Block 10: Inference of network processes

ELEC 573: Network Science and Analytics

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You are here

Wk.	Date	Topic	HW	Project
1	23-Aug	Introduction to course	HW0 out	
2	30-Aug	Graph theory	HW0 solutions posted	
3	6-Sep	LABOR DAY (no class)	HW1 out	
4	13-Sep	Centrality measures / Community detection		
5	20-Sep	Community detection		
6	27-Sep	Signal Processing and Deep learning for graphs	HW1 due	
7	4-Oct	Signal Processing and Deep learning for graphs	HW2 out	
8	11-Oct	FALL BREAK (no class)		
9	18-Oct	Network models	HW2 due	
10	25-Oct	Network models	HW3 out	Project proposal due
11	1-Nov	Inference of network topologies and features		
12	8-Nov	Inference of network topologies and features	HW3 due	
13	15-Nov	Inference of network topologies and features		
14	22-Nov	Epidemics		Project progress report
15	29-Nov	Inference of network processes		
	13-Dec	Project presentation (video recording) and final report due		

Nearest neighbors

Processes on networks

- Motivation: study complex systems of elements and their interactions
  - So far studied graphs as representations of these systems
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  1) Behaviors and beliefs influenced by social interactions
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  3) Spread of epidemics influenced by proximity of individuals
- Can think of these quantities as random processes defined on graphs
  - Static $\{X_i\}_{i \in V}$ and dynamic processes $\{X_i(t)\}_{i \in V}$ for $t \in \mathbb{N}$ or $\mathbb{R}_+$

Nearest-neighbor prediction

- Consider prediction of a static process $\mathbf{X} := \{X_i\}_{i \in V}$ on a graph
    - Process may be truly static, or a snapshot of a dynamic process

Static network process prediction

Predict X_i, given observations of the adjacency matrix $\mathbf{Y} = \mathbf{y}$ and of all attributes $\mathbf{X}^{(-i)} = \mathbf{x}^{(-i)}$ but X_i.

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- Idea: exploit the network structure in $\mathbf{y}$ for prediction

- For binary $X_i \in \{0, 1\}$, say, simple nearest-neighbor method predicts

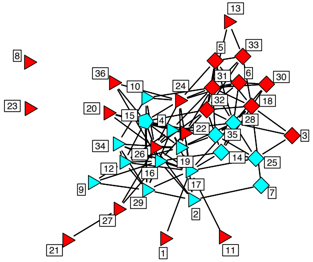
$$\hat{X}_i = \mathbb{I}\left\{ \frac{\sum_{j \in \mathcal{N}_i} x_j}{|\mathcal{N}_i|} > \tau \right\}$$

$\Rightarrow$ Average of the observed process in the neighborhood of i

$\Rightarrow$ Called 'guilt-by-association' or graph-smoothing method

Example: predicting law practice

- Network G^{obs} of working relationships among lawyers [Lazega'01]
  - Nodes are $N_v = 36$ partners, edges indicate partners worked together



- Data includes various node-level attributes $\{X_i\}_{i \in V}$ including
  $\Rightarrow$ Type of practice, i.e., litigation (red) and corporate (cyan)

- Suspect lawyers collaborate more with peers in same legal practice
  $\Rightarrow$ Knowledge of collaboration useful in predicting type of practice

Example: predicting law practice (cont.)

- Q: In predicting practice X_i, how useful is the value of one neighbor?

  $\Rightarrow$ Breakdown of 115 edges based on practice of incident lawyers

	Litigation	**Corporate**
Litigation	29	43
Corporate	43	43

- Looking at the rows in this table
  - Litigation lawyers collaborators are 40% litigation, 60% corporate
  - Collaborations of corporate lawyers are evenly split

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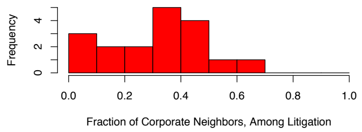
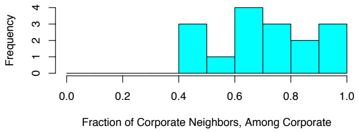
- But 60% (29+43=72) of edges join lawyers with common practice

  ⇒ Suggests on aggregate knowledge of collaboration informative

Example: predicting law practice (cont.)

- Incorporate information of all collaborators as in nearest-neighbors
  - Let $X_i = 0$ if lawyer i practices litigation, and $X_i = 1$ for corporate





- Nearest-neighbor prediction rule

$$\hat{X}_i = \mathbb{I}\left\{ \frac{\sum_{j \in \mathcal{N}_i} x_j}{|\mathcal{N}_i|} > 0.5 \right\}$$

$\Rightarrow$ Infers correctly 13 of the 16 corporate lawyers (i.e., 81%)

$\Rightarrow$ Infers correctly 16 of the 18 litigation lawyers (i.e., 89%)

