CS 7535 Markov Chain Monte Carlo Methods **Fall 2017**

Lecture 1: August 22

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For an undirected graph $G = (V, E)$, where $n = |V|$ is even, let $\mathcal{P}$ be the set of perfect matchings of G. Can we compute $|\mathcal{P}|$ in poly(n) time? In general, no, but yes in some special situations.

- #P complete for bipartite G. *#P complete is counting analog of NP complete* (next class)
- Poly-time algorithm for planar graphs, using the determinant so $O(n^3)$ time.

Recall that the determinant for an $n \times n$ matrix A is:

$$det\,(A) = \sum_{\sigma \in S_n} sgn\,(\sigma) \prod_{i \in [n]} A\,(i, \sigma\,(i)) \tag{1.1}$$

Where:

- S_n is the set of permutations of $[n] = \{0, 1, \ldots, n-1\}$
- $sgn\,(\sigma) = (-1)^{N(\sigma)}$ for $N\,(\sigma) = \#$ of inversions in σ. $\{i, j : i < j, \sigma\,(j) < \sigma\,(i)\}$

It will be useful to consider some equivalent forms of $sgn\,(\sigma)$:

Let $\sigma = \gamma_1 \ldots \gamma_k$ be its cycle decomposition.

Then:

$$sgn\,(\sigma) = \prod_{i=1}^{k} sgn\,(\gamma_i) \tag{1.2}$$

and

$$sgn\,(\gamma_i) = \begin{cases} -1 \text{ if } |\gamma_i| \text{ is even} \\ 1 \text{ if } |\gamma_i| \text{ is odd} \end{cases} \tag{1.3}$$

Thus

$$sgn\,(\sigma) = (-1)^{[\text{number even cycles in } \sigma]} \tag{1.4}$$

Also, since $sgn(\sigma_i) = (-1)^{|\gamma_i|-1}$ we have:

$$sgn(\sigma) = \prod_i (-1)^{|\gamma_i|-1} = (-1)^{n-k} \tag{1.5}$$

Where $n-k$ is the number of cycles in σ.

We are going to orient the edges of undirected G to make a directed graph $\vec{G}$. An orientation is a mapping of undirected edges to directed. For each edge $(i,j) \in E$ we replace it by $i\vec{j}$ or $j\vec{i}$. The original undirected graph is $G = (V, E)$ and the new directed graph is $\vec{G} = (V, \vec{E})$. Let A be the adjacency matrix of G and we'll use $\vec{A}$ for the skew symmetric adjacency matrix of $\vec{G}$:

$$\vec{A}(i,j) = \begin{cases} 1 \text{ if } i\vec{j} \in E \\ -1 \text{ if } j\vec{i} \in E \\ 0 \text{ if } (i,j) \notin E \end{cases} \tag{1.6}$$

We'll show the determinant of the adjacency matrix equals the square of the number of perfect matchings in G. To do this, we'll exploit even cycles and pfaffians:

Definition: an even cycle C in graph G, is oddly oriented in $\vec{G}$ if there are an odd number of edges opposite to traversal. *Doesn't matter which way you go around, every even length cycle can only be split even / even or odd / odd.*

Definition: A directed graph $\vec{G}$ is Pfaffian if $\forall P, P' \in \mathcal{P}$, all cycles in $P \cup P'$ are oddly oriented. *Union of two perfect matchings contains only even cycles and single edges.*

Theorem: for a pfaffian $\vec{G}$, its corresponding matrix A has determinant: $det(A) = |\mathcal{P}|^2$

1.1 How to find a pfaffian $\vec{G}$ for a planar graph G

Lemma: For a planar G, we can construct a pfaffian orientation $\vec{G}$ in poly-time. *Not only does G have to be planar, we also need embedding (actual drawing of it in plane).*

Proof Overview

1. Make an orientation $\vec{G}$ where every face, except possibly outer face, has an odd number of clockwise edges.

2. Prove orientation is pfaffian

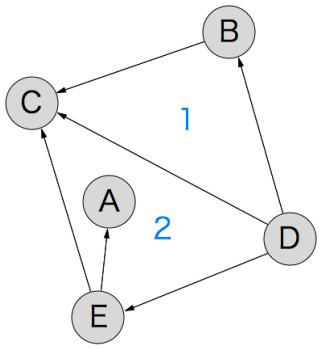


Figure 1.1: Simple directed graph. A, B, C, D, E are vertices, 1 and 2 are faces.

1.2 Clockwise / Counterclockwise

Edge $\vec{DC}$ is clockwise with respect to face 1, and counter clockwise with respect to face 2 in Fig. 1.1. Look at the face, and see what direction the edge goes around the face. Compare to clock.

Dangling Edges: $\vec{EA}$ is a bit ambiguous in terms of clockwise-ness. Classification of these edges doesn't matter, as long as the classification is consistent. We proposed a system in class: perform the dot product: $\left(\text{destination}_{xy} - \text{origin}_{xy}\right) \cdot \left(\text{face center}_{xy} - \text{origin}_{xy}\right)$, where:

- destination_{xy} is the *2d coordinates* of the destination vertex of the edge in the planar embedding
- origin_{xy} is the *2d coordinates* of the origin vertex of the edge in the planar embedding
- face center_{xy} is the mean of the *2d coordinates* of all vertices on face border.

