Appendix

On Triangular versus Edge Representations — Towards Scalable Modeling of Networks

A Full Mixed-Membership Triangular Model (MMTM)

In the main text, we presented the generative process of our model when the community index triplets are restricted to the case of x < y < z, where x, y, z are the ordered values of the community indices $s_{i,jk}, s_{j,ik}, s_{k,ij}$ belonging to a triangle E_{ijk} . Here, we shall address the remaining cases x = y = z, x = y < z, and x < y = z. Recall that the generative process restricted to x < y < z is:

- Triangle tensor $B_{xyz} \sim \text{Dirichlet}(\lambda)$ for all $x, y, z \in \{1, \dots, K\}$, where x < y < z
- Community admixture vectors $\theta_i \sim \text{Dirichlet}(\alpha)$ for all $i \in \{1, \dots, N\}$
- For each triplet (i, j, k) where i < j < k,
 - Community indices $s_{i,jk} \sim \text{Discrete}(\theta_i), s_{j,ik} \sim \text{Discrete}(\theta_j), s_{k,ij} \sim \text{Discrete}(\theta_k).$
 - Generate the triangular motif E_{ijk} based on $B_{xyz} \in \Delta_3$ and how the values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$ happen to be ordered; see Table 1 for the exact conditional probabilities. There are 6 entries in Table 1, corresponding to the 6 possible orderings of $s_{i,jk}, s_{j,ik}, s_{k,ij}$.

The difficulty with the cases x = y = z, x = y < z, and x < y = z stems from isomorphism in labeled graphs. To understand why, we must take note of the following two points: first, in these 3 cases, some of the community indices are equal and therefore indistinguishable. Second, the 2-triangles Δ_2 are *asymmetric*: the center vertex is not equivalent to the two peripheral vertices (though the peripheral vertices are equivalent to each other). In turn, these points imply that certain 2-triangles that would otherwise be distinct under x < y < z, become indistinguishable under x = y = z, x = y < z, or x < y = z.

To illustrate, consider the 2-triangle whose center vertex has community index x. When x < y < z, the 2-triangle's community structure could look like either y - x - z, or the isomorphism z - x - y (since the peripheral vertices are symmetric). This underscores an important point: we are really interested in generating the equivalence class $\{(y - x - z), (z - x - y)\}$, rather than a specific instance within this class. Notice that such isomorphisms on peripheral vertices are implicitly covered by our triangular representation $E_{ijk} \in \{1, 2, 3, 4\}$, because the 2-triangle cases 1, 2, 3 are defined only by their center vertex. However, if we now suppose that x = y < z, then the equivalence class grows to $\{(y - x - z), (z - x - y), (x - y - z), (z - y - x)\}$, i.e. we cannot distinguish the 2-triangle with x in the center from that with y in the center (because x = y). If we go further and let x = y = z, then the equivalence class grows to encompass all 6 orderings of x, y, z, i.e. $\{(y - x - z), (z - x - y), (x - y - x), (x$

Order	Conditional probability of $E_{ijk} \in \{1, 2, 3, 4\}$
$s_{i,jk} < s_{j,ik} < s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}, B_{xyz,3}, B_{xyz,4}])$
$s_{i,jk} < s_{k,ij} < s_{j,ik}$	$Discrete([B_{xyz,1}, B_{xyz,3}, B_{xyz,2}, B_{xyz,4}])$
$s_{j,ik} < s_{i,jk} < s_{k,ij}$	$Discrete([B_{xyz,2}, B_{xyz,1}, B_{xyz,3}, B_{xyz,4}])$
$s_{j,ik} < s_{k,ij} < s_{i,jk}$	$Discrete([B_{xyz,3}, B_{xyz,1}, B_{xyz,2}, B_{xyz,4}])$
$s_{k,ij} < s_{i,jk} < s_{j,ik}$	$Discrete([B_{xyz,2}, B_{xyz,3}, B_{xyz,1}, B_{xyz,4}])$
$s_{k,ij} < s_{j,ik} < s_{i,jk}$	$Discrete([B_{xyz,3}, B_{xyz,2}, B_{xyz,1}, B_{xyz,4}])$

Table 1: Conditional probabilities of E_{ijk} given $s_{i,jk}, s_{j,ik}$ and $s_{k,ij}$. We define x, y, z to be the ordered (i.e. sorted) values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$. Note that this table applies only to cases where x < y < z.