$\Rightarrow$ Overall error rate is just under 15%

Modeling static network processes

- Nearest-neighbor methods may seem rather informal and simple

  $\Rightarrow$ But competitive with more formal, model-based approaches

- Still, model-based methods have certain potential advantages:

  a) Probabilistically rigorous predictive statements;

  b) Formal inference for model parameters; and

  c) Natural mechanisms for handling missing data

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- Still, model-based methods have certain potential advantages:
  - a) Probabilistically rigorous predictive statements;
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  - c) Natural mechanisms for handling missing data
- Model the process $\mathbf{X} := \{X_i\}_{i \in V}$ given an observed graph $\mathbf{Y} = \mathbf{y}$
  - $\Rightarrow$ Markov random field (MRF) models
  - $\Rightarrow$ Kernel-regression models using graph kernels

Markov random fields

Markov random field models

- Consider a graph $G(V, E)$ with given adjacency matrix $\mathbf{A}$
  - $\Rightarrow$ Collection of discrete RVs $\mathbf{X} = [X_1, \ldots, X_{N_v}]^\top$ defined on V

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$$\mathrm{P}\left[X_i = x_i \,\middle|\, \mathbf{X}^{(-i)} = \mathbf{x}^{(-i)}\right] = \mathrm{P}\left[X_i = x_i \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right], \quad i \in V$$

  - X_i conditionally independent of other X_k, given neighbors values
  - 'Spatial' Markov property, generalizing Markov chains in time
  - G defines neighborhoods $\mathcal{N}_i$, hence dependencies

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- Roots in statistical mechanics, Ising model of ferromagnetism [Ising ’25]

  $\Rightarrow$ MRFs used extensively in spatial statistics and image analysis

MRFs and Gibbs random fields

- MRFs equivalent to Gibbs random fields $\mathbf{X}$, having joint distribution

$$\mathrm{P}\left[\mathbf{X} = \mathbf{x}\right] = \left(\frac{1}{\kappa}\right) \exp\{U(\mathbf{x})\}$$

$\Rightarrow$ Energy function $U(\cdot)$, partition function $\kappa = \sum_{\mathbf{x}} \exp\{U(\mathbf{x})\}$

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- Energy function decomposable over the cliques in G

$$U(\mathbf{x})=\sum_{c\in\mathcal{C}}U_c(\mathbf{x})$$

$\Rightarrow$ Defined clique potentials $U_c(\cdot)$, set $\mathcal{C}$ of cliques in G

- Can show $\mathrm{P}\left[X_i \,\middle|\, \mathbf{X}^{(-i)}\right]$ depends only on cliques involving vertex i

Example: auto-logistic MRFs

- May specify MRFs through choice of clique potentials $U_c(\cdot)$
- Ex: Class of auto models are defined through the constraints:
  (i) Only cliques $c \in \mathcal{C}$ of size one and two have $U_c \neq 0$
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- For binary RVs $X_i \in \{0, 1\}$, the energy function takes the form

$$U(\mathbf{x}) = \sum_{i \in V} \alpha_i x_i + \sum_{(i,j) \in E} \beta_{ij} x_i x_j$$

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- Resulting MRF is known as auto-logistic model, because

$$\mathrm{P}\left[X_i = 1 \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right] = \frac{\exp\{\alpha_i + \sum_{j \in \mathcal{N}_i} \beta_{ij} x_j\}}{1 + \exp\{\alpha_i + \sum_{j \in \mathcal{N}_i} \beta_{ij} x_j\}}$$

$\Rightarrow$ Logistic regression of x_i on its neighboring x_j's

$\Rightarrow$ Ising model a special case, when G is a regular lattice

Homogeneity assumptions

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$$\log\left[\frac{\mathrm{P}\left[X_i = 1 \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right]}{\mathrm{P}\left[X_i = 0 \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right]}\right] = \alpha + \beta \sum_{j \in \mathcal{N}_i} x_j$$

$\Rightarrow$ Linear in the number of neighbors j of i with $X_j = 1$

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- Ex: Specifying $\alpha_i = \alpha + |\mathcal{N}_i|\beta_2$ and $\beta_{ij} = \beta_1 - \beta_2$ yields

$$\log \left[\frac{\mathrm{P}\left[X_i = 1 \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right]}{\mathrm{P}\left[X_i = 0 \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right]} \right] = \alpha + \beta_1 \sum_{j \in \mathcal{N}_i} x_j + \beta_2 \sum_{j \in \mathcal{N}_i} (1 - x_j)$$

$\Rightarrow$ Linear also in the number of neighbors j of i with $X_j = 0$

MRFs for continuous random variables

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- Ex: auto-Gaussian model specifies Gaussian $X_i \,\big|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}$, with

$$\mathbb{E}\left[X_i \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right] = \alpha_i + \sum_{j \in \mathcal{N}_i} \beta_{ij}(x_j - \alpha_j)$$

$$\text{var}\left[X_i \,\middle|\, \mathbf{X}_{\mathcal{N}_i} = \mathbf{x}_{\mathcal{N}_i}\right] = \sigma^2$$

  - $\Rightarrow$ Values X_i modeled as weighted combinations of i's neighbors

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- Let $\boldsymbol{\mu} = [\alpha_1, \ldots, \alpha_{N_v}]^\top$ and $\boldsymbol{\Sigma} = \sigma^2(\mathbf{I} - \mathbf{B})^{-1}$, where $\mathbf{B} = [\beta_{ij}]$
  $\Rightarrow$ Under $\beta_{ii} = 0$ and $\beta_{ij} = \beta_{ji} \to \mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

