S&DS 365 / 665

Intermediate Machine Learning

Discrete Data Graphs and Graph Neural Networks

October 26

A rare lull

- Assignment 3 out; due next Wednesday
- Assignment 4 posted next week

Graphs

- A natural language for describing various data
- Give information about relationships between variables
- Associated with each multivariate distribution

Undirected Graphs

A graph $G = (V, E)$ has vertices V, edges E.

If $X = (X_1, \ldots, X_p)$ is a random variable, we will study graphs where there are p vertices, one for each X_j.

The graph will encode conditional independence relations among the variables.

Undirected graphs

Simplest case:

Here $V = \{X, Y, Z\}$ and $E = \{(X, Y), (Y, Z)\}$.

This encodes the independence relation

$$X \perp\!\!\!\perp Z \mid Y$$

which means that *X and Z are independent conditioned on Y*.

Markov Property

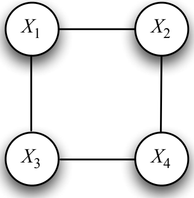
A probability distribution P satisfies the *global Markov property* with respect to a graph G if:

for any disjoint vertex subsets A, B, and C such that C separates A and B,

$$X_A \perp\!\!\!\perp X_B \mid X_C.$$

- X_A are the random variables X_j with $j \in A$.
- C separates A and B means that there is no path from A to B that does not pass through C.

Example

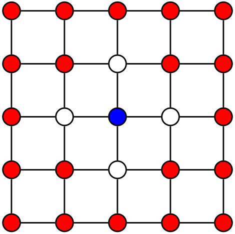


$$X_1 \perp\!\!\!\perp X_4 \mid X_2, X_3$$

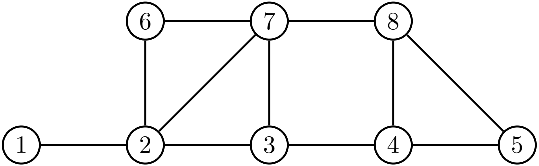
$$X_2 \perp\!\!\!\perp X_3 \mid X_1, X_4$$

Example: 2-dimensional grid

The blue node is independent of the red nodes given the white nodes.



Example



$C = \{3, 7\}$ separates $A = \{1, 2\}$ and $B = \{4, 8\}$. Hence,

$$\{X_1, X_2\} \perp\!\!\!\perp \{X_4, X_8\} \quad \Big| \quad \{X_3, X_7\}$$

Special case

If $(i, j) \notin E$ then

$$X_i \perp\!\!\!\perp X_j \;\middle|\; \{X_k : k \neq i, j\}$$

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Lack of an edge from i to j implies that X_i and X_j are independent given all of the other random variables.

Graph estimation

- A graph G represents the class of distributions, $\mathcal{P}(G)$, the distributions that are Markov with respect to G
- Graph estimation: Given n samples $X_1, \ldots, X_n \sim P$, estimate the graph G.

Factored form

Theorem (Hammersley, Clifford, Besag)

A positive distribution over random variables $Z_1, \ldots, Z_p$ satisfies the Markov properties of graph G if and only if it can be represented as

$$p(Z) \propto \prod_{c \in \mathcal{C}} \psi_c(Z_c)$$

where $\mathcal{C}$ is the set of cliques in the graph G.

Gaussian case

Let $\Omega = \Sigma^{-1}$ be the precision matrix.

A zero in Ω indicates a *lack of the corresponding edge* in the graph

So, the adjacency matrix of the graph is

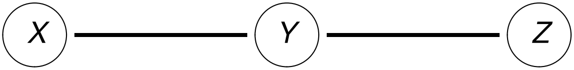
$$A = \big(\mathbb{1}(\Omega_{ij} \neq 0)\big)$$

That is,

$$A_{ij} = \begin{cases} 1 & \text{if } |\Omega_{ij}| > 0 \\ 0 & \text{otherwise} \end{cases}$$

Gaussian case

$$\Omega \equiv \Sigma^{-1} = \begin{pmatrix} * & * & 0 \\ * & * & * \\ 0 & * & * \end{pmatrix}$$



Gaussian case

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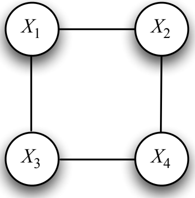

$$X_1 \perp\!\!\!\perp X_4 \mid X_2, X_3$$

Gaussian case: Algorithms

Two approaches:

- parallel lasso
- graphical lasso

Parallel Lasso:

1. For each $j = 1, \ldots, p$ (in parallel): Regress X_j on all other variables using the lasso.
2. Put an edge between X_i and X_j if each appears in the regression of the other.