Figure 1: Graphical model representation for full MMTM, our admixture model over triangular motifs.

Our solution to the isomorphism problem is simple: we first draw a triangle equivalence class for i, j, k. This equivalence class is denoted by C_{ijk} , which is a subset of $\{1, 2, 3, 4\}$. That is to say, C_{ijk} is a set containing the values of E_{ijk} that fall in the equivalence class. Then, we draw a specific triangular motif E_{ijk} uniformly at random from the equivalence class C_{ijk} . The 4 cases are as follows:

- 1. When x < y < z, there are 4 equivalence classes, so we have $B_{xyz} \in \Delta_3$, i.e. the 3-simplex. Here, $B_{xyz,1}$, $B_{xyz,2}$, $B_{xyz,3}$ represent the 2-triangle probabilities (for triangles centered on x, y, z respectively), and $B_{xyz,4}$ represents the full-triangle probability.
- 2. When x = y < z, it turns out there are only 3 equivalence classes, so $B_{xyz} \in \Delta_2$. Now, $B_{xyz,1}, B_{xyz,2}$ represent the 2-triangle probabilities (for triangles centered on x = y and z respectively), and $B_{xyz,3}$ represents the full-triangle probability.
- 3. The case x < y = z is almost identical to x = y < z. The only difference is that $B_{xyz,1}$ represents the 2-triangle probability for triangles centered on x, and $B_{xyz,2}$ represents the 2-triangle probability for triangles centered on y = z.
- 4. Finally, when x = y = z, there are only 2 equivalence classes, and $B_{xyz} \in \Delta_1$. Here, $B_{xyz,1}$ represents the probability of generating a 2-triangle (regardless of the center vertex's community), and $B_{xyz,2}$ represents the full-triangle probability.

With the structure of B_{xyz} in mind, our full generative model over triangular motifs is as follows; see Figure 1 for a graphical model representation.

- Triangle tensor elements B_{xyz} , where $x, y, z \in \{1, ..., K\}$ and $x \leq y \leq z$. All the Dirichlet distributions are symmetric, so we only need one scalar parameter λ .
 - When x < y < z, draw $B_{xyz} \in \Delta_3$ according to $B_{xyz} \sim \text{Dirichlet}(\lambda)$
 - When x = y < z, draw $B_{xyz} \in \Delta_2$ according to $B_{xyz} \sim \text{Dirichlet}(\lambda)$
 - When x < y = z, draw $B_{xyz} \in \Delta_2$ according to $B_{xyz} \sim \text{Dirichlet}(\lambda)$
 - When x = y = z, draw $B_{xyz} \in \Delta_1$ according to $B_{xyz} \sim \text{Dirichlet}(\lambda)$ (equivalent to $\text{Beta}(\lambda, \lambda)$)
- Community admixture vectors $\theta_i \sim \text{Dirichlet}(\alpha)$ for all $i \in \{1, \dots, N\}$
- For each triplet (i, j, k) where i < j < k,
 - Community indices $s_{i,jk} \sim \text{Discrete}(\theta_i), s_{j,ik} \sim \text{Discrete}(\theta_j), s_{k,ij} \sim \text{Discrete}(\theta_k).$
 - Generate the triangle equivalence class C_{ijk} based on B_{xyz} and how the values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$ happen to be ordered; see Table 2 for the exact conditional probabilities. There are 13 entries in Table 2.
 - Generate the triangular motif $E_{ijk} \in C_{ijk}$: draw E_{ijk} uniformly at random from the set of elements in C_{ijk} . In the case where all three community indices $s_{i,jk}, s_{j,ik}, s_{k,ij}$ are distinct, each equivalence class C_{ijk} is a singleton, and the corresponding generative process is consistent with the description in the main text.