- Homogeneity assumptions can be imposed, simplifying expressions
  $\Rightarrow$ Further set $\alpha_i = \alpha$ and $\beta_{ij} = \beta \to \mathbf{X} \sim \mathcal{N}(\alpha\mathbf{1}, \sigma^2(\mathbf{I} - \beta\mathbf{A})^{-1})$

Inference and prediction for MRFs

- In studying process $\mathbf{X} = \{X_i\}_{i \in V}$ of interest to predict some or all of $\mathbf{X}$
- MRF models we have seen for this purpose are of the form

$$\mathrm{P}_\theta(\mathbf{X} = \mathbf{x}) = \left(\frac{1}{\kappa(\boldsymbol{\theta})}\right) \exp\{U(\mathbf{x}; \boldsymbol{\theta})\}$$

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- Predictions can be generated based on the distribution $\mathrm{P}_\theta(\cdot)$

$\Rightarrow$ Knowledge of $\boldsymbol{\theta}$ is necessary, and typically $\boldsymbol{\theta}$ is unknown

- Unlike nearest-neighbors prediction, MRFs requires inference of θ first

Inference for MRFs

- Estimation of $\boldsymbol{\theta}$ most naturally approached via maximum-likelihood
- Even though the log-likelihood function takes a simple form

$$\ell(\theta) = \log \mathsf{P}_\theta(\mathbf{X} = \mathbf{x}) = U(\mathbf{x}; \boldsymbol{\theta}) - \log \kappa(\boldsymbol{\theta})$$

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- Popular alternative is maximum pseudo-likelihood, i.e., maximize

$$\sum_{i \in V} \log \mathrm{P}_\theta \left(X_i = x_i \,\middle|\, \mathbf{X}^{(-i)} = \mathbf{x}^{(-i)} \right)$$

$\Rightarrow$ Ignores dependencies beyond the neighborhood of each X_i

$\Rightarrow$ Probabilities depend on clique potentials U_c, not on $\kappa(\boldsymbol{\theta})$

Gibbs sampler

- Given a value of $\boldsymbol{\theta}$, consider predicting some or all of $\mathbf{X}$ from $\mathrm{P}_{\theta}(\cdot)$

  $\Rightarrow$ Computing $\mathrm{P}_{\theta}(\cdot)$ hard, can draw from it using a Gibbs sampler

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- Gibbs sampler exploits $P_\theta\left(X_i \,\middle|\, \mathbf{X}^{(-i)} = \mathbf{x}^{(-i)}\right)$ in simple closed form
  - New value $\mathbf{X}_{(k)}$ obtained from $\mathbf{X}_{(k-1)} = \mathbf{x}_{(k-1)}$ by drawing

$$\begin{aligned} X_{1,(k)} \quad &\text{from} \quad P_\theta\left(X_1 \,\middle|\, \mathbf{X}^{(-1)} = \mathbf{x}^{(-1)}_{(k-1)}\right) \\ &\vdots \\ X_{N_v,(k)} \quad &\text{from} \quad P_\theta\left(X_{N_v} \,\middle|\, \mathbf{X}^{(-N_v)} = \mathbf{x}^{(-N_v)}_{(k-1)}\right) \end{aligned}$$

  $\Rightarrow$ Generated sequence $\mathbf{X}_{(1)}, \mathbf{X}_{(2)}, \ldots$ forms a Markov chain

- Under appropriate conditions, stationary distribution equals $P_\theta(\cdot)$

Prediction with MRFs

- Given large sample from $\mathrm{P}_\theta(\cdot)$, predict $\mathbf{X}$ using empirical distributions
  Ex: for binary $\mathbf{X}$ use empirical marginal frequencies to predict X_i, i.e.,

$$\hat{X}_i = \mathbb{I}\left\{ \frac{1}{n} \sum_{k=m+1}^{m+n} X_{i,(k)} > 0.5 \right\} \quad \text{for large } m, n$$

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- Suppose we observe some elements $\mathbf{X}^{obs} = \mathbf{x}^{obs}$, and wish to predict $\mathbf{X}^{miss}$

  $\Rightarrow$ Draw from the relevant $\mathrm{P}_\theta\left(\mathbf{X}^{miss} \,\middle|\, \mathbf{X}^{obs} = \mathbf{x}^{obs}\right)$ as

$$X_{i,(k)} \quad \text{from} \quad \mathrm{P}_\theta\left(X_i \,\middle|\, \mathbf{X}^{obs} = \mathbf{x}^{obs}, \mathbf{X}^{(-i),miss} = \mathbf{x}^{(-i),miss}_{(k-1)}\right)$$

  $\Rightarrow$ Prediction from empirical distributions analogous

- Prior inference of $\boldsymbol{\theta}$ based on limited data $\mathbf{X}^{obs} = \mathbf{x}^{obs}$ non-trivial

Network of the week (the last one!)

