

### Graph Signal Processing

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Network as graph G(V, E): encode pairwise relationships

- Desiderata: Process, analyze and learn from network data [Kolaczyk'09]
   ⇒ Use G to study graph signals, data associated with nodes in V
- Ex: Opinion profile, buffer congestion levels, neural activity, epidemic



### Graph signal processing: Motivation and fundamentals

Learning graphs from observations of smooth signals

Case study: Discriminative graph learning for emotion recognition

# Graph signal processing (GSP)



Graph G with adjacency matrix A
 ⇒ A<sub>ij</sub> = proximity between i and j
 Signal x ∈ ℝ<sup>N<sub>v</sub></sup> on top of the graph
 ⇒ x<sub>i</sub> = signal value at node i



- ▶ Graph Signal Processing  $\rightarrow$  Exploit structure encoded in **A** to process **x**
- Q: Graph signals common and interesting as networks are?
- Q: Why do we expect the graph structure to be useful in processing x?

A. Ortega et al, "Graph signal processing: Overview, challenges, and applications," *Proc. IEEE*, 2018



- Bureau of Economic Analysis of the U.S. Department of Commerce
  - $A_{ij} =$ Output of sector *i* that becomes input to sector *j* (62 sectors)



- Oil extraction (OG), Petroleum and coal products (PC), Construction (CO)
- Administrative services (AS), Professional services (MP)
- Credit intermediation (FR), Securities (SC), Real state (RA), Insurance (IC)
- Only interactions stronger than a threshold are shown



Bureau of Economic Analysis of the U.S. Department of Commerce
 A<sub>ij</sub> = Output of sector *i* that becomes input to sector *j* (62 sectors)



- A few sectors have widespread strong influence (services, finance, energy)
- Some sectors have strong indirect influences (oil)
- The heavy last row is final consumption
- This is an interesting network  $\Rightarrow$  Signals on this graph are as well



Signal x = output per sector = disaggregated GDP

 $\Rightarrow$  Network structure used to, e.g., reduce GDP estimation noise



Signal is as interesting as the network itself. Arguably more

- Same is true for brain connectivity and fMRI brain signals, ...
- Gene regulatory networks and gene expression levels, ...
- Online social networks and information cascades, ...

Signal and Information Processing is about exploiting signal structure

- Discrete time described by cyclic graph  $\Rightarrow$  Time *n* follows time n-1
  - $\Rightarrow$  Signal value  $x_n$  similar to  $x_{n-1}$
- Formalized with the notion of frequency









**Fourier transform**  $\Rightarrow$  Projection on eigenvector space of cycle



► Random signal with mean E [x] = 0 and covariance C<sub>x</sub> = E [xx<sup>H</sup>] ⇒ Eigenvector decomposition C<sub>x</sub> = VAV<sup>H</sup>

Covariance matrix A = C<sub>x</sub> is a graph
 ⇒ Not a very good graph, but still

Precision matrix C<sub>x</sub><sup>-1</sup> a common graph too
 ⇒ Conditional dependencies of Gaussian x



► Covariance matrix structure  $\Rightarrow$  Principal components (PCA)  $\Rightarrow \tilde{\mathbf{x}} = \mathbf{V}^{H} \mathbf{x}$ 

- ▶ PCA transform ⇒ Projection on eigenvector space of (inverse) covariance
- Q: Can we extend these principles to general graphs and signals?



- ► Adjacency **A**, Laplacian **L**, or, generically graph shift  $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$  $\Rightarrow S_{ij} = 0$  for  $i \neq j$  and  $(i, j) \notin E$  (captures local structure in *G*)
- ► The Graph Fourier Transform (GFT) of x is defined as

$$ilde{\mathsf{x}} = \mathsf{V}^{-1}\mathsf{x}$$

▶ While the inverse GFT (iGFT) of x̃ is defined as

#### $\mathbf{x} = \mathbf{V} \tilde{\mathbf{x}}$

 $\Rightarrow$  Eigenvectors  $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_{N_v}]$  are the frequency basis (atoms)