Order	Conditional probability distribution over classes C_{ijk}	Possible classes C_{ijk} (each being a set of E_{ijk} values)
$s_{i,jk} < s_{j,ik} < s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}, B_{xyz,3}, B_{xyz,4}])$	$\{1\},\{2\},\{3\},\{4\}$
$s_{i,jk} < s_{k,ij} < s_{j,ik}$		$\{1\},\{3\},\{2\},\{4\}$
$s_{j,ik} < s_{i,jk} < s_{k,ij}$		$\{2\},\{1\},\{3\},\{4\}$
$s_{j,ik} < s_{k,ij} < s_{i,jk}$		$\{2\},\{3\},\{1\},\{4\}$
$s_{k,ij} < s_{i,jk} < s_{j,ik}$		$\{3\},\{1\},\{2\},\{4\}$
$s_{k,ij} < s_{j,ik} < s_{i,jk}$		$\{3\},\{2\},\{1\},\{4\}$
$s_{i,jk} = s_{j,ik} < s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}, B_{xyz,3}])$	$\{1,2\},\{3\},\{4\}$
$s_{i,jk} = s_{k,ij} < s_{j,ik}$		$\{1,3\},\{2\},\{4\}$
$s_{j,ik} = s_{k,ij} < s_{i,jk}$		$\{2,3\},\{1\},\{4\}$
$s_{i,jk} < s_{j,ik} = s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}, B_{xyz,3}])$	$\{1\}, \{2,3\}, \{4\}$
$s_{j,ik} < s_{i,jk} = s_{k,ij}$		$\{2\}, \{1,3\}, \{4\}$
$s_{k,ij} < s_{i,jk} = s_{j,ik}$		$\{3\},\{1,2\},\{4\}$
$s_{i,jk} = s_{j,ik} = s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}])$	$\{1, 2, 3\}, \{4\}$

Table 2: Full table of conditional probabilities of C_{ijk} given $s_{i,jk}, s_{j,ik}$ and $s_{k,ij}$. We define x, y, z to be the ordered (i.e. sorted) values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$. This table is structured differently from Table 1: within each row, for each element of the discrete distribution (which is the probability for some equivalence class C_{ijk}), we give the value of the corresponding equivalence class C_{ijk} (which is a set of elements $E_{ijk} \in \{1, 2, 3, 4\}$). For example, suppose that $s_{i,jk} = s_{j,ik} < s_{k,ij}$ and we draw the first element of the discrete distribution (with probability $B_{xyz,1}$), then $C_{ijk} = \{1, 2\}$, i.e. the equivalence class of triangles centered on vertex $i (E_{ijk} = 1)$ or $j (E_{ijk} = 2)$.

B Modeling Community Assumptions via the Conditional Probability Distributions of C_{ijk}

The MMTM, as just described, does not assume communities should have mostly Δ_3 motifs (full triangles) rather than Δ_2 (2-edge triangles). In other words, it does not assume that communities are characterized by a *high clustering coefficient*. Because this assumption is common in network analysis, we show how to modify the MMTM to better match this assumption. Note that all MMTM experiments in the main text make use of this high CC modification.

Our approach to incorporating the high CC assumption is simple: we just modify the distributions $C_{ijk} | s_{i,jk}, s_{j,ik}, s_{k,ij}, B$ (the distribution of triangular equivalence classes given community assignments). The basic idea is to prevent 2-edge triangles Δ_2 from receiving community assignments of the form a - b - a, where the peripheral nodes have the same community a, but the middle node has a different community b. These assignments are undesirable as they put nodes that do not share edges into the same community; by preventing these assignments from occuring, we force the model to choose other assignments such as a - a - b or a - b - c that do not contradict the high clustering coefficient assumption. To implement this idea, we set the generative probability of certain equivalence classes C_{ijk} to zero, which in turn causes the undesirable values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$ to have zero posterior probability. Refer to Table 3 for a full explanation.

