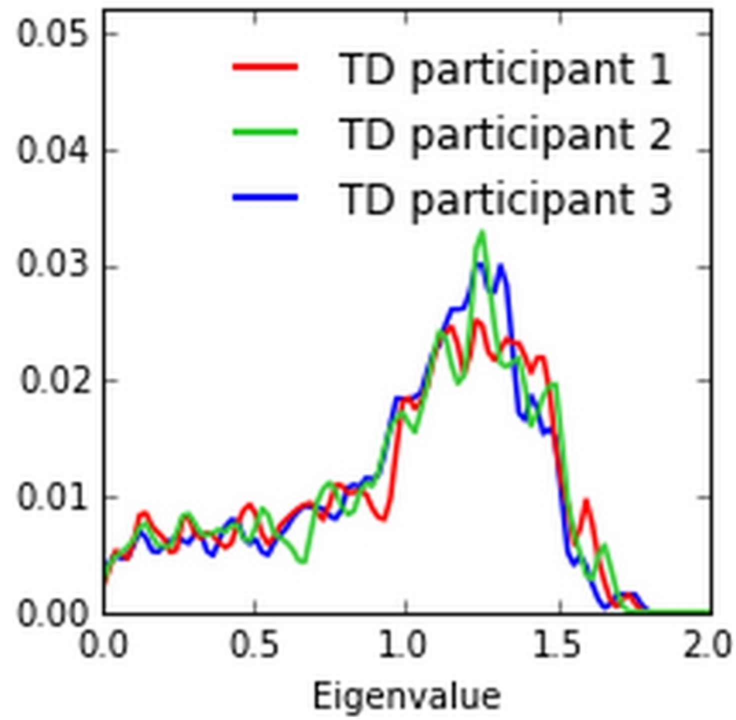
Rudie, J.D., Brown, J.A., Beck-Pancer, D., Hernandez, L.M., Dennis, E.L., Thompson, P.M., et al.: Altered functional and structural brain network organization in autism. Neuroimage Clin 2, 79–94 (2013)

Brown, J.A., Rudie, J.D., Bandrowski, A., Van Horn, J.D., Bookheimer, S.Y. (2012) The UCLA multimodal connectivity database: a web-based platform for brain connectivity matrix sharing and analysis. Frontiers in Neuroinformatics 6, 28.