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- Collaborators of Paul Erdős
- Character co-appearance in Les Miserables
- Zachary's karate club
- Blogosphere of US 2014 elections
- C. elegans neuronal connectome
- Internet has no Achilles heel
- Collaboration between network scientists
- Coloring problem on human subjects
- Co-citation network in particle physics
- Ebola epidemics on Africa

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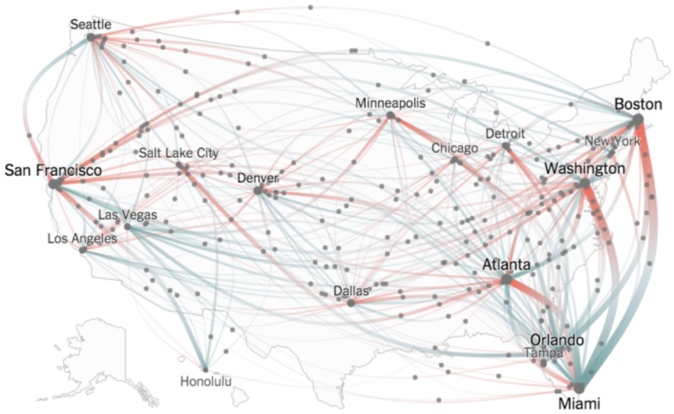

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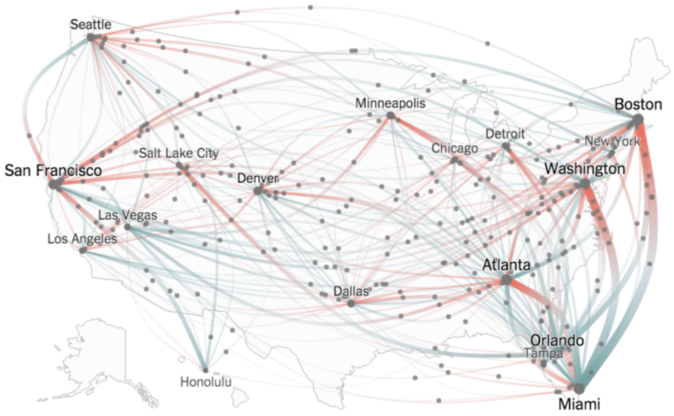
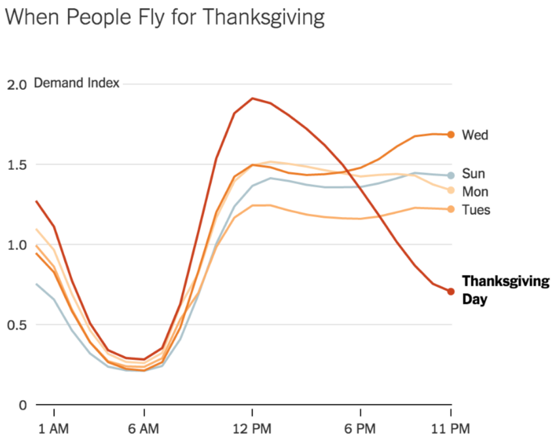


- Additional flight demand (Google flights) for Thanksgiving
- Origins in red and destinations in blue (New York Times, 2015)
- Boston and Seattle vs. Miami and Las Vegas

Network of the week (the last one!)

- Times of flight also tell a story



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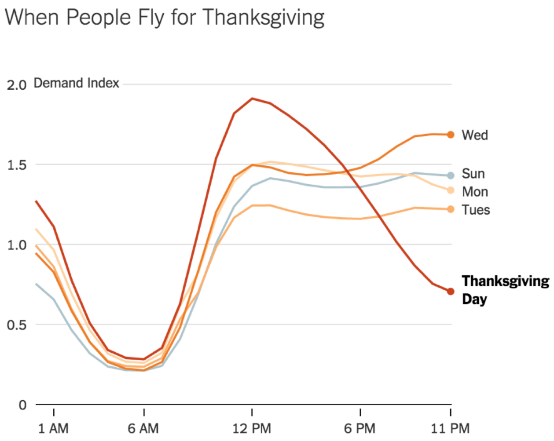

- Take the week off or leave late (Tuesday uncommon)

Kernel-based regression

Kernel methods

- MRFs specify precise dependency structures in $\mathbf{X}$, given the graph G
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- Methods such as LS regression relate data in Euclidean space
- Q2: Can these methods be tuned to accommodate graph-indexed data?

  A2: Yes! Kernel methods consisting of:

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- Key innovation here is the construction of graph kernels

Kernel regression on graphs

- Let $G(V, E)$ be a graph and $\mathbf{X} = \{X_i\}_{i \in V}$ a vertex attribute process
  - $\Rightarrow$ Suppose we observe $X_i = x_i$ for $i \in V^{obs} \subset V$, with $n = |V^{obs}|$

Regression on graphs

Learn $\hat{h} : V \mapsto \mathbb{R}$ describing how attributes vary across vertices.