In general, the $C_{ijk} | s_{i,jk}, s_{j,ik}, s_{k,ij}, B$ table can be modified to suit other kinds of community assumptions. Importantly, we are not restricted to merely preventing specific classes C_{ijk} from being generated, rather, we are free to place *any* discrete distribution over the possible C_{ijk} 's. For the aforementioned high CC assumption, we simply used distributions that gave certain classes C_{ijk} zero probability.

C Gibbs Sampler Inference Equations

We adopt a collapsed, blocked Gibbs sampling approach, where θ , B and C have been integrated out. Thus, only the community indices s need to be sampled. For each triplet (i, j, k) where i < j < k,

$$\mathbb{P}\left(s_{i,jk}, s_{j,ik}, s_{k,ij} \mid \mathbf{s}_{-ijk}, \mathbf{E}, \alpha, \lambda\right) \propto \mathbb{P}\left(E_{ijk} \mid \mathbf{E}_{-ijk}, \mathbf{s}, \lambda\right) \mathbb{P}\left(s_{i,jk} \mid \mathbf{s}_{i,-jk}, \alpha\right) \mathbb{P}\left(s_{j,ik} \mid \mathbf{s}_{j,-ik}, \alpha\right) \mathbb{P}\left(s_{k,ij} \mid \mathbf{s}_{k,-ij}, \alpha\right),$$

where s_{-ijk} is the set of all community memberships except for $s_{i,jk}, s_{j,ik}, s_{k,ij}$, and $s_{i,-jk}$ is the set of all community memberships of vertex i except for $s_{i,jk}$. The last three terms are predictive distributions of a multinomial-Dirichlet model,

Order	Conditional probability distribution over classes C_{ijk}	Possible classes C_{ijk} (each being a set of E_{ijk} values)
$s_{i,jk} < s_{j,ik} < s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}, B_{xyz,3}, B_{xyz,4}])$	$\{1\},\{2\},\{3\},\{4\}$
$s_{i,jk} < s_{k,ij} < s_{j,ik}$		$\{1\},\{3\},\{2\},\{4\}$
$s_{j,ik} < s_{i,jk} < s_{k,ij}$		$\{2\},\{1\},\{3\},\{4\}$
$s_{j,ik} < s_{k,ij} < s_{i,jk}$		$\{2\},\{3\},\{1\},\{4\}$
$s_{k,ij} < s_{i,jk} < s_{j,ik}$		$\{3\},\{1\},\{2\},\{4\}$
$s_{k,ij} < s_{j,ik} < s_{i,jk}$		$\{3\},\{2\},\{1\},\{4\}$
$s_{i,jk} = s_{j,ik} < s_{k,ij}$	NormalizedDiscrete($[B_{xyz,1}, 0, B_{xyz,3}]$)	$\{1,2\},\{3\},\{4\}$
$s_{i,jk} = s_{k,ij} < s_{j,ik}$		$\{1,3\},\{2\},\{4\}$
$s_{j,ik} = s_{k,ij} < s_{i,jk}$		$\{2,3\},\{1\},\{4\}$
$s_{i,jk} < s_{j,ik} = s_{k,ij}$	NormalizedDiscrete($[0, B_{xyz,2}, B_{xyz,3}]$)	$\{1\}, \{2,3\}, \{4\}$
$s_{j,ik} < s_{i,jk} = s_{k,ij}$		$\{2\}, \{1,3\}, \{4\}$
$s_{k,ij} < s_{i,jk} = s_{j,ik}$		$\{3\},\{1,2\},\{4\}$
$s_{i,jk} = s_{j,ik} = s_{k,ij}$	$Discrete([B_{xyz,1}, B_{xyz,2}])$	$\{1, 2, 3\}, \{4\}$

