# CLUSTERING IN A GROWING NETWORK: A DYNAMIC EXTENSION OF STOCHASTIC BLOCK MODEL\*

By Zitong Zhang<sup>†,‡,¶</sup>, Shizhe Chen<sup>§,¶</sup>
University of California Davis<sup>¶</sup>

The abstract should summarize the contents of the paper. It should be clear, descriptive, self-explanatory and not longer than 200 words.

#### 1. Introduction.

Topic introduction and motivation.

- Networks arise in many disciplines. [Cite some applied papers.]
- One major topic in network analysis is the study of node classification. [Introduce its application in neuroscience, social science, etc.]
- In this paper, we focus on the problem of clustering cell types of neurons in a developing network. We observe the time of the appearance of edges in the network, and the edges do not disappear once developed. Neurons of the same type have similar active time and connecting patterns.
- While existing dynamic stochastic block models show promising performance on some real datasets, they do not fit our dataset for the following reasons. (i) Most of the dynamic stochastic block models are designed for the snapshots of a network. But in our case, the network is sparse in the sense that there is at most one event (occurrence of an edge) for each pair of neurons. For this reason, one cannot model the snapshots by (dynamic) stochastic block models. (ii) The assumption that all the nodes within the same cluster are statistically equivalent is violated. In our network, neurons only develop edges with their neighbor neurons. So two neurons from the same cluster may connect with two different subsets of neurons from another cluster.
- We address these problems by an extension of the stochastic block model.

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<sup>\*</sup>Footnote to the title with the "thankstext" command.

<sup>†</sup>Some comment

<sup>&</sup>lt;sup>‡</sup>First supporter of the project

<sup>§</sup>Second supporter of the project

## Contribution.

- We integrate the point processes in order to obtain the statistical equivalence of nodes from the same cluster.
- We derive a k-means (or least square) estimator and show its consistency (or the oracle inequality). This is similar to Pensky [10], except that we also incorporate time lag and spatial position which may lower the estimation precision.
- For inference, we (hopefully) propose a convex relaxation method that convexify over both clustering matrix and time lags. We also obtain the proximity condition for this convex relaxation method to recover the global optima. (Convex relaxation can also be adapted to solve the penalized least square problem in Pensky [10].)

#### Related work.

- There are many dynamic extensions of stochastic block model. Yang et al. [14], Xu and Hero [13], Matias and Miele [7], Xu [12] use the Markov chain to model the time-varying connecting probabilities and/or the clustering matrix. EM algorithm or iterative optimization algorithm is commonly used for inference. Pensky [10] proposes a vectorization technique and derives a penalized least square estimator that satisfies an oracle inequality and attains the minimax lower bound for the risk.
- However, these methods are based on snapshots of networks where data are aggregated on some time intervals. Aggregating data will lose much information, and the results can be crucially influenced by the choice of time intervals.
- Matias, Rebafka and Villers [8] address this problem by extending the stochastic block model to recurrent interaction events in continuous time, where the time-varying connecting probabilities are characterized by intensity functions.
- While this model gives reasonable interpretation on some real datasets, it does not guarantee to recover the clusters determined by the connecting pattern of each node. Moreover, the model comes without theoretical guarantees for the estimation precision.
- Convex relaxation methods for community detection have been studied in Li, Chen and Xu [3], Li et al. [4], Peng and Wei [9].
- Degree-corrected model?

# Organization.

# 2. Model.

2.1. Stochastic block model. A set of n nodes  $\Gamma = \{v_1, \dots, v_n\}$  is partitioned into k clusters  $\Gamma_1, \dots, \Gamma_k$ . For simplicity, we use the notation  $i \in \Gamma_l$  to denote that  $v_i \in \Gamma_l$ . The cluster of node  $v_i$  is represented by  $z_i \in \{1, \dots, k\}$ , and the vector of clusters is  $\mathbf{z} = (z_i)_{i=1}^n$ . Define the adjacency matrix  $\mathbf{A} \in \{0, 1\}^{n \times n}$  where  $\mathbf{A}_{i,j} = 1$  if an edge is observed between  $v_i$  and  $v_j$  and  $\mathbf{A}_{i,j} = 0$  otherwise. We set  $\mathbf{A}_{i,i} \equiv 0$  for any  $i = 1, \dots, n$ , and assume that  $\mathbf{A}_{i,j}$ 's are conditionally independent given the cluster vector  $\mathbf{z}$ :

$$\mathbf{A}_{i,j}|z_i = q, z_j = l \stackrel{ind}{\sim} \text{Bernoulli}(\mathbf{C}_{q,l}), \quad i \neq j,$$

where  $\mathbf{C} \in [0,1]^{k \times k}$  denote the connecting probability matrix.