Additional structure

 $\Rightarrow$  If **S** is normal, then  $\mathbf{V}^{-1} = \mathbf{V}^H$  and  $\tilde{x}_k = \mathbf{v}_k^H \mathbf{x} = \langle \mathbf{v}_k, \mathbf{x} \rangle$ 

 $\Rightarrow$  Parseval holds,  $\|\mathbf{x}\|^2 = \|\mathbf{\tilde{x}}\|^2$ 

► GFT ⇒ Projection on eigenvector space of graph shift operator S

### Frequency modes of the Laplacian



Total variation of signal x with respect to L

$$\mathsf{TV}(\mathbf{x}) = \mathbf{x}^{\top} \mathsf{L} \mathbf{x} = \sum_{i,j=1,j>i}^{N_v} A_{ij} (x_i - x_j)^2$$

⇒ Smoothness measure on the graph G (Dirichlet energy)
For Laplacian eigenvectors V = [v<sub>1</sub>,..., v<sub>N<sub>v</sub></sub>] ⇒ TV(v<sub>k</sub>) = λ<sub>k</sub> ⇒ Can view 0 = λ<sub>1</sub> < ··· ≤ λ<sub>N<sub>v</sub></sub> as frequencies
Ex: gene network, N<sub>v</sub>=10, k=1, k=2, k=9



- ▶ Particularized to cyclic graphs  $\Rightarrow$  GFT  $\equiv$  Fourier transform
- Also for covariance graphs  $\Rightarrow$  GFT  $\equiv$  PCA transform
- ▶ But really, this is an empirical question. GFT of disaggregated GDP



► Spectral domain representation characterized by a few coefficients ⇒ Notion of bandlimitedness:  $\mathbf{x} = \sum_{k=1}^{K} \tilde{x}_k \mathbf{v}_k$ ⇒ Sampling, compression, filtering, pattern recognition



▶ GFT of brain signals during a visual-motor learning task [Huang et al'16]
 ⇒ Decomposed into low, medium and high frequency components



Brain: Complex system where regularity coexists with disorder [Sporns'11]
 ⇒ Signal energy mostly in the low and high frequencies
 ⇒ In brain regions akin to the visual and sensorimotor cortices



- Learning graphs from nodal observations
- Key in neuroscience
  - $\Rightarrow$  Functional network from fMRI signals



- ▶ Most GSP works: how known graph **S** affects signals and filters
- ▶ Here, reverse path: how to use GSP to infer the graph topology?
  - Graphical models [Egilmez et al'16], [Rabbat'17], [Kumar et al'19], ...
  - Smooth signals [Dong et al'15], [Kalofolias'16], [Sardellitti et al'17], ...
  - ▶ Graph filtering models [Shafipour et al'17], [Thanou et al'17], ...
  - Stationary signals [Pasdeloup et al'15], [Segarra et al'16], ...
  - Directed graphs [Mei-Moura'15], [Shen et al'16], ...







In Deduction Medices data analysis and preserving tails typically invol-large uris of simultaneil data, where the structure carries cell

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#### Topology Identification and Learning Over Graphs: Accounting for Nonlinearities and Dynamics

This article focuses on the problem of learning graphs from data, in particular, to capture the nonlinear and dynamic dependencies.

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Recent tutorials on learning graphs from data (with a GSP flavor) IEEE Signal Processing Magazine and Proceedings of the IEEE



### Graph signal processing: Motivation and fundamentals

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Case study: Discriminative graph learning for emotion recognition

### Problem formulation

#### Rationale

- Seek graphs on which data admit certain regularities
  - Nearest-neighbor prediction (a.k.a. graph smoothing)
  - Semi-supervised learning
  - Efficient information-processing transforms
- Many real-world graph signals are smooth
  - Graphs based on similarities among vertex attributes
  - Network formation driven by homophily, proximity in latent space

#### **Problem statement**

Given observations  $\mathcal{X} := {\mathbf{x}_p}_{p=1}^P$ , identify a graph G such that signals in  $\mathcal{X}$  are smooth on G.