UCLA Autism: spectral distributions



Spectra of the group average matrices



Spectra of the individual matrices of TD class

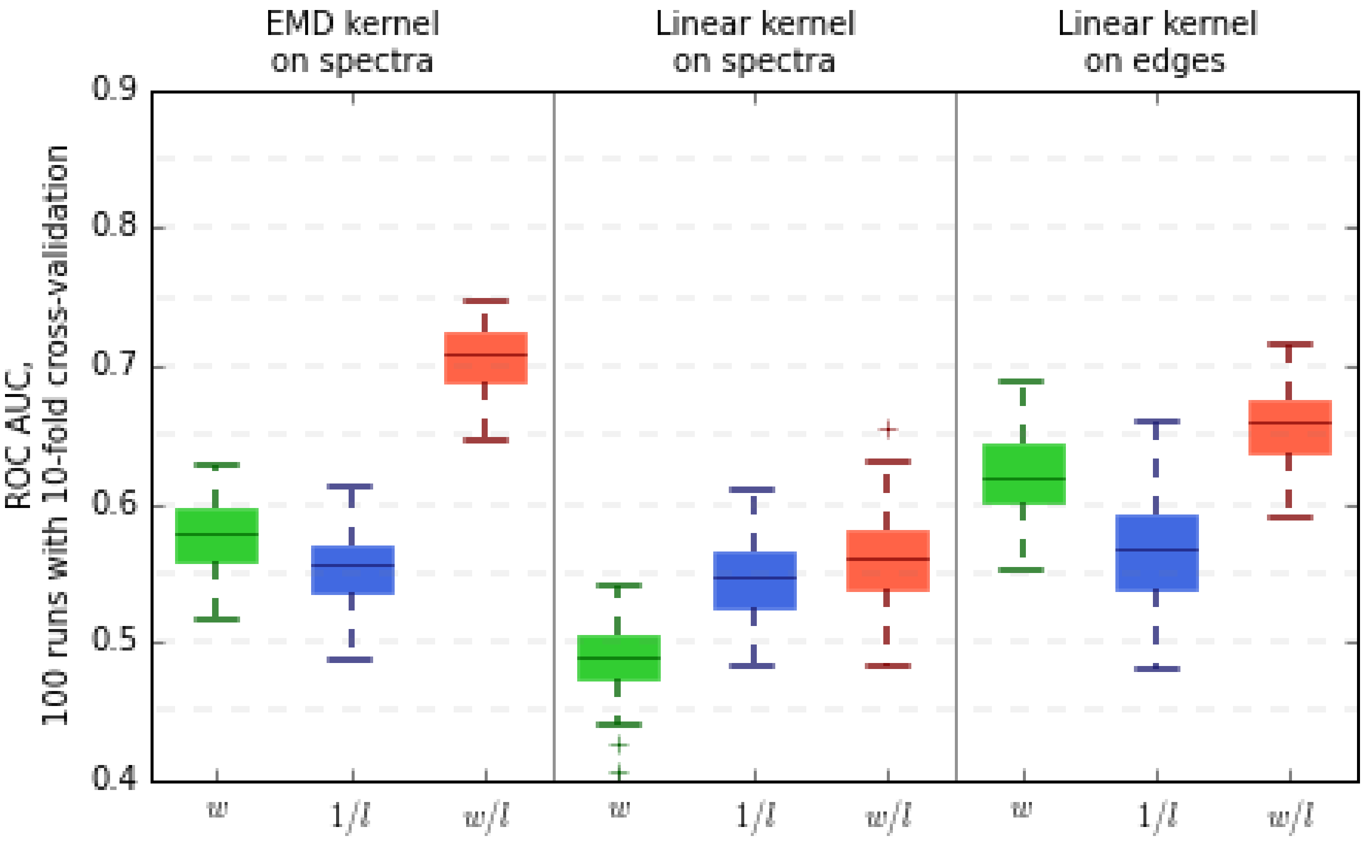
UCLA Autism: classification

- Run parallel analysis on connectomes with three different weighting schemes:
  - weights proportional do the number of streamlines
  - weights proportional to the inverse Euclidean distance between the centers of the respective regions
  - combined the above weights
- Compare performance of the proposed pipeline against the linear SVM classifiers on the vectors of edges and the vectors of sorted eigenvalues

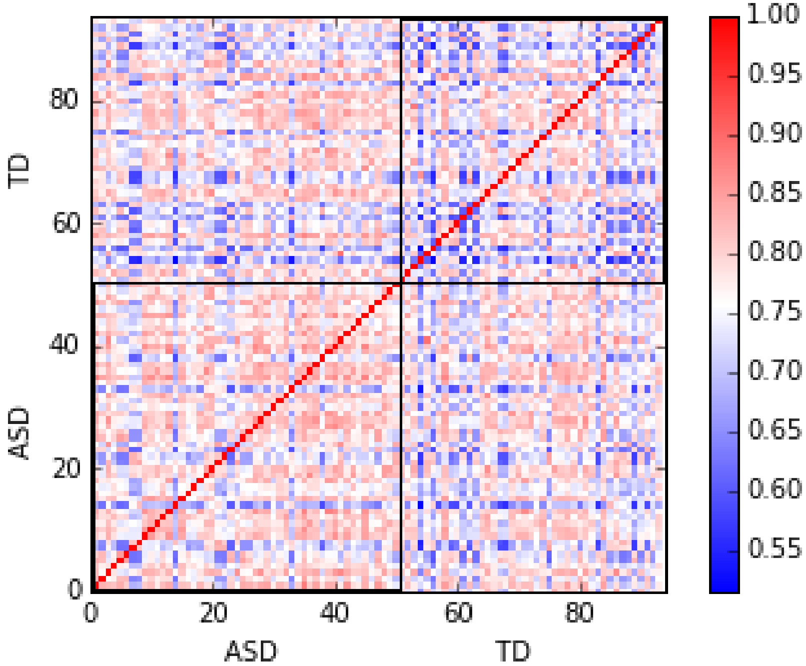
.

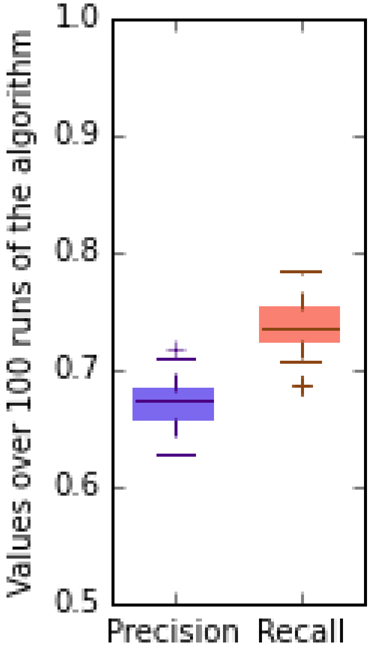
- Area under the ROC-curve (ROC AUC), 10-fold cross-validation, 100 runs with different splits

UCLA Autism: results



UCLA Autism: results





Gram matrix based on the EMD between the normalized Laplacian spectra: the TD group shows larger variability

Precision and recall values: Algorithm performs quite well Identifying ASD subjects, but tends to classify TD subjects as pathological

Conclusions

- Spectral distributions of the normalized Laplacians capture some meaningful **structural properties** of brain networks which make them different from other network classes
- Spectral distributions of connectomes can help to **distinguish normal and pathological brain networks**
- **Further studies are needed** to explore whether these findings generalize to other classification tasks and other schemes of network construction

Thank you!

Q?

dodonova@iitp.ru

Kernel Classification of Connectomes Based on Earth Mover’s Distance between Graph Spectra

Yulia Dodonova, Mikhail Belyaev, Anna Tkachev,
Dmitry Petrov, and Leonid Zhukov