2.2. Dynamic generalization of the stochastic block model. Consider a growing dynamic network where edges appear over time. Assume that the edges will not disappear once constructed, and that the observed point processes  $N_{i,j}(\cdot) \in \{0,1\}$  are independent realizations of intensity functions

$$\lambda_{i,j}(t) = f_{z_i,z_j}(t - \tau_{i,j}) \cdot g(d_{i,j}), \quad t \in [0,T], \quad i,j = 1,\dots, n,$$

where [0,T] is overall time period,  $\tau_{i,j}$  is the time lag of the edge from  $v_i$  to  $v_j$ ,  $d_{i,j}$  is the spatial distance between  $v_i$  and  $v_j$ ,  $f_{z_i,z_j}(\cdot)$  is the connecting intensity function from cluster  $z_i$  to  $z_j$ , and  $g(\cdot)$  is a decreasing function that accounts for the decay of connection as the distance between any pair of nodes increases. Similar to the stochastic block model, we set  $\lambda_{i,i}(\cdot) \equiv 0$  for  $i = 1, \dots, n$ .

The integrated point process  $N_{i,\cdot}(\cdot) := \sum_{j\neq i} N_{i,j}(\cdot)$  can be viewed as a realization of the intensity function  $\lambda_{i,\cdot}(\cdot) = \sum_{j\neq i} \lambda_{i,j}(\cdot)$ . For convenience, we denote  $N_{i,\cdot}(\cdot)$  by  $N_{i}(\cdot)$ , and  $\lambda_{i,\cdot}(\cdot)$  by  $\lambda_{N_{i}}(\cdot)$ .

In many applications, the edge from  $v_i$  to  $v_j$  is determined only by the activity of  $v_i$ . So we may have the following assumption.

Assumption 1.  $\tau_{i,j}$  only depends on  $v_i$ , that is,  $\tau_{i,j} = \tau_i$  for all  $j \neq i, i = 1, \dots, n$ .

With Assumption 1,  $\lambda_{N_i}(\cdot)$  can be written as

$$\lambda_{N_i}(t) = \sum_{l=1}^k \left( f_{z_i,l}(t - \tau_i) \cdot \sum_{j \in \Gamma_l, j \neq i} g(d_{i,j}) \right)$$
$$=: \sum_{l=1}^k f_{z_i,l}(t - \tau_i) \cdot w_{i,l}.$$

Here  $w_{i,l}$  measures the overall distance between node  $v_i$  and cluster  $\Gamma_l$ . For example, if the nodes represent neurons and are clustered by cell types,  $w_{i,l}$  represents the distance between  $v_i$  and its neighbor cells which belong to cell types l. We assume that the cell types are distributed uniformly in the sense that  $w_{i,l}$  and  $w_{j,l}$  are identically distributed for any i,j such that  $z_i = z_j$ . More formally, we have the following assumption.

Assumption 2.  $w_{i,l} = \bar{w}_{z_i,l} + \epsilon_{i,l}$  where  $\{\epsilon_{i,l}\}_{i \in \Gamma_l, l=1,\cdots,k}$  are i.i.d. random variables with mean 0 and variance  $\sigma^2 < \infty$ .

By Assumption 1 and 2,  $\lambda_{N_i}(t) = \lambda_{z_i}(t-\tau_i) + \sum_{l=1}^k f_{z_i,l}(t-\tau_i)\epsilon_{i,l}$  for  $t \in [0,T]$ , where  $\lambda_{z_i}(t) := \sum_{k=1}^l f_{z_i,l}(t) \cdot \bar{w}_{z_i,l}$ .

