Graph Completion

Tuan Dinh University of Wisconsin - Madison

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1 Introduction

Recovering signal from partially observed samples is recently active with related development in matrix completion, collaborative filtering. Wavelet transform is a widely used transform and recently extended to the graph domain[1]. Matrix completion is currently an active research area with recent novel research and theory [2].

Most modern datasets however have additional information, either as features or as pairwise relationships between variables. For example, in the case of recommender systems, one can have demographic information or a social network for users. In sensor networks, one might have pairwise similarity information based on the actual locations of sensors. It makes sense to assume that using this additional information will aid in making predictions, and recently, several methods have been proposed to do the same [6], [7].

In this work, we consider a practical setting of a neuroimaging study. Each patient has 2 types of measurement: cheap measurement (cognition, genetic, roi) and expensive measurement (CSF NFL, Ab142, pTau, hTau). For cheap measurements, we have access to full data of every patients while we have only a small proportion of the expensive one. For example, among 100 patients, we have all 100 data points of congition data while having only 20 records of CSF data. Our goal is to recover 80 missing records from these given data.

2 Ideas

The idea behind: both cheap data and expensive data share mutual information about the underlying brain-disease relationship between patients. Therefore, we can build up a relation network based on the fully cheap data, then apply graph completion on this to recover expensive data points.

This can be modeled as an **optimization problem**:

$$|P_w(Mg - y)|_2^2 + \gamma h(g)$$

where g is the recovered signal, y is the observed data vector, P_w is the importance value, M is the projection matrix (to observed samples only) and the righthand term is the regularizer.

Assumptions and conditions: cognitive data contains relationship information about CSF, and the adjacency matrix contains true connection in terms of CSF between nodes.

Why not machine learning? the problem of small dataset and the nature of signal.

3 Problem setup, our method, and theory

We can divide the overall process into 2 main steps: Graph construction and Graph completion. Firstly, given fully cheap dataset and partially observed expensive dataset, we construct a Adjacency matrix that represents relationship between people. Using it, Graph completion part recovers the missing part of CSF signal. The whole pipeline of process is given as below:

3.1 Pre-processing

As the first step, we do feature scaling into the interval (0, 1) that makes every features equal and remove outliers to clean noise.

Secondly, we select only a few important features among tens of features because multiple trivial features can affect the true distance metric. Features having high correlation with the target CSF are selected or using lasso to filter important features

3.2 Graph Construction

The goal of construction is to extact near-CSF-related connection between patients based on the cognitive one. The construction part can be divided into 3 steps [Tony]: metric learning, sparsification and reweight the matrix.

The important part is metric learning: how we measure CSF-similarity between two patients using their cognition, that is the kernel k so that $k(cog1, cog2) \approx sim(csf1, csf2)$. We also apply variant methods to learn this similary measures.

Metric learning: learn similarity, learn connection

- Kernel learning: rbf, laplacian, linear, polynomial, sigmoid, cosine
- Learn CSF directly (lasso, ensemble), then using predicted CSF to build the graph: few data points
- Learn CSF pair-distance, then use it to predict the weight of each connection
- Classify connection: consider only binary connection, learn from observed data points to classify each connection as 0 or 1
- MMD linear transformation
- ITML (Information Theoretic ML): using the given threshold to assign label (+/-) to each node, then using ITML to learn the metric between them
- Semi-supervised ITML

Sparsification is used to keep only strong connection. We apply kNN, thresholding - weighted or binary.

- kNN using a new sigma (Dk/3) Tony's paper
- b-Matching: supervised learning
- Percentile threshold
- Unweighted connection

3.3 Graph Completion

Laplacian extraction, Intialize pre-used energy, Random Sampling, Recovery Optimization, Select and recover.

3.4 Post-processing

Control unreasonable prediction

3.5 Evaluation

RMSE, Error percentage, Recovery accuracy, Precision.

3.6 Baseline methods

Linear regression, Lasso.

4 Experiments

4.1 Setting

Datasets: CSF: 5 x 147, Cog: 27 features, 147 matches; Genetic: 65 - 27, 126 matches; ROI: 60 matches; Combined.

Default Params: CSF: Ab142, Available: 0.4, Max Samples:0.6, nSelected: 10, preSigma: 0.1, kernel: RBF, Threshold: 0.9, weighted: binary, KNN: 12, metric learning: ITML, rBand: 0.8, alpha - regularization: 0.1, gamma: 10

Cross-validation: Fold: 5 (shift), Iters: 100, Methods: randomly permutate.