Table 3: Modified table of conditional probabilities of C_{ijk} , incorporating the assumption that communities should have a high clustering coefficient ("high CC" MMTM). Specifically, we set the probability of generating particular values of C_{ijk} to zero whenever exactly two of $s_{i,jk}, s_{j,ik}, s_{k,ij}$ are equal. Refer to the second column of the table for full details; any differences with the "regular" MMTM in Table 2 are highlighted in red. In particular, "NormalizedDiscrete" refers to a discrete distribution that first normalizes its parameters to sum to 1. These changes ensure that the posterior distribution over $s_{i,jk}, s_{j,ik}, s_{k,ij}$ has zero probability mass on "bad" community assignments that do not favor a high within-community clustering coefficient, for example a - b - a on 2-edge motifs Δ_2 .

with the multinomial parameter θ marginalized out:

$$\mathbb{P}(s_{i,jk} \mid \mathbf{s}_{i,-jk}, \alpha) = \frac{\#[\mathbf{s}_{i,-jk} = s_{i,jk}] + \alpha}{\#[\mathbf{s}_{i,-jk}] + K\alpha}.$$

The first term $\mathbb{P}(E_{ijk}|\mathbf{E}_{-ijk}, \mathbf{s}, \lambda)$ is another multinomial-Dirichlet predictive distribution, and its exact form depends on how the values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$ happen to be ordered, as well as whether we are using the "regular" MMTM (Table 2) or the "high clustering coefficient" MMTM (Table 3). All experiments in the main text were performed with the "high CC" MMTM.

C.1 Regular MMTM

Letting x, y, z be the ordered values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$,

1. When x < y < z,

$$\mathbb{P}(E_{ijk}|\mathbf{E}_{-ijk},\mathbf{s},\lambda) = \frac{Q_1f_1 + Q_2f_2 + Q_3f_3 + Q_4f_4 + \lambda}{Q_1 + Q_2 + Q_3 + Q_4 + 4\lambda}$$

where

 $\begin{array}{ll} Q_1 &=& \# \left[\mathbf{E}_{-ijk} \in \{1,2,3\} \text{ with node communities } x,y,z \text{ and center node having community } x \right] \\ Q_2 &=& \# \left[\mathbf{E}_{-ijk} \in \{1,2,3\} \text{ with node communities } x,y,z \text{ and center node having community } y \right] \\ Q_3 &=& \# \left[\mathbf{E}_{-ijk} \in \{1,2,3\} \text{ with node communities } x,y,z \text{ and center node having community } z \right] \\ Q_4 &=& \# \left[\mathbf{E}_{-ijk} = 4 \text{ with node communities } x,y,z \right] \end{array}$

and

$$f_1 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } x]$$

$$f_2 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } y]$$

$$f_3 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } z]$$

$$f_4 = \mathbb{I}[E_{ijk} = 4]$$

2. When x = y < z,

$$\mathbb{P}\left(E_{ijk}|\mathbf{E}_{-ijk},\mathbf{s},\lambda\right) = \frac{\frac{1}{2}(Q_1+\lambda)f_1 + (Q_2+\lambda)f_2 + (Q_3+\lambda)f_3}{Q_1+Q_2+Q_3+3\lambda}$$

where

 $Q_1 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\}$ with node communities x, y, z and center node having community x or y] $Q_2 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\}$ with node communities x, y, z and center node having community z] $Q_3 = \# [\mathbf{E}_{-ijk} = 4$ with node communities x, y, z]

and

 $f_1 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } x \text{ or } y]$ $f_2 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } z]$ $f_3 = \mathbb{I}[E_{ijk} = 4]$