Graphical Lasso (glasso)

- Assume a multivariate Gaussian model
- Subtract out the sample mean
- Minimize the negative log-likelihood of the data, subject to a constraint on the sum of the absolute values of the inverse covariance

Graphical Lasso (glasso)

The glasso optimizes the parameters of $\Omega = \Sigma^{-1}$ by minimizing:

$$\text{trace}(\Omega S_n) - \log|\Omega| + \lambda \sum_{j \neq k} |\Omega_{jk}|$$

where $|\Omega|$ is the determinant and S_n is the sample covariance

$$S_n = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T$$

There is a blockwise gradient descent algorithm to minimize this, using iterative lassos

Discrete Graphical Models

Challenges of handling discrete data:

- Models don't have closed from; can't compute normalizing constant
- Need to use Gibbs sampling, variational inference
- No analogue of the graphical lasso

Discrete Graphical Models

- Positive distributions can be represented by an exponential family,

$$p(Z;\beta) \propto \exp\left(\sum_{c\in\mathcal{C}} \beta_c \phi_c(Z_c)\right)$$

- Special case: Ising Model (discrete Gaussian)

$$p(Z;\beta) \propto \exp\left(\sum_{i\in V} \beta_i Z_i + \sum_{(i,j)\in E} \beta_{ij} Z_i Z_j\right).$$

Discrete Gaussian?

Note that we can write a multivariate Gaussian as follows:

$$p(z) \propto \exp\left(\sum_i \beta_i z_i + \sum_{i,j} \beta_{ij} z_i z_j\right)$$

From edges to cliques

Take $\beta_i \equiv 0$ for simplicity

If we have a triangle (i, j, k) in the graph then the potential function corresponds to

$$\begin{aligned}\psi_{(ijk)}(Z_i, Z_j, Z_k) &= e^{\beta_{ij} Z_i Z_j} \cdot e^{\beta_{jk} Z_j Z_k} \cdot e^{\beta_{ik} Z_i Z_k} \\ &= e^{\beta_{ij} Z_i Z_j + \beta_{jk} Z_j Z_k + \beta_{ik} Z_i Z_k}\end{aligned}$$

Ising

We have a graph with edges E and vertices V. Each node i has a random variable Z_i that can be "up" ($Z_i = 1$) or "down" ($Z_i = 0$)

$$\mathbb{P}_\beta(z_1, \ldots, z_n) \propto \exp\left(\sum_{s \in V} \beta_s z_s + \sum_{(s,t) \in E} \beta_{st} z_s z_t\right)$$

Since $2Z_i - 1 \in \{-1, 1\}$ if $Z_i \in \{0, 1\}$, can re-parameterize in terms of sample space $Z_i = \pm 1$.

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E are the set of edges, V are the vertices. Imagine the Z_i are votes of politicians, and the edges encode the social network of party affiliations

Since $2Z_i - 1 \in \{-1, 1\}$ if $Z_i \in \{0, 1\}$, can re-parameterize in terms of sample space $Z_i = \pm 1$.

Stochastic approximation

Gibbs sampler

Iterate until converged:

1. Choose vertex $s \in V$ at random
2. Sample z_s holding others fixed

$$\theta_s = \text{sigmoid}\left(\beta_s + \sum_{t \in N(s)} \beta_{st} z_t\right)$$

$$Z_s \mid \theta_s \sim \text{Bernoulli}(\theta_s)$$

---

sigmoid$(u) = 1/(1 + e^{-u})$

Deterministic approximation

Mean field variational algorithm

Iterate until converged:

1. Choose vertex $s \in V$ at random
2. Update mean μ_s holding others fixed

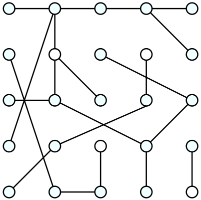
$$\mu_s = \text{sigmoid}\left(\beta_s + \sum_{t \in N(s)} \beta_{st}\, \mu_t\right)$$

---

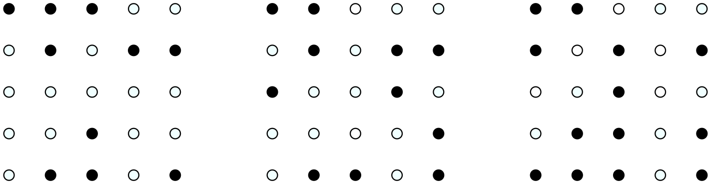
sigmoid$(u) = 1/(1 + e^{-u})$

Graph Estimation

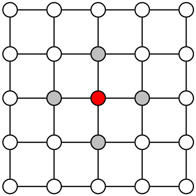
- Given n i.i.d. samples from an Ising distribution, $\{Z_i, i = 1, \ldots, n\}$, (each is a p-vector of $\{0, 1\}$ values) identify underlying graph