4.2 Evaluation

5 Discussion

5.1 Analysis

- A good graph needs to be: sparse, full band
- Regularization doesn't help
- observed data always get nearly 100
- $ROI \ge Genetic \ge Cog$
- other CSFs don't really help

Questions

- Role of wavelet
- Optimization overfit
- Nature of data/problem
- former questions

5.2 TODO

- Obtain good graph metric learning? How to evaluate a graph being well-constructed? check if 2 signals are related? (cross-correlation); semi-supervised approach
- Strengthen optimization for uncertain graph: the current approach strongly depends on the graph (Leverage values)
- Hybrid

Table 1: Dataset 1

| Dataset | Selection | Learning | Sparse | ole 1: Data Binary | Unobserved | Observed |
|---------|-----------|----------|--------|-----------------------|-----------------------|----------------------|
| 1 | 0 | 1 | 0 | 0 | 1.54961642086494E+57 | 41 |
| 1 | 0 | 1 | 0 | 1 | 231 | 46 |
| 1 | 0 | 1 | 80 | 0 | 1.10132257451605E+86 | 2.96574466415869E+69 |
| 1 | 0 | 1 | 80 | 1 | 225 | 47 |
| 1 | 0 | 1 | 90 | 0 | 1.09866432626114E+65 | 35 |
| 1 | 0 | 1 | 90 | 1 | 1104 | 46 |
| 1 | 0 | 3 | 0 | 0 | 3.71675892880196E+101 | 1.01917511102594E+85 |
| 1 | 0 | 3 | 0 | 1 | 222 | 47 |
| 1 | 0 | 3 | 80 | 0 | 1.72638716966231E+74 | 1.8791754897833E+58 |
| 1 | 0 | 3 | 80 | 1 | 282 | 46 |
| 1 | 0 | 3 | 90 | 0 | 6.36406024670921E+50 | 30 |
| 1 | 0 | 3 | 90 | 1 | 225 | 46 |
| 1 | 0 | 4 | 0 | 0 | 440 | 47 |
| 1 | 0 | 4 | 0 | 1 | 187 | 173 |
| 1 | 0 | 4 | 80 | 0 | 454 | 48 |
| 1 | 0 | 4 | 80 | 1 | 198 | 75 |
| 1 | 0 | 4 | 90 | 0 | 475 | 48 |
| 1 | 0 | 4 | 90 | 1 | 237 | 59 |
| 1 | 10 | 1 | 0 | 0 | 2.42644453862811E+32 | 35 |
| 1 | 10 | 1 | 0 | 1 | 218 | 60 |
| 1 | 10 | 1 | 80 | 0 | 4.35973959870523E+109 | 37 |
| 1 | 10 | 1 | 80 | 1 | 214 | 62 |
| 1 | 10 | 1 | 90 | 0 | 2.08978550566874E+216 | 41 |
| 1 | 10 | 1 | 90 | 1 | 246 | 62 |
| 1 | 10 | 3 | 0 | 0 | 1.74358185482125E+39 | 39 |
| 1 | 10 | 3 | 0 | 1 | 212 | 65 |
| 1 | 10 | 3 | 80 | 0 | 5.93262384782626E+48 | 2733 |
| 1 | 10 | 3 | 80 | 1 | 426 | 60 |
| 1 | 10 | 3 | 90 | 0 | 4.166170379216E+92 | 36 |
| 1 | 10 | 3 | 90 | 1 | 218 | 62 |
| 1 | 10 | 4 | 0 | 0 | 188 | 171 |
| 1 | 10 | 4 | 0 | 1 | 190 | 170 |
| 1 | 10 | 4 | 80 | 0 | 199 | 81 |
| 1 | 10 | 4 | 80 | 1 | 200 | 80 |
| 1 | 10 | 4 | 90 | 0 | 220 | 66 |
| 1 | 10 | 4 | 90 | 1 | 216 | 67 |