Criterion: Dirichlet energy on the graph G with Laplacian L

$$\mathsf{TV}(\mathsf{x}) = \mathsf{x}^{\top}\mathsf{L}\mathsf{x}$$





Baker's yeast data, formally known as *Saccharomyces cerevisiae* 

▶ Graph: 134 vertices (proteins) and 241 edges (protein interactions)



Signal: functional annotation intracellular signaling cascade (ICSC)

- Signal transduction, how cells react to the environment
- ▶  $x_i = 1$  if protein *i* annotated ICSC (yellow),  $x_i = 0$  otherwise (blue)

### Example: Predicting law practice



Working relationships among lawyers [Lazega'01]

Graph: 36 partners, edges indicate partners worked together



Signal: various node-level attributes  $\mathbf{x} = \{x_i\}_{i \in V}$  including

 $\Rightarrow$  Type of practice, i.e., litigation (red) and corporate (cyan)



Consider an unknown graph G with Laplacian L = VΛV<sup>⊤</sup> ⇒ Adopt GFT basis V as signal representation matrix

► Factor analysis model for the observed graph signal

 $\mathbf{x} = \mathbf{V} \boldsymbol{\chi} + \boldsymbol{\epsilon}$ 

 $\Rightarrow$  Latent variables  $\chi \sim \mathcal{N}(\mathbf{0}, \mathbf{\Lambda}^{\dagger}) \ (\approx$  GFT coefficients)

 $\Rightarrow$  Isotropic error term  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ 

- Smoothness: prior encourages low-pass bandlimited x
  - $\Rightarrow$  Small eigenvalues of L (low freq.)  $\rightarrow$  High-power factor loadings

X. Dong et al, "Learning Laplacian matrix in smooth graph signal representations," *IEEE Trans. Signal Process.*, 2016



 $\blacktriangleright$  Maximum a posteriori (MAP) estimator of the latent variables  $\chi$ 

$$\hat{\boldsymbol{\chi}}_{\mathsf{MAP}} = \arg\min_{\boldsymbol{\chi}} \left\{ \| \mathbf{x} - \mathbf{V} \boldsymbol{\chi} \|^2 + \alpha \boldsymbol{\chi}^\top \mathbf{\Lambda} \boldsymbol{\chi} \right\}$$

 $\Rightarrow$  Parameterized by the unknown  ${\bm V}$  and  ${\bm \Lambda}$ 

• Define predictor  $\mathbf{y} := \mathbf{V} \boldsymbol{\chi}$ , regularizer expressible as

$$\boldsymbol{\chi}^{\top} \boldsymbol{\Lambda} \boldsymbol{\chi} = \boldsymbol{\mathsf{y}}^{\top} \boldsymbol{\mathsf{V}} \boldsymbol{\Lambda} \boldsymbol{\mathsf{V}}^{\top} \boldsymbol{\mathsf{y}} = \boldsymbol{\mathsf{y}}^{\top} \boldsymbol{\mathsf{L}} \boldsymbol{\mathsf{y}} = \mathsf{TV}(\boldsymbol{\mathsf{y}})$$

 $\Rightarrow$  Laplacian-based TV denoiser of **x**, smoothness prior on **y** 

 $\Rightarrow$  Kernel-ridge regression with unknown **K** := **L**<sup>†</sup> (graph filter)

**Idea:** jointly search for **L** and denoised representation  $\mathbf{y} = \mathbf{V} \boldsymbol{\chi}$ 

$$\min_{\mathbf{L},\mathbf{y}} \left\{ \|\mathbf{x} - \mathbf{y}\|^2 + \alpha \mathbf{y}^\top \mathbf{L} \mathbf{y} \right\}$$



▶ Given signals 
$$\mathcal{X} := \{\mathbf{x}_{\rho}\}_{\rho=1}^{P}$$
 in  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_P] \in \mathbb{R}^{N_v \times P}$ , solve

$$\min_{\mathbf{L},\mathbf{Y}} \left\{ \|\mathbf{X} - \mathbf{Y}\|_{F}^{2} + \alpha \operatorname{trace}\left(\mathbf{Y}^{\top}\mathbf{L}\mathbf{Y}\right) + \frac{\beta}{2}\|\mathbf{L}\|_{F}^{2} \right\}$$

s. to 
$$\operatorname{trace}(\mathbf{L}) = N_{v}, \ \mathbf{L}\mathbf{1} = \mathbf{0}, \ L_{ij} = L_{ji} \leq 0, \ i \neq j$$