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- Graph-indexed data not Euclidean $\Rightarrow$ kernel regression methods

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- **Def:** A function $K : V \times V \mapsto \mathbb{R}$ is a called a kernel if for each $m = 1, \ldots, N_v$ and subset of vertices $\{i_1, \ldots, i_m\} \subseteq V$, matrix

  $\mathbf{K}^{(m)} = [K(i_j, i_{j'})] \in \mathbb{R}^{m \times m}$ is symmetric and positive semi-definite

- Think of kernels as functions that produce similarity matrices
  - $\Rightarrow$ Kernel regression builds predictors from such similarities
  - $\Rightarrow$ Need to also decide on the space $\mathcal{H}$ where to search for $\hat{h}$

Reproducing-kernel Hilbert spaces

- Since V is finite, represent functions h on V as vectors $\mathbf{h} \in \mathbb{R}^{N_v}$
  - $\Rightarrow$ Form $\mathbf{K}^{(N_v)} \in \mathbb{R}^{N_v \times N_v}$ by evaluating K in all pairs $(i, j) \in V^{(2)}$
  - $\Rightarrow$ Suppose $\mathbf{K}^{(N_v)}$ admits an eigendecomposition

$$\mathbf{K}^{(N_v)} = \boldsymbol{\Phi}\boldsymbol{\Delta}\boldsymbol{\Phi}^\top$$

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Kernel regression

Given kernel K and data $\mathbf{x}^{obs}$, kernel regression seeks $\hat{\mathbf{h}}$ from the class

$$\mathcal{H}_K = \{\mathbf{h} \in \mathbb{R}^{N_v} : \mathbf{h} = \mathbf{\Phi}\boldsymbol{\beta} \text{ and } \boldsymbol{\beta}^\top \mathbf{\Delta}^{-1}\boldsymbol{\beta} < \infty\}$$

- $\mathcal{H}_K$ is the reproducing-kernel Hilbert space induced by K
  - $\Rightarrow$ Members $\mathbf{h} \in \mathcal{H}_K$ are linear combinations of eigenvectors of $\mathbf{K}^{(N_v)}$
  - $\Rightarrow$ Constrained to finite norm $\|\mathbf{h}\|_{\mathcal{H}} = \|\mathbf{\Phi}\boldsymbol{\beta}\|_{\mathcal{H}} := \boldsymbol{\beta}^\top \mathbf{\Delta}^{-1}\boldsymbol{\beta} < \infty$

Penalized regression in RKHS

- Choose appropriate $\hat{\mathbf{h}} \in \mathcal{H}_K$ using penalized kernel regression
- Q: Appropriate? Data fidelity and small norm (i.e., low complexity)

$$\hat{\mathbf{h}} = \boldsymbol{\Phi}\hat{\beta}, \quad \text{where} \quad \hat{\beta} = \arg\min_{\boldsymbol{\beta}} \left[\sum_{i \in V^{obs}} C(x_i, [\boldsymbol{\Phi}\beta]_i) + \lambda \boldsymbol{\beta}^\top \boldsymbol{\Delta}^{-1} \beta \right]$$

  - Convex loss $C(\cdot, \cdot)$ encourages goodness of fit to $\mathbf{x}^{obs}$
  - The term $\|\mathbf{h}\|_{\mathcal{H}} = \boldsymbol{\beta}^\top \boldsymbol{\Delta}^{-1} \boldsymbol{\beta}$ penalizes excessive complexity
  - Tuning parameter λ trades off data fidelity and complexity

- Generalized ridge-regression with columns of $\boldsymbol{\Phi}$ as predictors

  $\Rightarrow$ Eigenvectors with small eigenvalues penalized more harshly

Representer theorem

- Need to compute the entire $\mathbf{\Phi}$ to find the regression function $\hat{\mathbf{h}}$

  $\Rightarrow$ Complex to evaluate K for all vertex pairs $V^{(2)}$ and find $\mathbf{\Phi}$

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  - $\Rightarrow$ The Representer theorem asserts that $\hat{\mathbf{h}}$ equivalently given by

$$\hat{\mathbf{h}} = \mathbf{K}^{(N_v,n)}\hat{\boldsymbol{\alpha}}, \text{ where } \hat{\boldsymbol{\alpha}} = \arg\min_{\boldsymbol{\alpha}} \left[\sum_{i \in V^{obs}} C(x_i, [\mathbf{K}^{(n)}\boldsymbol{\alpha}]_i) + \lambda \boldsymbol{\alpha}^\top \mathbf{K}^{(n)} \boldsymbol{\alpha} \right]$$

- Just need to evaluate K in $V^{obs} \times V^{obs}$ to form $\mathbf{K}^{(n)}$
  - $\Rightarrow$ Complexity scales with the number of observations n, not N_v

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  - $\Rightarrow$ Complexity scales with the number of observations n, not N_v
- Because $\hat{\mathbf{h}} = \mathbf{K}^{(N_v,n)}\hat{\boldsymbol{\alpha}}$, can predict value in $i \in V^{miss}$ via

$$\hat{h}_i = \sum_{j \in V^{obs}} \hat{\alpha}_j K(i,j)$$

Example: Kernel ridge regression

- Let the X_i be continuous and the loss quadratic, i.e., $C(x, a) = (x - a)^2$
- The optimization problem defining $\hat{\alpha}$ thus specializes to

$$\min_{\boldsymbol{\alpha}} \left[\|\mathbf{x}^{obs} - \mathbf{K}^{(n)}\boldsymbol{\alpha}\|_2^2 + \lambda \boldsymbol{\alpha}^\top \mathbf{K}^{(n)} \boldsymbol{\alpha} \right]$$