Table 2: Dataset 2

| Dataset | Selection | Learning | Sparse | ole 2: Data Binary | Unobserved | Observed |
|---------|-----------|----------|--------|------------------------------|-----------------------|-----------------------|
| 2 | 0 | 1 | 0 | 0 | 1.45882402120812E+50 | 63025804323189 |
| 2 | 0 | 1 | 0 | 1 | 229 | 45 |
| 2 | 0 | 1 | 80 | 0 | 1.43340247001959E+206 | 9.55489627082001E+117 |
| 2 | 0 | 1 | 80 | 1 | 252 | 49 |
| 2 | 0 | 1 | 90 | 0 | 2.99211738552092E+126 | 5710390983 |
| 2 | 0 | 1 | 90 | 1 | 258 | 47 |
| 2 | 0 | 3 | 0 | 0 | 1.90619837413455E+109 | 1.69474525741715E+92 |
| 2 | 0 | 3 | 0 | 1 | 233 | 48 |
| 2 | 0 | 3 | 80 | 0 | 2.69648070080857E+281 | 1.03591070221205E+79 |
| 2 | 0 | 3 | 80 | 1 | 227 | 45 |
| 2 | 0 | 3 | 90 | 0 | 5.87605647756047E+76 | 40 |
| 2 | 0 | 3 | 90 | 1 | 241 | 48 |
| 2 | 0 | 4 | 0 | 0 | 465 | 48 |
| 2 | 0 | 4 | 0 | 1 | 187 | 174 |
| 2 | 0 | 4 | 80 | 0 | 448 | 48 |
| 2 | 0 | 4 | 80 | 1 | 194 | 76 |
| 2 | 0 | 4 | 90 | 0 | 459 | 48 |
| 2 | 0 | 4 | 90 | 1 | 229 | 59 |
| 2 | 10 | 1 | 0 | 0 | 1.23852856051863E+52 | 37 |
| 2 | 10 | 1 | 0 | 1 | 216 | 65 |
| 2 | 10 | 1 | 80 | 0 | 1444906301113 | 37 |
| 2 | 10 | 1 | 80 | 1 | 212 | 63 |
| 2 | 10 | 1 | 90 | 0 | 3.3266124244703E+54 | 977562 |
| 2 | 10 | 1 | 90 | 1 | 211 | 61 |
| 2 | 10 | 3 | 0 | 0 | 10384246327 | 37 |
| 2 | 10 | 3 | 0 | 1 | 215 | 61 |
| 2 | 10 | 3 | 80 | 0 | 7.3046669499928E + 76 | 150 |
| 2 | 10 | 3 | 80 | 1 | 214 | 62 |
| 2 | 10 | 3 | 90 | 0 | 23245 | 35 |
| 2 | 10 | 3 | 90 | 1 | 212 | 62 |
| 2 | 10 | 4 | 0 | 0 | 186 | 173 |
| 2 | 10 | 4 | 0 | 1 | 189 | 171 |
| 2 | 10 | 4 | 80 | 0 | 201 | 82 |
| 2 | 10 | 4 | 80 | 1 | 196 | 82 |
| 2 | 10 | 4 | 90 | 0 | 221 | 63 |
| 2 | 10 | 4 | 90 | 1 | 226 | 61 |

Table 3: Dataset 3

| Dataset | Selection | Learning | Sparse | ole 3: Data Binary | Unobserved | Observed |
|---------|-----------|----------|--------|------------------------------|-----------------------|-----------------------|
| 3 | 0 | 1 | 0 | 0 | 1.54903473090918E+33 | 1543012929119330 |
| 3 | 0 | 1 | 0 | 1 | 224 | 46 |
| 3 | 0 | 1 | 80 | 0 | 3.02737251340352E+23 | 33 |
| 3 | 0 | 1 | 80 | 1 | 222 | 45 |
| 3 | 0 | 1 | 90 | 0 | 2.69696418741955E+17 | 34 |
| 3 | 0 | 1 | 90 | 1 | 237 | 44 |
| 3 | 0 | 3 | 0 | 0 | 3.70926447247101E+179 | 2109477941248780 |
| 3 | 0 | 3 | 0 | 1 | 9277 | 44 |
| 3 | 0 | 3 | 80 | 0 | 1.53574797954259E+30 | 28270776028301 |
| 3 | 0 | 3 | 80 | 1 | 785 | 44 |
| 3 | 0 | 3 | 90 | 0 | 5.28506607280535E+122 | 9.66525191036136E+105 |
| 3 | 0 | 3 | 90 | 1 | 223 | 53 |
| 3 | 0 | 4 | 0 | 0 | 463 | 48 |
| 3 | 0 | 4 | 0 | 1 | 189 | 172 |
| 3 | 0 | 4 | 80 | 0 | 448 | 45 |
| 3 | 0 | 4 | 80 | 1 | 199 | 74 |
| 3 | 0 | 4 | 90 | 0 | 453 | 47 |
| 3 | 0 | 4 | 90 | 1 | 240 | 60 |
| 3 | 10 | 1 | 0 | 0 | 1.41374441607731E+90 | 44 |
| 3 | 10 | 1 | 0 | 1 | 212 | 62 |
| 3 | 10 | 1 | 80 | 0 | 1083854 | 37 |
| 3 | 10 | 1 | 80 | 1 | 219 | 60 |
| 3 | 10 | 1 | 90 | 0 | 3.40420221788906E+48 | 633312622368 |
| 3 | 10 | 1 | 90 | 1 | 215 | 61 |
| 3 | 10 | 3 | 0 | 0 | 3.45974604529664E+85 | 37 |
| 3 | 10 | 3 | 0 | 1 | 232 | 62 |
| 3 | 10 | 3 | 80 | 0 | 4.29195739957084E+43 | 36 |
| 3 | 10 | 3 | 80 | 1 | 216 | 59 |
| 3 | 10 | 3 | 90 | 0 | 3.11387913408208E+31 | 38 |
| 3 | 10 | 3 | 90 | 1 | 216 | 62 |
| 3 | 10 | 4 | 0 | 0 | 186 | 172 |
| 3 | 10 | 4 | 0 | 1 | 187 | 172 |
| 3 | 10 | 4 | 80 | 0 | 200 | 78 |
| 3 | 10 | 4 | 80 | 1 | 199 | 81 |
| 3 | 10 | 4 | 90 | 0 | 219 | 65 |
| 3 | 10 | 4 | 90 | 1 | 220 | 65 |