 $\Rightarrow \mbox{Objective function: Fidelity} + \mbox{smoothness} + \mbox{edge sparsity} \\ \Rightarrow \mbox{Not jointly convex in } L \mbox{ and } Y, \mbox{ but bi-convex} \\$ 

• Algorithmic approach: alternating minimization (AM),  $O(N_v^3)$  cost (S1) Fixed Y: solve for L via interior-point method, ADMM (more soon) (S2) Fixed L: low-pass, graph filter-based smoother of the signals in X  $Y = (I + \alpha L)^{-1} X$ 



• Generate multiple signals on a synthetic Erdős-Rényi graph  $\Rightarrow$  Recover the graph for different values of  $\alpha$  and  $\beta$ 



- $\blacktriangleright$  More edges promoted by increasing  $\beta$  and decreasing  $\alpha$
- ▶ In the low noise regime, the ratio  $\beta/\alpha$  determines behavior



- ▶  $N_v = 89$  stations measuring monthly temperature averages (1981-2010)
  - $\Rightarrow$  Learn a graph G on which the temperatures vary smoothly
- ► Geographical distance not a good idea ⇒ different altitudes



▶ Recover altitude partition from spectral clustering on G
 ⇒ Red (high stations) and blue (low stations) clusters
 ▶ K-means applied directly to the temperatures (right) fails

# Signal smoothness meets edge sparsity



▶ Recall  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_P] \in \mathbb{R}^{N_v \times P}$ , let  $\bar{\mathbf{x}}_i^\top \in \mathbb{R}^{1 \times P}$  denote its *i*-th row ⇒ Euclidean distance matrix  $\mathbf{Z} \in \mathbb{R}_+^{N_v \times N_v}$ , where  $Z_{ij} := \|\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_j\|^2$ 

Neat trick: link between smoothness and sparsity

$$\sum_{\rho=1}^{P} \mathsf{TV}(\mathbf{x}_{\rho}) = \mathsf{trace}(\mathbf{X}^{\top} \mathbf{L} \mathbf{X}) = \frac{1}{2} \| \mathbf{A} \circ \mathbf{Z} \|_{1}$$

 $\Rightarrow$  Sparse *E* when data come from a smooth manifold

 $\Rightarrow$  Favor candidate edges (i, j) associated with small  $Z_{ij}$ 

Shows that edge sparsity on top of smoothness is redundant

Parameterize graph learning problems in terms of A (instead of L)
 Advantageous since constraints on A are decoupled

V. Kalofolias, "How to learn a graph from smooth signals," *AISTATS*, 2016



General purpose model for learning graphs [Kalofolias'16]

$$\begin{split} \min_{\mathbf{A}} & \left\{ \|\mathbf{A} \circ \mathbf{Z}\|_1 - \alpha \mathbf{1}^\top \log(\mathbf{A}\mathbf{1}) + \frac{\beta}{2} \|\mathbf{A}\|_F^2 \right\}\\ \text{s. to} \quad \text{diag}(\mathbf{A}) = \mathbf{0}, \ A_{ij} = A_{ji} \geq 0, \ i \neq j \end{split}$$

 $\Rightarrow$  Logarithmic barrier forces positive degrees

#### $\Rightarrow$ Penalize large edge-weights to control sparsity

- ▶ Primal-dual solver amenable to parallelization,  $O(N_v^2)$  cost
- Laplacian-based factor analysis encore. Tackle (S1) as

$$\begin{split} \min_{\mathbf{A}} & \left\{ \|\mathbf{A} \circ \mathbf{Z}\|_1 - \log(\mathbb{I}\left\{\|\mathbf{A}\|_1 = N_v\right\}) + \frac{\beta}{2} \left(\|\mathbf{A}\mathbf{1}\|^2 + \|\mathbf{A}\|_F^2\right) \right\}\\ \text{s. to} \quad \text{diag}(\mathbf{A}) = \mathbf{0}, \ A_{ij} = A_{ji} \geq 0, \ i \neq j \end{split}$$