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- Define $\boldsymbol{\theta} := (\mathbf{K}^{(n)})^{1/2}\boldsymbol{\alpha}$ and $\mathbf{M} := (\mathbf{K}^{(n)})^{1/2}$. An equivalent problem is

$$\min_{\boldsymbol{\theta}} \left[\|\mathbf{x}^{obs} - \mathbf{M}\boldsymbol{\theta}\|_2^2 + \lambda \boldsymbol{\theta}^\top \boldsymbol{\theta} \right]$$

- Standard ridge regression with solution $\hat{\boldsymbol{\theta}} = (\mathbf{M}^\top \mathbf{M} + \lambda \mathbf{I})^{-1} \mathbf{M}^\top \mathbf{x}^{obs}$

$\Rightarrow$ The kernel regression function is $\hat{\mathbf{h}} = \mathbf{K}^{(N_v, n)} (\mathbf{K}^{(n)})^{-1/2} \hat{\boldsymbol{\theta}}$

Example: Kernel logistic regression

- Let binary $X_i \in \{-1, 1\}$ indicate class membership, for two classes
- A natural choice in this context is the logistic loss, given by

$$C(x, a) = \ln\left(1 + e^{-xa}\right)$$

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- Kernel logistic regression selects $\hat{\boldsymbol{\alpha}}$ via the optimization problem

$$\min_{\boldsymbol{\alpha}} \left[\sum_{i \in V^{obs}} \ln\left(1 + e^{-x_i [\mathbf{K}^{(n)} \boldsymbol{\alpha}]_i}\right) + \lambda \boldsymbol{\alpha}^\top \mathbf{K}^{(n)} \boldsymbol{\alpha} \right]$$

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- Given $\hat{\mathbf{h}} = \mathbf{K}^{(N_v, n)} \hat{\boldsymbol{\alpha}}$, prediction of X_i for $i \in V^{miss}$ based on

$$\hat{\mathrm{P}}\left(X_i = 1 \,\middle|\, \mathbf{X}^{obs} = \mathbf{x}^{obs}\right) = \frac{e^{\hat{h}_i}}{1 + e^{\hat{h}_i}}$$

Designing kernels on graphs

- In designing a kernel K on a graph G, desired properties are:
  - P1) $\mathbf{K}^{(N_v)}$ is symmetric and positive semi-definite
  - P2) K captures suspected similarity among vertices in V
- Presumption: proximity of vertices in G already indicative of similarity

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  $\Rightarrow$ Most kernels proposed are related to the topology of G
- Ex: the Laplacian kernel is $\mathbf{K}^{(N_v)} := \mathbf{L}^{\dagger}$, where † denotes pseudo-inverse
  $\Rightarrow$ Penalty term $\|\mathbf{h}\|_{\mathcal{H}} = \boldsymbol{\beta}^{\top}\boldsymbol{\Delta}^{-1}\boldsymbol{\beta}$ takes the form

$$\begin{aligned}\boldsymbol{\beta}^{\top}\boldsymbol{\Delta}^{-1}\boldsymbol{\beta} &= \boldsymbol{\beta}^{\top}\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi}\boldsymbol{\Delta}^{-1}\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi}\boldsymbol{\beta}\\ &= \mathbf{h}^{\top}\mathbf{K}^{\dagger}\mathbf{h} = \mathbf{h}^{\top}\mathbf{L}\mathbf{h}\\ &= \sum_{(i,j)\in E}(h_i - h_j)^2\end{aligned}$$

- Kernel regression seeks smooth $\hat{\mathbf{h}}$ with respect to the topology of G

Diffusion kernels

- Laplacian kernel $\mathbf{K} = \mathbf{L}^{\dagger}$ encodes similarity among vertices through $\mathbf{A}$

  $\Rightarrow$ Can encode similarity through paths, powers of $\mathbf{A}$ and $\mathbf{L}$

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$$\mathbf{K} = e^{-\zeta \mathbf{L}} := \sum_{m=0}^{\infty} \frac{(-\zeta)^m}{m!} \mathbf{L}^m$$

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- Treating $\mathbf{K}$ as a function of ζ yields the differential equation

$$\frac{\partial \mathbf{K}}{\partial \zeta} = -\mathbf{L}\mathbf{K}$$

  $\Rightarrow$ Parallels the heat equation in physics, motivating its name

Regularized Laplacian kernels

- Let $\mathbf{L} = \mathbf{\Phi}\mathbf{\Gamma}\mathbf{\Phi}^\top$, with $\mathbf{\Gamma} = [\gamma_1, \ldots, \gamma_{N_v}]^\top$ and $\mathbf{\Phi} = [\phi_1, \ldots, \phi_{N_v}]$
- Laplacian and diffusion kernels within class of regularization kernels

$$\mathbf{K} = \sum_{i=1}^{N_v} r^{-1}(\gamma_i)\phi_i\phi_i^\top$$

$\Rightarrow$ **K** is the inverse of the regularized Laplacian $r(\mathbf{L}) := \mathbf{\Phi} r(\mathbf{\Gamma})\mathbf{\Phi}^\top$

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$\Rightarrow$ $\mathbf{K}$ is the inverse of the regularized Laplacian $r(\mathbf{L}) := \mathbf{\Phi} r(\mathbf{\Gamma})\mathbf{\Phi}^\top$

- Regularization function $r(\cdot) \geq 0$ is increasing, including:

  Ex: Identity function $r(\gamma) = \gamma$

  Ex: Exponential function $r(\gamma) = \exp(\zeta\gamma)$

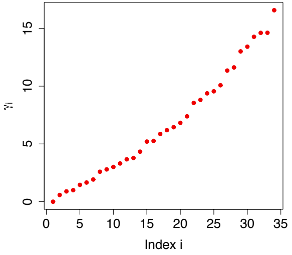
  Ex: Linear inverse function $r(\gamma) = (1 - \frac{\gamma}{\gamma_{\max}})^{-1}$

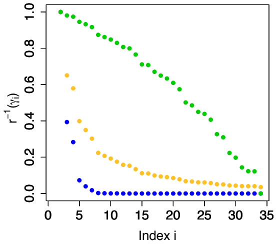
- All $\mathbf{K}$ have identical eigenvectors, just vary the eigenvalues $r^{-1}(\gamma_i)$

  $\Rightarrow$ Same predictors in the kernel regression, different penalty

Example: kernels in the lawyer collaboration graph

- Network of lawyer collaboration, connected component with $N_v = 34$

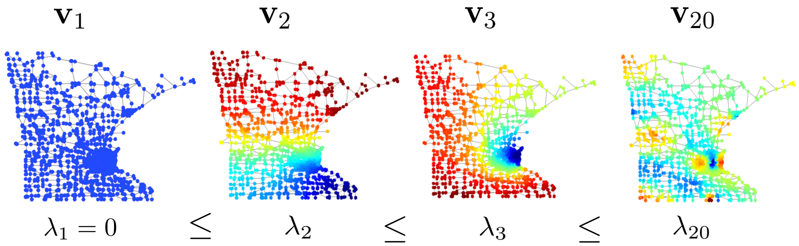




  - Left figure shows eigenvalues $\gamma_1, \ldots, \gamma_{34}$ of $\mathbf{L}$, recall $\gamma_1 = 0$
  - Right figure shows values of $r^{-1}(\gamma_i)$, for $i = 2, \ldots, 34$

- Regularizers: identity, exponential, and linear inverse functions
  - $\Rightarrow$ First two damp most eigenvalues, only few ϕ_i affect $\mathbf{K}$
  - $\Rightarrow$ Small decay in the last, all ϕ_i play a substantial role in $\mathbf{K}$

Visual representation of eigenvectors

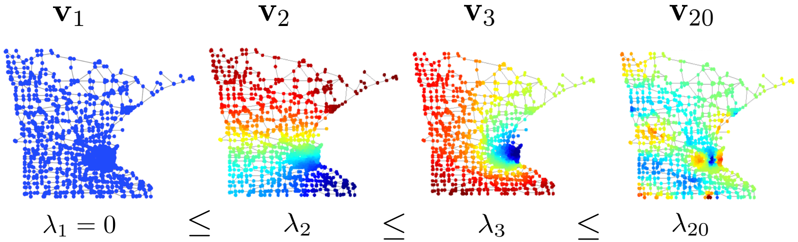

$\mathbf{v}_1$
$\mathbf{v}_2$
$\mathbf{v}_3$
$\mathbf{v}_{20}$
$\lambda_1 = 0 \quad \leq \quad \lambda_2 \quad \leq \quad \lambda_3 \quad \leq \quad \lambda_{20}$

- Early eigenvectors have entries relatively more uniform color

  $\Rightarrow$ Eigenvectors become less ‘smooth’ with increasing eigenvalue

Visual representation of eigenvectors

$$\mathbf{v}_k^T \mathbf{L} \mathbf{v}_k = \sum_{(i,j)\in\mathcal{E}} A_{ij}([\mathbf{v}_k]_i - [\mathbf{v}_k]_j)^2 = \mathrm{TV}(\mathbf{v}_k)$$



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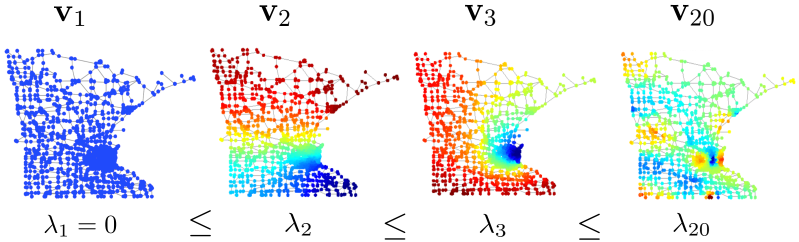

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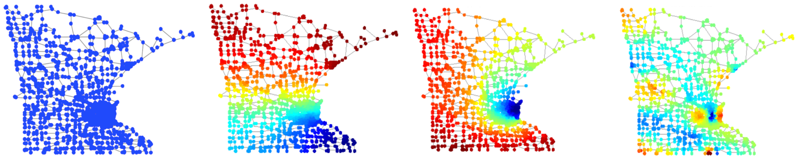

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Case study

Predicting protein function

- Proteins integral to complex biochemical processes within organisms
  $\Rightarrow$ Understanding their function is critical in biology and medicine
- But $\sim$ 70% of genes code for proteins with unknown function
  $\Rightarrow$ Prediction of protein function a task of great importance