3. When x < y = z,

$$\mathbb{P}\left(E_{ijk}|\mathbf{E}_{-ijk},\mathbf{s},\lambda\right) = \frac{(Q_1+\lambda)f_1 + \frac{1}{2}(Q_2+\lambda)f_2 + (Q_3+\lambda)f_3}{Q_1+Q_2+Q_3+3\lambda}$$

where

 $Q_1 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\} \text{ with node communities } x, y, z \text{ and center node having community } x]$ $Q_2 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\} \text{ with node communities } x, y, z \text{ and center node having community } y \text{ or } z]$ $Q_3 = \# [\mathbf{E}_{-ijk} = 4 \text{ with node communities } x, y, z]$

and

 $f_1 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } x]$ $f_2 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } y \text{ or } z]$ $f_3 = \mathbb{I}[E_{ijk} = 4]$

4. When x = y = z,

$$\mathbb{P}(E_{ijk}|\mathbf{E}_{-ijk},\mathbf{s},\lambda) = \frac{\frac{1}{3}(Q_1+\lambda)f_1 + (Q_2+\lambda)f_2}{Q_1+Q_2+2\lambda}$$

where

$$Q_1 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\} \text{ with node communities } x, y, z]$$
$$Q_2 = \# [\mathbf{E}_{-ijk} = 4 \text{ with node communities } x, y, z]$$

and

$$\begin{array}{rcl} f_1 & = & \mathbb{I}[E_{ijk} \in \{1,2,3\}] \\ f_2 & = & \mathbb{I}[E_{ijk} = 4] \end{array}$$

C.2 High Clustering Coefficient MMTM

Letting x, y, z be the ordered values of $s_{i,jk}, s_{j,ik}, s_{k,ij}$,

- 1. Same as "regular" MMTM.
- 2. When x = y < z,

$$\mathbb{P}\left(E_{ijk}|\mathbf{E}_{-ijk},\mathbf{s},\lambda\right) = \begin{cases} \frac{\frac{1}{2}(Q_1+\lambda)f_1+(Q_3+\lambda)f_3}{Q_1+Q_3+2\lambda} & \text{if } E_{ijk} = 4 \text{ or } E_{ijk} \in \{1,2,3\} \text{ and its center node has community } x \text{ or } y \\ 0 & \text{otherwise (i.e. } E_{ijk} \in \{1,2,3\} \text{ and its center node has community } z) \end{cases}$$

where

 $Q_1 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\}$ with node communities x, y, z and center node having community x or y] $Q_3 = \# [\mathbf{E}_{-ijk} = 4$ with node communities x, y, z]

and

$$f_1 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\} \text{ and its center node has community } x \text{ or } y]$$

 $f_3 = \mathbb{I}[E_{ijk} = 4]$

3. When x < y = z,

$$\mathbb{P}\left(E_{ijk}|\mathbf{E}_{-ijk},\mathbf{s},\lambda\right) = \begin{cases} \frac{\frac{1}{2}(Q_2+\lambda)f_2+(Q_3+\lambda)f_3}{Q_2+Q_3+2\lambda} & \text{if } E_{ijk} = 4 \text{ or } E_{ijk} \in \{1,2,3\} \text{ and its center node has community } y \text{ or } z \in \{1,2,3\} \text{ and its center node has community } x \} \\ 0 & \text{otherwise (i.e. } E_{ijk} \in \{1,2,3\} \text{ and its center node has community } x \} \end{cases}$$

where

 $Q_2 = \# [\mathbf{E}_{-ijk} \in \{1, 2, 3\}$ with node communities x, y, z and center node having community y or z] $Q_3 = \# [\mathbf{E}_{-ijk} = 4$ with node communities x, y, z]

and

 $f_2 = \mathbb{I}[E_{ijk} \in \{1, 2, 3\}$ and its center node has community y or z] $f_3 = \mathbb{I}[E_{ijk} = 4]$

4. Same as "regular" MMTM.