If the dot product is ≥ 0, the face is clockwise. Again, this is arbitrary, and any consistent labeling system will work.

1.3 Constructing Orientation $\vec{G}$

Every face (except outer face) must have odd number of clockwise edges. A very simple algorithm to do this is outlined below. This algorithm takes in an undirected graph G, and returns a directed graph $\vec{G}$.

find_pfaffian(G)

if G has no edges:
    return empty digraph
end

pick $e \in E(G)$ on the outer face

recursively orient $G - e$

if G and $G - e$ have the same number of faces:
    orient e arbitrarily
else
    orient e such that the new face of G is oddly oriented
end

This algorithm recursively removes edges **on the outer face of the graph** until the graph contains no edges. Then, it adds those edges back in (with an orientation) one by one. There are two types of edges to add:

- Edges that do not create a new face: because there are no new faces this addition is unconstrained, the condition that *every face (except outer face) must have odd number of clockwise edges* is satisfied by any orientation.
- Edges that do create a new face: the new face must satisfy the condition that *every face (except outer face) must have odd number of clockwise edges*. Not counting the edge to be added, the new internal face either has an even or an odd number of clockwise edges. If it has an even number, the add the edge in clockwise orientation. If it has an odd number, add the edge in counter clockwise orientation.

By removing edges **on the outer face of the graph** first, the algorithm ensures that when adding edges back in, a new edge splits the outer face (and not any internal face) into two new sections. This is important because the constraint ignores the outer face, and leaves us with only one condition to satisfy (odd # of clockwise edges on new internal face). If the algorithm allowed a new edge to split an internal face into two new internal faces, the algorithm would breakdown if each internal face required a different orientation from the new edge to satisfy the constraint.

Rather than running the algorithm recursively until there are no edges left, it can be seeded with a MST. The MST will have no cycles, i.e. one face (the outer face), therefore any assignment of orientations for edges on the MST satisfies the *every face (except outer face) must have odd number of clockwise edges* constraint.

1.4 Proof that Orientation $\vec{G}$ is Pfaffian

Take a cycle C in $\vec{G}$. Look at the induced subgraph on C, including all edges and vertices on or inside C.

- Let $E_{on}^{clock}(C) = \#$ of clockwise edges on C
- Let $F = \#$ of non-outer faces in this subgraph
- Let $f_1, f_2, f_F = \#$ be theses outer faces

- Let $E_{on}(C), V_{on}(C) = \#$ of edges and vertices on C
- Let $E_{in}(C), V_{in}(C) = \#$ of other edges and vertices, inside C
- Let $E_{on}^{clock}(f_i) = \#$ of clockwise edges on the boundary of f_i

Start with Euler's formula (n, m, f, count vertices, edges, faces, resp.)

$$n - m + f = 2 \tag{1.7}$$

Simplify: $f = F$ *(internal faces)* $+1$ *(outer face)*

$$(V_{on} + V_{in}) - (E_{on} + E_{in}) + (F + 1) = 2 \tag{1.8}$$

C is a cycle so $V_{on} = E_{on}$

$$V_{in} - E_{in} + F = 1 \tag{1.9}$$

Our construction of G guarantees an odd number of clockwise edge on each internal face, that is:

$$\forall i, E_{on}^{clock}(f_i) \equiv 1 \mod 2 \tag{1.10}$$

Thus,

$$\sum_{i=1}^{F} E_{on}^{clock}(f_i) \equiv F \mod 2 \tag{1.11}$$

Observe:

- $E_{in}(C)$: each edge inside C is clockwise on exactly 1 non-outer face.
- $E_{on}^{clock}(C)$: each clockwise edge on C is clockwise on exactly 1 non-outer face.

Thus,

$$\sum_{i=1}^{F} E_{on}^{clock}(f_i) = E_{in} + E_{on}^{clock}(C) \tag{1.12}$$

Combine equations 1.11 and 1.13:

$$E_{in} + E_{on}^{clock}(C) \equiv F \mod 2 \tag{1.13}$$

Plugging in equation 1.9 yields:

$$(V_{in} + F - 1) + E_{on}^{clock}(C) \equiv F \mod 2 \tag{1.14}$$

Or simply:

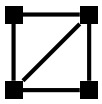
$$V_{in} + E_{on}^{clock}(C) \equiv 1 \mod 2 \tag{1.15}$$

This can be re-written as:

$$E_{on}^{clock}(C) \not\equiv V_{in} \mod 2 \tag{1.16}$$

Take a pair of perfect matchings $P, P' \in \mathcal{P}$: each component of $P \cup P'$ is an even cycle C. Crucially, the vertices interior to C can only match with other—otherwise, G would not be planar. It follows that $|V_{in}|$ is even, and hence $E_{on}^{clock}(C)$ is odd. Thus C is oddly oriented, and since C, P, P' were arbitrary, the orientation is Pfaffian.