Table 4: No learning metric

| Dataset | Selection | Learning | Sparse | Binary | Un | Ob |
|---------|-----------|----------|--------|--------|------------------------|------------------|
| 1 | 0 | 0 | 80 | 0 | 8.37534530699594e + 25 | 31.2283285940655 |
| 1 | 0 | 0 | 80 | 1 | 169.811589282339 | 67.1314233865849 |
| 1 | 0 | 0 | 90 | 0 | 3.92689474545834e + 27 | 31.2728103401116 |
| 1 | 0 | 0 | 90 | 1 | 8273.9478226901 | 48.2890713851527 |
| 1 | 10 | 0 | 80 | 0 | 188.89398953533 | 54.3337434394667 |
| 1 | 10 | 0 | 80 | 1 | 183.04721606027 | 76.3197172110488 |
| 1 | 10 | 0 | 90 | 0 | 210.232897671081 | 42.0337774719589 |
| 1 | 10 | 0 | 90 | 1 | 192.826607703433 | 52.8589041113998 |
| 2 | 0 | 0 | 80 | 0 | 8.47008277251517e+27 | 28.5544653381159 |
| 2 | 0 | 0 | 80 | 1 | 169.940921002443 | 66.3176891608828 |
| 2 | 0 | 0 | 90 | 0 | 1.03600604652679e + 28 | 27.3782107285531 |
| 2 | 0 | 0 | 90 | 1 | 200.374401628382 | 48.7501166393764 |
| 2 | 10 | 0 | 80 | 0 | 187.517883561345 | 55.1083756739318 |
| 2 | 10 | 0 | 80 | 1 | 179.418694210083 | 77.3653994805961 |
| 2 | 10 | 0 | 90 | 0 | 201.61394698689 | 41.2969962890936 |
| 2 | 10 | 0 | 90 | 1 | 189.715486090034 | 52.7498314968634 |
| 3 | 0 | 0 | 80 | 0 | 5.44110187416378e + 24 | 30.7053754138505 |
| 3 | 0 | 0 | 80 | 1 | 169.641393156147 | 65.4419378958738 |
| 3 | 0 | 0 | 90 | 0 | 1.13717210734559e + 27 | 26.7336754955024 |
| 3 | 0 | 0 | 90 | 1 | 217.120328737184 | 49.6705866635551 |
| 3 | 10 | 0 | 80 | 0 | 190.905175653626 | 54.8149733968542 |
| 3 | 10 | 0 | 80 | 1 | 178.03491250063 | 78.556383990529 |
| 3 | 10 | 0 | 90 | 0 | 208.987455065167 | 42.7130502325773 |
| 3 | 10 | 0 | 90 | 1 | 192.002262018352 | 52.0688875155099 |

Table 5: Random Matrix

| Sparse | Binary | Un | observed |
|--------|--------|----------|----------|
| 0 | 0 | 640.2203 | 34.7778 |
| 0 | 1 | 187.9999 | 172.1380 |
| 90 | 0 | 665.6549 | 33.7123 |
| 90 | 1 | 232.1691 | 60.5835 |

Table 6: Baseline Methods

| Dataset | Selection | Baseline | Unobserved | Observed |
|---------|-----------|----------|------------|----------|
| 1 | 0 | 1 | 199.1077 | 148.6310 |
| 1 | 1 | 1 | 200.7876 | 147.3206 |
| 2 | 0 | 1 | 468.6379 | 79.0458 |
| 2 | 1 | 1 | 480.6175 | 77.9348 |
| 3 | 0 | 1 | 362.6294 | 0 |
| 3 | 1 | 1 | 365.9741 | 0 |
| 1 | 0 | 2 | 200.2997 | 147.5909 |
| 1 | 1 | 2 | 202.8420 | 147.0311 |
| 3 | 0 | 2 | 223.1343 | 5.4357 |
| 3 | 1 | 2 | 216.0443 | 5.4199 |
| 1 | 0 | 3 | 247.0391 | 83 |
| 1 | 1 | 3 | 249.6211 | 82.8922 |
| 3 | 0 | 3 | 245.5798 | 76.6625 |
| 3 | 1 | 3 | 238.2402 | 79.0812 |