Minor comments. Let  $\mathbf{F}_{k\times k}=[f_{q,l}(\cdot)]_{q,l\in\{1,\cdots,k\}}, \mathbf{W}_{n\times k}=[w_{i,l}]_{i\in\{1,\cdots,n\},l\in\{1,\cdots,k\}},$   $\mathbf{Z}\in\{0,1\}^{n\times k}$  with  $\mathbf{Z}_{i,l}=1$  if  $z_i=l$  and 0 otherwise. Then

$$\begin{bmatrix} \lambda_{N_1}(\cdot + \tau_1) \\ \vdots \\ \lambda_{N_n}(\cdot + \tau_n) \end{bmatrix} = \operatorname{diag}\left(\mathbf{Z}\mathbf{F}\mathbf{W}^{\top}\right).$$

#### 3. Method.

3.1. k-means objective function. In what follows, we review the k-means objective function in the Euclidean space, and introduce the objective function in our case where the samples are realizations of point processes.

k-means in  $\mathbb{R}^d$ . Let  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$  be an i.i.d. sample from distribution function F. Denote by  $F_n$  the empirical distribution function. The k-means problem is to solve

$$A_n := \underset{A: A \subset \mathbb{R}^d, |A| = k}{\arg \min} W_n(A, F_n) = \underset{A: A \subset \mathbb{R}^d, |A| = k}{\arg \min} \int \underset{a \in A}{\min} \|\mathbf{x}_i - a\|^2 dF_n.$$

There are some theoretical guarantees of k-means. Pollard [11] shows that for a given k,  $A_n \to \bar{A}$  almost surely, where  $\bar{A} = \arg \min_A W(A, F)$  denotes the optimal population cluster centers. Bachem et al. [1] provides a uniform bound with a rate of  $\mathcal{O}\left(n^{-1/2}\right)$  for the deviation between the empirical loss and the expected loss. The bound is uniform in the sense that it holds for any set of k cluster centers.

Note that  $\bar{A}$  is a biased estimator of the true cluster centers (when they are well-defined). For example, if k=2 and  $F(x)=\frac{1}{2}\Phi(x;\mu_1,\sigma_1^2)+\frac{1}{2}\Phi(x;\mu_2,\sigma_2^2)$ 

is a mixture Gaussian distribution, and denote  $X_1 \sim N(\mu_1, \sigma_1^2)$ , then  $\bar{A} = \{a_1, a_2\}$  where  $a_1 = \mathbb{E}[X_1 \mathbf{1}_{X_1 \leq (\mu_1 + \mu_2)/2}] \neq \mu_1$  (and a similar expression for  $a_2$ ).

This problem can be re-formulated as following

(3.1) 
$$\min_{\{\Gamma_l\}_{l=1}^k} \frac{1}{n} \sum_{l=1}^k \sum_{i \in \Gamma_l} \|\mathbf{x}_i - \mathbf{c}_l\|^2,$$

where  $\{\Gamma_l\}_{l=1}^k$  represent the clusters and form a partition of  $\Gamma = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\}$ ,  $\mathbf{c}_l = 1/|\Gamma_l| \cdot \sum_{\mathbf{x}_i \in \Gamma_l} \mathbf{x}_i$  is the sample center of the l-th cluster. For simplicity, we denote  $\mathbf{x}_i \in \Gamma_l$  by  $i \in \Gamma_l$  henceforth. The notation  $\Gamma_l$  is introduced in 2.1 but for a different set of nodes. What is the appropriate way to re-define this notation? We now extend this objective function to the context of point process.

k-means in point processes. By Assumption 1 and 2,  $\lambda_{N_i}(t+\tau_i) \stackrel{d}{=} \lambda_{N_j}(t+\tau_j)$  for any i,j satisfying  $z_i = z_j$ . Thus  $F_{N_i}(t+\tau_i) \stackrel{d}{=} F_{N_j}(t+\tau_j)$  for any i,j satisfying  $z_i = z_j$ , where  $F_{N_i}(t) := \int_0^t \lambda_{N_i}(s) \mathrm{d}s / \int_0^T \lambda_{N_i}(s) \mathrm{d}s$ . So the k-means problem is to solve

(3.2) 
$$\min_{\{\Gamma_l\}_{l=1}^k} \frac{1}{n} \sum_{l=1}^k \left( \min_{\{\tau_i\}_{i \in \Gamma_l}, F_l} \sum_{i \in \Gamma_l} \|F_{N_i}^{obs}(\cdot + \tau_i) - F_l(\cdot)\|_2^2 \right),$$

where  $F_{N_i}^{obs}(t) := 1/N_i([0,T]) \cdot \sum_{j=1}^{N_i([0,T])} \mathbf{1}_{\{t_{N_i,j} \leq t\}}$  is the empirical distribution function of the occurrence time of edges,  $t_{N_i,j}$  is the occurrence time of the j-th edge of  $N_i(\cdot)$ , and  $F_l(t) = \mathbb{E}[F_{N_i}(t+\tau_i)](\forall i \in \Gamma_l)$  is the expected cumulative distribution function of the l-th cluster.