- Multiple examples are observed:



Local Distributions



- Consider Ising model $p_\beta(Z) \propto \exp\left(\sum_{i\in V} \beta_i Z_i + \sum_{(i,j)\in E} \beta_{ij} Z_i Z_j\right)$.
- Conditioned on $(z_2, \ldots, z_p)$, variable $Z_1 \in \{0, 1\}$ has probability mass function given by a logistic function,

$$\mathbb{P}(Z_1 = 1 \mid z_2, \ldots, z_p) \quad = \quad \text{sigmoid}\left(\beta_1 + \sum_{j\in\mathcal{N}(1)} \beta_{1j} z_j\right)$$

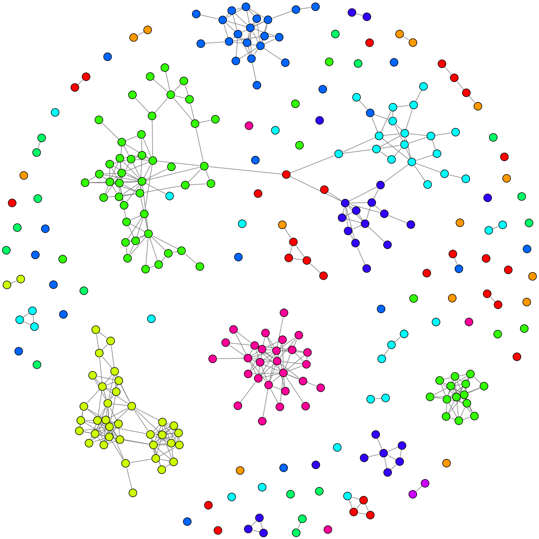
Parallel lasso (sparse logistic regressions)

Strategy

- Perform ℓ_1 regularized logistic regression of each node Z_i on $Z_{\setminus i} = \{Z_j,\ j \neq i\}$ to estimate neighbors $\widehat{\mathcal{N}}(i)$
- Two versions:
  - Create an edge (i, j) if $j \in \widehat{\mathcal{N}}(i)$ *and* $i \in \widehat{\mathcal{N}}(j)$
  - Create an edge (i, j) if $j \in \widehat{\mathcal{N}}(i)$ *or* $i \in \widehat{\mathcal{N}}(j)$

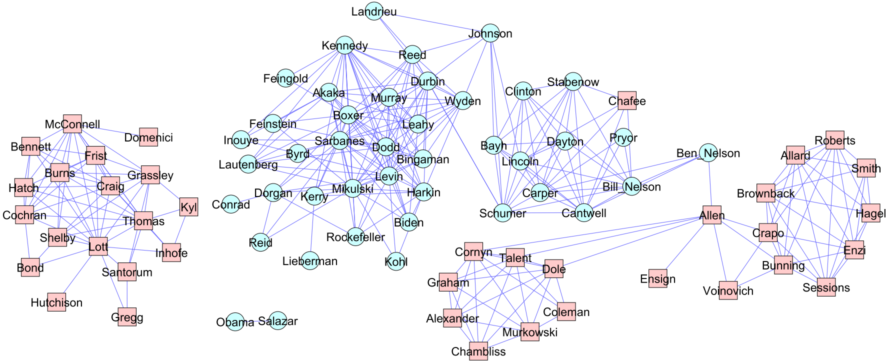
https://www.jstor.org/stable/20744454

S&P 500: Ising Model (Price up or down?)



Voting Data

Voting records of US Senate, 2006-2008



Scaling behavior: Performance with data size

Maximum degree d of the p variables. Sample size n must satisfy

Ising model:	$n \geq d^3 \log p$
Graphical lasso:	$n \geq d^2 \log p$
Parallel lasso:	$n \geq d \log p$
Lower bound:	$n \geq d \log p$

- Each method makes different *incoherence assumptions*:
  - Correlations between unrelated variables not too large

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Summary: Graphs for discrete data

- A positive distribution factors into product of potential functions on the cliques of the graph
- Graphs and independence relations are same for discrete data
- Ising models are discrete Gaussians
- No version of the graphical lasso holds for discrete data; instead, we use the parallel lasso