# Example: Learning the graph of USPS digits



- ▶ 1001 images of the 10 digits, but highly imbalanced (2.6*i*<sup>2</sup>)
   ⇒ 10 classes via graph recovery plus spectral clustering
- Compare two methods based on smoothness and k-NN graph



Performance more robust to graph density

 $\Rightarrow$  Likely attributable to non-singleton nodes



- Idea: parameterize the unknown topology via an edge indicator vector
- ► Complete graph on  $N_V$  nodes, having  $M := \binom{N_v}{2}$  edges ⇒ Incidence matrix  $\mathbf{B} := [\mathbf{b}_1, \dots, \mathbf{b}_M] \in \mathbb{R}^{N_v \times M}$

• Laplacian of a candidate graph G(V, E)

$$\mathbf{L}(\boldsymbol{\omega}) = \sum_{m=1}^{M} \omega_m \mathbf{b}_m \mathbf{b}_m^{\top}$$

⇒ Binary edge indicator vector  $\boldsymbol{\omega} := [\omega_1, \dots, \omega_M]^\top \in \{0, 1\}^M$ ⇒ Offers an explicit handle on the number of edges  $\|\boldsymbol{\omega}\|_0 = |E|$ 

**Problem:** Given observations  $\mathcal{X} := {\mathbf{x}_p}_{p=1}^{P}$ , learn an unweighted graph G(V, E) such that signals in  $\mathcal{X}$  are smooth on G and |E| = K.

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Natural formulation is to solve the non-convex problem

$$\min_{oldsymbol{\omega}\in\{0,1\}^M} ext{trace}(oldsymbol{X}^{ op}oldsymbol{L}(oldsymbol{\omega})oldsymbol{X}), \hspace{1em} ext{s. to} \hspace{1em} \|oldsymbol{\omega}\|_0=K$$

Solution obtained through a simple rank-ordering procedure

- Compute edge scores  $c_m := \text{trace}(\mathbf{X}^{\top}(\mathbf{b}_m \mathbf{b}_m^{\top})\mathbf{X})$
- Set  $\omega_m = 1$  for those K edges having the smallest scores

▶ More pragmatic AWGN setting where  $\mathbf{x}_p = \mathbf{y}_p + \boldsymbol{\epsilon}_p$ ,  $p = 1, \dots, P$ 

$$\min_{\mathbf{Y},\boldsymbol{\omega}\in\{0,1\}^M}\left\{\|\mathbf{X}-\mathbf{Y}\|_F^2 + \alpha \mathsf{trace}(\mathbf{Y}^{\top}\mathbf{L}(\boldsymbol{\omega})\mathbf{Y})\right\}, \quad \mathsf{s. to} \ \|\boldsymbol{\omega}\|_0 = K$$

### $\Rightarrow$ Tackle via AM or semidefinite relaxation (SDR)

S. Chepuri et al, "Learning sparse graphs under smoothness prior," *ICASSP*, 2017

### Comparative summary



Noteworthy features of the edge subset selection approach

- $\checkmark\,$  Direct control on edge sparsity
- $\checkmark\,$  Simple algorithm in the noise-free case
- ✓ Devoid of Laplacian feasibility constraints
- $\checkmark$  Does not guarantee connectivity of G
- X No room for optimizing edge weights

Scalable framework in [Kalofolias'16] also quite flexible

$$\begin{split} \min_{\mathbf{A}} \left\{ \|\mathbf{A} \circ \mathbf{Z}\|_1 + g(\mathbf{A}) \right\} \\ \text{s. to} \quad \text{diag}(\mathbf{A}) = \mathbf{0}, \ A_{ij} = A_{ji} \geq 0, \ i \neq j \end{split}$$

 $\Rightarrow$  Subsumes the factor-analysis model [Dong et al'16]

 $\Rightarrow$  Recovers Gaussian kernel weights  $A_{ij} := \exp\left(-\frac{\|ar{\mathbf{x}}_i - ar{\mathbf{x}}_j\|^2}{\sigma^2}
ight)$  for

$$g(\mathbf{A}) = \sigma^2 \sum_{i,j} A_{ij} (\log(A_{ij}) - 1)$$



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Case study: Discriminative graph learning for emotion recognition