- 3.2. Algorithm. The initialization method and the choice of the number of clusters k will be discussed later, now let us assume the initialization and k are given. To solve the problem (3.2), we iterate between two steps until convergence:
  - Re-cluster step: update the clustering  $\left\{\hat{\Gamma}_l\right\}_{l=1}^k$  based on the distance  $d(F_{N_i}^{obs}, \hat{F}_l)$  defined as

$$d(F_{N_i}^{obs}, \hat{F}_l) = \inf_{\tau \in [0, T]} \left( \int_{-T}^{T} \left| f_{\tau}(t) - g(t) \right|^2 \right)^{1/2},$$

where

(3.3)

$$f_{\tau}(t) = \begin{cases} 0, & t \in [-T, -\tau) \\ F_{N_i}^{obs}(t+\tau), & t \in [-\tau, T-\tau) \\ 1, & t \in [T-\tau, T] \end{cases}, g(t) = \begin{cases} 0, & t \in [-T, 0) \\ \hat{F}_l(t), & t \in [0, T] \end{cases}.$$

# The range of $\tau$ ?

• Re-center step: update the expected cumulative distribution functions  $\{\hat{F}_l\}_{l=1}^k$  using the method in Bigot and Gendre [2].

In the re-cluster step, the distance  $d(F_{N_i}^{obs}, \hat{F}_l)$  for each pair of node i and cluster l is evaluated by solving a (non-convex) optimization problem

$$\hat{\tau}_{i,l} = \underset{\tau \in [0,T]}{\operatorname{arg \, min}} \sum_{|j| \le m} \left| \theta_{i,j} e^{i2\pi j\tau} + \int_{T-\tau}^{T} e^{-i2\pi jt} dt - \gamma_{i,j} \right|^{2}$$

$$= \underset{\tau \in [0,T]}{\operatorname{arg \, min}} \sum_{|j| \le m} \left| \left( \theta_{i,j} + \frac{e^{-i2\pi jT}}{i2\pi j} \right) e^{i2\pi j\tau} - \left( \gamma_{i,j} + \frac{e^{-i2\pi jT}}{i2\pi j} \right) \right|^{2}$$

$$\stackrel{\triangle}{=} \underset{\tau \in [0,T]}{\operatorname{arg \, min}} \sum_{|j| \le m} \left| \theta'_{i,j} e^{i2\pi j\tau} - \gamma'_{i,j} \right|^{2},$$

where  $\theta_{i,j}$  and  $\gamma_{i,j}$ ,  $j \in \mathbb{Z}$ , are the Fourier coefficients of  $F_{N_i}^{obs}$  and  $\hat{F}_l$ , respectively, m is a positive integer which will be specified later. Gradient descent is used to solve problem (3.4) with gradient

(3.5) 
$$\nabla = 4\pi \sum_{|j| < m} j \cdot \operatorname{Im} \left( \theta'_{i,j} \overline{\gamma'_{i,j}} e^{i2\pi j \tau} \right).$$

# Initialization and step size?

In the re-center step, let  $\{\theta_{i,j}\}_{j\in\mathbb{Z}}$  be the Fourier coefficients of  $F_{N_i}^{obs}$  and  $f_{\tau}(t)$  be as defined in (3.3). The Fourier coefficients of  $f_{\tau}(t)$  are

$$\left(\theta_{i,j} + \frac{e^{-i2\pi jT}}{i2\pi j}\right)e^{i2\pi j\tau_i} - \frac{e^{-i2\pi jT}}{i2\pi j} \stackrel{\triangle}{=} \theta'_{i,j}e^{i2\pi j\tau_i} - C.$$