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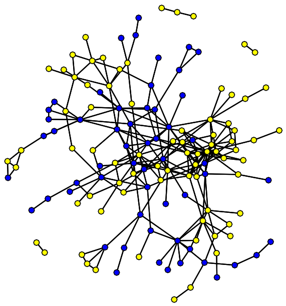
- But $\sim 70\%$ of genes code for proteins with unknown function
  - $\Rightarrow$ Prediction of protein function a task of great importance
- Methodologies explored so far:
  - (i) Traditional experiment-intensive approaches
  - (ii) Methods based on sequence-similarity, protein structure
  - (iii) Network-based methods
- Networks of protein-protein interactions natural in the latter

Protein-protein interaction network

- Baker's yeast data, formally known as *Saccharomyces cerevisiae*
  - Graph: 134 vertices (proteins) and 241 edges (protein interactions)



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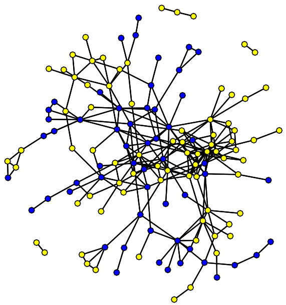


- Predict functional annotation intracellular signaling cascade (ICSC)

  $\Rightarrow$ Signal transduction, how cells react to the environment

- Let $\mathbf{X} = \{X_i\}_{i \in V}$ denote the vertex process of the annotation ICSC
  - $X_i = 1$ if protein i annotated ICSC (yellow), $X_i = 0$ otherwise (blue)

Methods to predict protein function

Method 1: nearest-neighbor (NN) prediction with varying threshold τ

Method 2: MRF with predictors counting nodes with and without ICSC

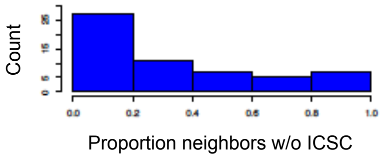
- Parameters $(\alpha, \beta_1, \beta_2)$ estimated via maximum pseudo-likelihood
- Drew 1,000 samples of vertex annotations using a Gibbs sampler
- Predictions based on empirical estimates of $\mathrm{P}\left[X_i = 1 \,\middle|\, \mathbf{X}^{obs} = \mathbf{x}^{obs}\right]$

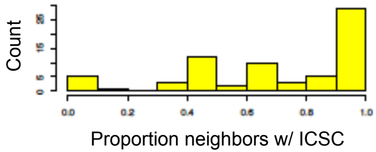
Method 3: kernel logistic regression (KLR) with $\mathbf{K} = \mathbf{L}^{\dagger}$ and $\lambda = 0.01$

- In all cases predictions generated using 10-fold cross validation
  - $\Rightarrow$ 90% of the labels used to train the prediction methods
  - $\Rightarrow$ Remaining 10% used to test obtained predictors

Nearest-neighbor prediction

- Empirical proportions of neighbors with and without ICSC





$\Rightarrow$ Classes less-well separated than for the lawyer data

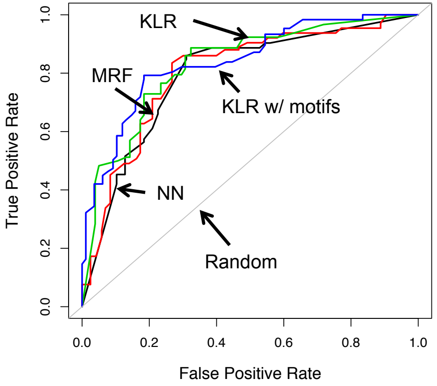
- Recall nearest-neighbor prediction rule for $\tau = 0.5$ is

$$\hat{X}_i = \mathbb{I}\left\{ \frac{\sum_{j \in \mathcal{N}_i} x_j}{|\mathcal{N}_i|} > 0.5 \right\}$$

$\Rightarrow$ Yields a decent missclasification rate of roughly 23%

Receiver operating characteristic

- ROC curves depict predictive performance



- All methods performed comparably. Area under the curve values:

  NN - 0.80, MRF - 0.82, KLR - 0.83, KLR w/motifs - 0.85

Closing remarks

- Not surprising that all three methods performed similarly
  - $\Rightarrow$ NN and MRF use same statistics $\sum_{j \in \mathcal{N}_i} x_j$ and $\sum_{j \in \mathcal{N}_i} (1 - x_j)$
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  - $\Rightarrow$ $\mathbf{L}$ key to many graph partitioning algorithms
- Simple NN prediction comparable to sophisticated classification methods
  - $\Rightarrow$ MRF and kernels flexible to incorporate information beyond G
- Ex: certain DNA sequence motifs useful for function prediction
  - 114 out of 134 proteins associated with one or more of 154 motifs
  - Encode associations in $\mathbf{M} \in \{0, 1\}^{134 \times 154}$, construct kernel $\bar{\mathbf{K}} = \mathbf{M}\mathbf{M}^\top$
  - $\Rightarrow$ Improvement in performance with the combined kernel

$$\mathbf{K} = 0.5 \times \mathbf{L}^\dagger + 0.5 \times \mathbf{M}\mathbf{M}^\top$$

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- We did not go into too much detail within each topic
- Act as trigger for future exploration and inspiration for project
- Feel free to contact me (even after this semester) if you want to discuss