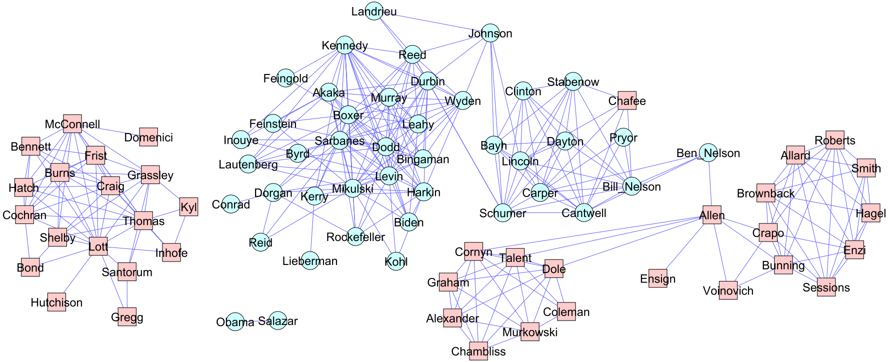
Graph neural networks

Next, we'll discuss graph neural networks, following this article:

`https://distill.pub/2021/understanding-gnns/`

Recall: Voting Data

Voting records of US Senate, 2006-2008

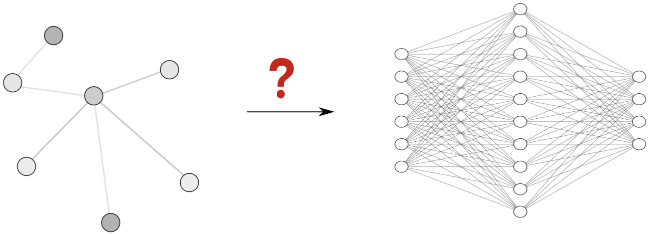


Suppose we have the graph and other covariates for each node or edge.
How can we classify the senators according to political orientation?

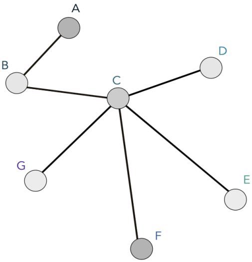
Graph neural networks

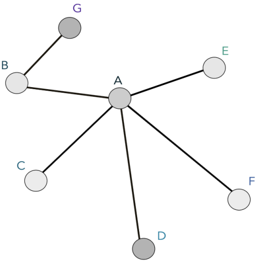
- We'll dicuss how GNNs correspond to CNNs
- The graph Laplacian plays a central role

Equivariance problem

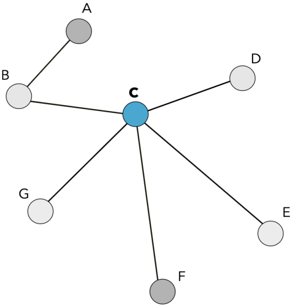


Equivariance problem





Graph Laplacian



Input Graph G

$$
\begin{array}{c}
\\ A \\ B \\ \mathbf{C} \\ D \\ E \\ F \\ G
\end{array}
\begin{array}{c}
\begin{array}{ccccccc} A & B & \mathbf{C} & D & E & F & G \end{array} \\
\begin{bmatrix}
1 & -1 & & & & & \\
-1 & 2 & -1 & & & & \\
 & -1 & 5 & -1 & -1 & -1 & -1 \\
 & & -1 & 1 & & & \\
 & & -1 & & 1 & & \\
 & & -1 & & & 1 & \\
 & & -1 & & & & 1
\end{bmatrix}
\end{array}
$$

Laplacian L of G

Polynomials of the Laplacian

$$p_w(L) = w_0 I_n + w_1 L + w_2 L^2 + \cdots w_d L^d$$

If $\text{dist}(u, v) > i$ then the (u, v) entry of L^i is zero

- This is analogous to a CNN filter (kernel)
- The weights w_i play role of filter coefficients
- Degree d of polynomial plays role of the size of the kernel

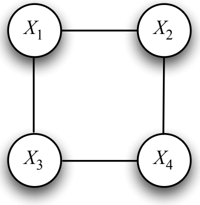
The Laplacian is a Mercer kernel

- Symmetric $L_{uv} = L_{vu}$
- Positive-definite:

$$f^T L f = \sum_{(u,v) \in E} (f_u - f_v)^2 \geq 0$$

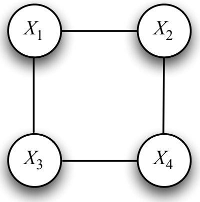
For more on properties of such kernels: https://www.ml.cmu.edu/research/dap-papers/kondor-diffusion-kernels.pdf, https://mlg.eng.cam.ac.uk/zoubin/papers/ssl-book.pdf

Sanity checks



What is the Laplacian L?