Then  $\{\hat{\tau}_i\}_{i=1}^n$  are obtained by

$$\begin{split} \{\hat{\tau}_i\}_{i \in \Gamma_l} &= \mathop{\arg\min}_{\min\{\tau_i\}_{i \in \Gamma_l} = 0} \frac{1}{|\Gamma_l|} \sum_{i \in \Gamma_l} \sum_{|j| \leq m} \left| \theta'_{i,j} e^{\mathrm{i} 2\pi j \tau_i} - \frac{1}{|\Gamma_l|} \sum_{i' \in \Gamma_l} \theta'_{i',j} e^{\mathrm{i} 2\pi j \tau_{i'}} \right|^2 \\ &\stackrel{\triangle}{=} \mathop{\arg\min}_{\min\{\tau_i\}_{i \in \Gamma_l} = 0} L(\{\tau_i\}_{i \in \Gamma_l}). \end{split}$$

Again, gradient descent is applied with gradients

$$\frac{\partial L}{\partial \tau_i} = \frac{1}{|\Gamma_l|^2} \sum_{|j| \le m} 4\pi j \left( \operatorname{Im} \left( \theta'_{i,j} e^{i2\pi j \tau_i} \cdot \overline{A_j} \right) + \left( \frac{1}{|\Gamma_l|} - 2 \right) \operatorname{Im}(A_j) \cdot 2\operatorname{Re} \left( \theta'_{i,j} e^{i2\pi j \tau_i} \right) \right),$$

where  $A_j = \frac{1}{|\Gamma_l|} \sum_{i \in \Gamma_l} \theta'_{i,j} e^{i2\pi j \tau_i}$ . Therefore, the expected c.d.f. is estimated as the average of shifted empirical distribution functions. Initialization? Step size?

Truncate  $\hat{F}_l$  at zero?

Initialization. We need good initialization of mean curves.

Choosing k. Model selection.

3.3. Convex relaxation of k-means type clustering.

Semidefinite programming relaxation. We briefly introduce a semidefinite programming relaxation (Peng-Wei relaxation) of k-means proposed by Peng and Wei [9]. The k-means objective function in (3.1) can be re-written as

$$\sum_{l=1}^{k} \sum_{i \in \Gamma_l} \|\mathbf{x}_i - \mathbf{c}_l\|^2 = \frac{1}{2} \sum_{l=1}^{k} \frac{1}{|\Gamma_l|} \sum_{i,j \in \Gamma_l} \|\mathbf{x}_i - \mathbf{x}_j\|^2$$
$$= \frac{1}{2} \sum_{l=1}^{k} \frac{1}{|\Gamma_l|} \langle \mathbf{1}_{\Gamma_l} \mathbf{1}_{\Gamma_l}^{\top}, \mathbf{D} \rangle$$

where  $\mathbf{D} \in \mathbb{R}^{n \times n}$  with entries  $\mathbf{D}_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|^2$ . Hence (3.1) can be relaxed to

$$\min_{\mathbf{Z}} \langle \mathbf{Z}, \mathbf{D} \rangle$$
s.t.  $\mathbf{Z} \succeq 0$ ,  $\mathbf{Z} \ge 0$ ,  $\mathbf{Z} \mathbf{1}_n = \mathbf{1}_n$ ,  $\operatorname{Tr}(\mathbf{Z}) = k$ .

Proximity conditions are discussed in 4.3.

In our case, (??) is equivalent to

(3.6) 
$$\min_{\mathbf{Z}, \{\tau_i\}_{i=1}^n} \langle \mathbf{Z}, \mathbf{D}(\tau_1, \cdots, \tau_n) \rangle$$

where  $\mathbf{Z} = 1/2 \cdot \sum_{l=1}^{k} (1/|\Gamma_l| \cdot \mathbf{1}_{\Gamma_l} \mathbf{1}_{\Gamma_l}^{\top}), \ \mathbf{D}_{i,j} = \|\hat{\lambda}_{N_i}(t+\tau_i) - \hat{\lambda}_{N_j}(t+\tau_j)\|_2^2$ . Using Fourier transformation,

$$\mathbf{D}_{i,j} = \int_{0}^{T} \left( \int_{0}^{\infty} \hat{h}_{N_i}(\xi) e^{i2\pi\xi(t+\tau_i)} - \hat{h}_{N_j}(\xi) e^{i2\pi\xi(t+\tau_j)} d\xi \right)^2 dt$$

where  $\hat{h}_{N_i}(\xi)$  is the Fourier transform of  $\hat{\lambda}_{N_i}(t)$ . How to convexify?