A celebrated result of McCuaig, Robertson, Seymour, and Thomas is a poly-time algorithm to decide whether a bipartite graph has a Pfaffian orientation.



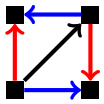


Figure 2.2: Non-Pfaffian orientation.

CS 7535 Markov Chain Monte Carlo Methods **Fall 2017**

Lecture 2: August 24

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Disclaimer: *These notes have not been subjected to the usual scrutiny reserved for formal publications. They may be distributed outside this class only with the permission of the Instructor.*

Let G be an undirected graph with vertex set $[n] := \{0, 1, \ldots, n-1\}$ and $\mathcal{P}$ denote the set of all perfect matchings in G. We would like an an algorithm, polynomial in n, for computing $|\mathcal{P}|$. This is "hard" to compute exactly for general graphs, but attainable when G is *planar*. Last time, we gave an algorithm due to Kasteleyn which takes a plane-embedded graph and outputs a **Pfaffian orientation**—that is, an orientation $\vec{G}$ such that for all $P, P' \in \mathcal{P}$, every (necessarily even) cycle in $P \cup P'$ has an odd number of edges opposite of its traverse sequence (see Figure 2.2.)

Given a Pfaffian orientation $\vec{G}$, consider the $n \times n$ skew-symmetric adjacency matrix defined by

$$\vec{A}[i,j] = \begin{cases} 1 & \text{if} \quad \overrightarrow{ij} \in E(\vec{G}), \\ -1 & \text{if} \quad \overrightarrow{ji} \in E(\vec{G}), \\ 0 & \text{else.} \end{cases}$$

The following theorem, paired with Kastelyn's algorithm and a linear-time planar embedding algorithm, shows that the problem of counting perfect matchings in planar graphs is in **P**.

Theorem 2.1 *If $\vec{G}$ is Pfaffian, then* $\det \vec{A} = |\mathcal{P}|^2$.

Proof: Construct a digraph $D = ([n], A)$, where A consists of each edge in G in either possible orientation. We begin by showing that

$$|\mathcal{E}| = |\mathcal{P}|^2,$$

where $\mathcal{E}$ is the set of even cycle covers in D.[1] Noting the natural ordering on $[n]$, consider the map $f : \mathcal{P} \times \mathcal{P} \to \mathcal{E}$ which takes a pair (P, P') and directs each cycle $C \subset P \cup P'$ starting from the lowest vertex present (say i) to its unique C-neighbor (say j) such that $ij \in P$. To see that f is invertible, fix a cycle cover in $\mathcal{E}$. We may order the edges of any cycle appearing in this cover as $\overrightarrow{i_1 i_2}, \ldots, \overrightarrow{i_L i_1}$ with i_1 minimal—with this ordering scheme, f^{-1} takes our cycle cover to the pair ("odd edges", "even edges") $\in \mathcal{P}$.

We may now evaluate the determinant

$$\det \vec{A} = \sum_{\sigma \in S_n} \operatorname{sgn} \sigma \prod_{i \in n} \vec{A}[i, \sigma(i)]$$

[1] For us an **even cycle cover** of D is a collection of vertex-disjoint directed cycles of even length in D such that each vertex of D is contained in a cycle.

by taking an arbitrary permutation with cycle decomposition $\sigma = \gamma_1 \cdots \gamma_k$ and finding its contribution to the sum by considering cases:

1) If σ has a cycle of odd length, let γ_i denote the leftmost one and define $\sigma' = \gamma_1 \cdots \gamma_{i-1} \gamma_i^{-1} \gamma_{i+1} \cdots \gamma_k$. We have that

$$\operatorname{sgn}\sigma = (-1)^{n-k} = \operatorname{sgn}\sigma' \quad \text{and} \quad \prod_{i\in n} \vec{A}[i,\sigma'(i)] = (-1) \times \prod_{i\in n} \vec{A}[i,\sigma(i)].$$

   Thus, noting $\sigma'' = \sigma$, the total contribution from such σ is zero.

2) For the case where all cycles in σ have even length, the product

$$\prod_{i\in[n]} \vec{A}[i,\sigma(i)] \tag{*}$$

   is nonzero iff the γ_i determine a cycle cover for D. Here, we use the fact that the orientation is Pfaffian. Each directed cycle corresponding to γ_i in turn corresponds to an even cycle formed by the union of two perfect matchings in G—since $\vec{G}$ oddly orients this cycle, we see that each γ_i contributes -1 to the product (*). Now

$$\operatorname{sgn}\sigma \times \prod_{i=1}^{k} \operatorname{contrib}(\gamma_i) = (-1)^{n-k} \times (-1)^k = (-1)^n,$$

   gives a total contribution of $(-1)^n |\mathcal{E}| = |\mathcal{E}|$, the last equality being clear for n even and trivial for n odd, since then $|\mathcal{E}| = 0$.

■

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