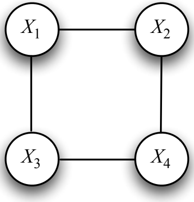
Sanity checks



What is the Laplacian L?

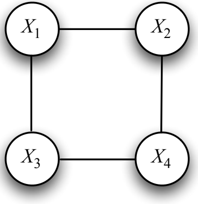
$$L = \begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix}$$

Sanity checks



What is L^2?

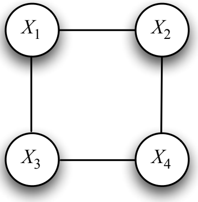
Sanity checks



What is L^2?

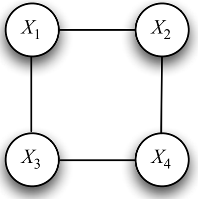
$$L^2 = \begin{pmatrix} 6 & -4 & -4 & 2 \\ -4 & 6 & 2 & -4 \\ -4 & 2 & 6 & -4 \\ 2 & -4 & -4 & 6 \end{pmatrix}$$

Sanity checks



If $x = (1, 2, 3, 4)^T$ what is $h = \text{ReLU}(Lx)$?

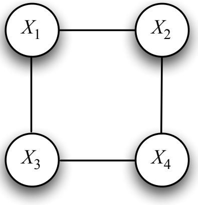
Sanity checks



If $x = (1, 2, 3, 4)^T$ what is $h = \text{ReLU}(Lx)$?

$$\text{ReLU}(Lx) = \text{ReLU}((-3, -1, 1, 3)^T) = (0, 0, 1, 3)^T$$

Sanity checks



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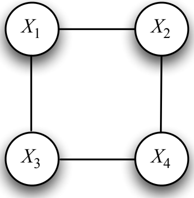

If $x = (1, 2, 3, 4)^T$ what is $x^T L x$?

$$x^T L x = \sum_{(u,v) \in E} (x_u - x_v)^2 = 10$$

Whence equivariance

A transformation $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is equivariant if

$$f(Px) = Pf(x)$$

for any permuation matrix P, where $PP^T = I$.

The transformed data and Laplacian are

$$\begin{aligned} x &\longrightarrow Px \\ L &\longrightarrow PLP^T \\ L^i &\longrightarrow PL^iP^T \end{aligned}$$

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The transformed polynomial kernels are

$$\begin{aligned} f(Px) &= \sum_{i=0}^{d} w_i (PL^i P^T) Px \\ &= \sum_{i=0}^{d} w_i PL^i x \\ &= P \sum_{i=0}^{d} w_i L^i x \\ &= Pf(x) \end{aligned}$$

Building layers

Let $h^{(k)}$ be the neurons at layer k.

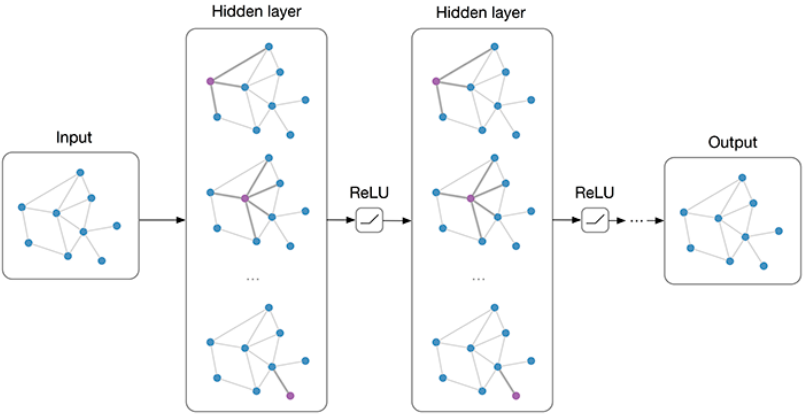
We start with $h^{(0)} = x$, a value x_j at each node j

The next layer is

$$h^{(k+1)} = \varphi\left(p_w(L)h^{(k)}\right)$$

See tutorial for other ways of building layers

Building layers



https://tkipf.github.io/graph-convolutional-networks/

Course ad

CPSC 483: Deep Learning on Graphs

Instructor: Rex Ying

Summary: Graph neural nets

- Certain data have natural graphical structure
- GNNs are analogues of CNNs for graphs
- Based on use of graph Laplacian
- Independent of ordering of nodes (equivariant)

Next topic: Reinforcement learning