# 4. Theory.

4.1. Minimax optimality of the estimator. For the case in (??), denote  $\theta = \left(\{\Gamma_l\}_{l=1}^k, \{\tau_i\}_{i=1}^n, \{\lambda_l\}_{l=1}^k\right)$ , show the convergence rate of

$$\hat{\theta}_n := \operatorname*{arg\,min}_{\{\Gamma_l\}_{l=1}^k, \{\tau_i\}_{i=1}^n, \{\lambda_l\}_{l=1}^k} \frac{1}{n} \sum_{l=1}^k \sum_{i \in \Gamma_l} \|\hat{\lambda}_{N_i}(\cdot + \tau_i) - \lambda_l(\cdot)\|_2^2$$

to

$$\theta_n := \underset{\{\Gamma_l\}_{l=1}^k, \{\tau_i\}_{i=1}^n, \{\lambda_l\}_{l=1}^k}{\arg \min} \frac{1}{n} \sum_{l=1}^k \sum_{i \in \Gamma_l} \|\lambda_{N_i}(\cdot + \tau_i) - \lambda_l(\cdot)\|_2^2.$$

Papers about shape invariant model might be useful.

4.2. Convergence of Lloyd's algorithm using shape invariant model.

Guarantees of Lloyd's algorithm. Lu and Zhou [6] provides a weak initialization condition under which Lloyd's algorithm converges to the optimal label estimators of sub-Gaussian mixture model. Also, see the reference therein.

4.3. Proximity condition of the convex relaxation. See Ling and Strohmer [5], Li et al. [4], Peng and Wei [9], Zhao, Levina and Zhu [15] for theory and proof. Ling and Strohmer [5] proposed a proximity condition under which the convex relaxation of RatioCuts is exactly the global optimal to the original ratio cut problem. The theorem is then applied to spectral clustering (as a special case of graph cuts) to obtain the theoretical guarantees for spectral clustering

Li, Chen and Xu [3] surveys recent theoretical advances in convex optimization approaches for community detection. Li et al. [4] compare different convex relaxations by relating them to corresponding proximity conditions. They present an improved proximity condition under which the relaxation proposed by Peng and Wei [9] recovers the underlying clusters exactly. The proximity condition states that for any  $a \neq b$ , the following holds

$$\min_{i \in \Gamma_a} \left\langle \mathbf{x}_i - \frac{\mathbf{c}_a + \mathbf{c}_b}{2}, \mathbf{w}_{b,a} \right\rangle > \frac{1}{2} \sqrt{\left(\sum_{l=1}^k \left\| \overline{\mathbf{X}}_l \right\|^2\right) \left(\frac{1}{n_a} + \frac{1}{n_b}\right)}$$

where  $\mathbf{w}_{b,a} = \frac{\mathbf{c}_a - \mathbf{c}_b}{\|\mathbf{c}_a - \mathbf{c}_b\|}$  is the unit vector pointing from  $\mathbf{c}_b$  to  $\mathbf{c}_a$ ,  $\overline{\mathbf{X}}_l$  is the centered data matrix of the l-th cluster,  $\|\overline{\mathbf{X}}_l\|$  is the operator norm of  $\overline{\mathbf{X}}_l$ ,

and  $n_a = |\Gamma_a|, n_b = |\Gamma_b|.$ 

Translate into point processes if (3.6) can be convexified.

- 5. Simulation.
- 6. Conclusion.

## APPENDIX A: APPENDIX SECTION

## TO DO:

- 1. Selection of k; initialization.
- 2. Simulation.
- 3. Write introduction, and sketch of proof.
- 4. Basic knowledge about point process (reading).
- 5. Convex relaxation/FPCA (reading).

# **A.1.** Appendix subsection. See Appendix A.

# ACKNOWLEDGEMENTS

See Supplement A for the supplementary material example.

# SUPPLEMENTARY MATERIAL

# Supplement A: Title of the Supplement A

(http://www.e-publications.org/ims/support/dowload/imsart-ims.zip). Dum esset rex in accubitu suo, nardus mea dedit odorem suavitatis. Quoniam confortavit seras portarum tuarum, benedixit filiis tuis in te. Qui posuit fines tuos

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ADDRESS OF THE FIRST AND SECOND AUTHORS USUALLY A FEW LINES LONG

E-MAIL: zztzhang@ucdavis.edu