► Labeled graph signals X<sub>c</sub> := {x<sub>p</sub><sup>(c)</sup>}<sub>p=1</sub><sup>P<sub>c</sub></sup> from C different classes ⇒ Signals in each class possess a very distinctive structure

▶ As.: Class c signals are smooth w.r.t. unknown  $G_c(V, E_c)$ 

Multiple linear subspace model

 $\Rightarrow$  Signals spanned by few Laplacian modes (GFT components)

 $\Rightarrow$  Like susbpace clustering [Vidal'11], but with supervision

#### **Problem statement**

Given training signals  $\mathcal{X} = \bigcup_{c=1}^{C} \mathcal{X}_c$ , learn discriminative graphs  $\mathbf{A}_c$  under smoothness priors to classify test signals via GFT projections.



 $\blacktriangleright$  Discriminative graph learning per class c

$$\min_{\mathbf{A}_{c}} \left\{ \|\mathbf{A}_{c} \circ \mathbf{Z}_{c}\|_{1} - \alpha \mathbf{1}^{\top} \log(\mathbf{A}_{c}\mathbf{1}) + \frac{\beta}{2} \|\mathbf{A}_{c}\|_{F}^{2} - \gamma \sum_{k \neq c}^{C} \|\mathbf{A}_{c} \circ \mathbf{Z}_{k}\|_{1} \right\}$$

s. to 
$$\operatorname{diag}(\mathbf{A}_c) = \mathbf{0}, \ [\mathbf{A}_c]_{ij} = [\mathbf{A}_c]_{ji} \ge 0, \ i \neq j$$

 $\Rightarrow Capture the underlying graph topology (class c structure)$  $\Rightarrow Discriminability to boost classification performance$ 

- Q: Given graphs  $\{\hat{\mathbf{A}}_c\}_{c=1}^C$ , how do we classify a test signal x?
- Pass x through a filter-bank with C low-pass filters (LPFs)

$$\tilde{\mathbf{x}}_{F,c} = \mathsf{diag}(\tilde{\mathbf{h}}) \hat{\mathbf{V}}_c^\top \mathbf{x} \quad \Rightarrow \quad \hat{c} = \operatorname*{argmax}_c \left\{ \|\tilde{\mathbf{x}}_{F,c}\|^2 \right\}$$

 $\Rightarrow$  LPF frequency response  $\tilde{\mathbf{h}}_{\text{r}}$  learned class-c GFT basis  $\hat{\mathbf{V}}_{c}$ 



- Discriminative graph learning for emotion recognition from EEG signals
- ▶ DEAP dataset  $\Rightarrow$  32 subjects watch music videos (40 trials each)
  - Asked to rate videos: valence, arousal, like/dislike, dominance
  - Focus on valence labels: low (1-5 rating) and high (6-10 rating)
  - Signals acquired from  $N_v = 32$  EEG channels
- ► We perform a subject-specific valence classification task
  - $\Rightarrow$  Learn C = 2 graphs and project onto the 8 smoothest modes
  - $\Rightarrow$  Report leave-one (trial)-out classification accuracy
- Mean classification accuracy over subjects is 92.73%

S. S. Saboksayr et al, "Online discriminative graph learning from multi-class smooth signals," *Signal Processing*, 2022

### Valence classification



#### Q: What information do we glean from the class-conditional graphs? Centr Centra Tempor Tempor Parieta Occipit Frontal Central Temporal Parietal Occipita Frontal Central Temporal Parietal Occipital Low valence High valence Different connections (p=0.002) Connectivity increases with emotion intensity (frontal lobe links) High valence Low valence



Asymmetric frontal activity apparent from the 8 smoothest modes





- Graph signal
- Graph signal processing
- Fourier transform
- Covariance matrix
- Principal component analysis
- Graph shift operator
- Graph Fourier transform
- Topology identification
- Smooth signal
- Dirichlet energy
- Factor analysis model

- Alternating minimization
- Euclidean distance matrix
- Edge subset selection
- Gaussian kernel graph
- Multiple subspace model
- Subspace clustering
- Discriminative graphs
- Low-pass graph filter
- Emotion recognition
- EEG signals
- Valence classification