Clustering-based State Aggregation of Dynamical Networks

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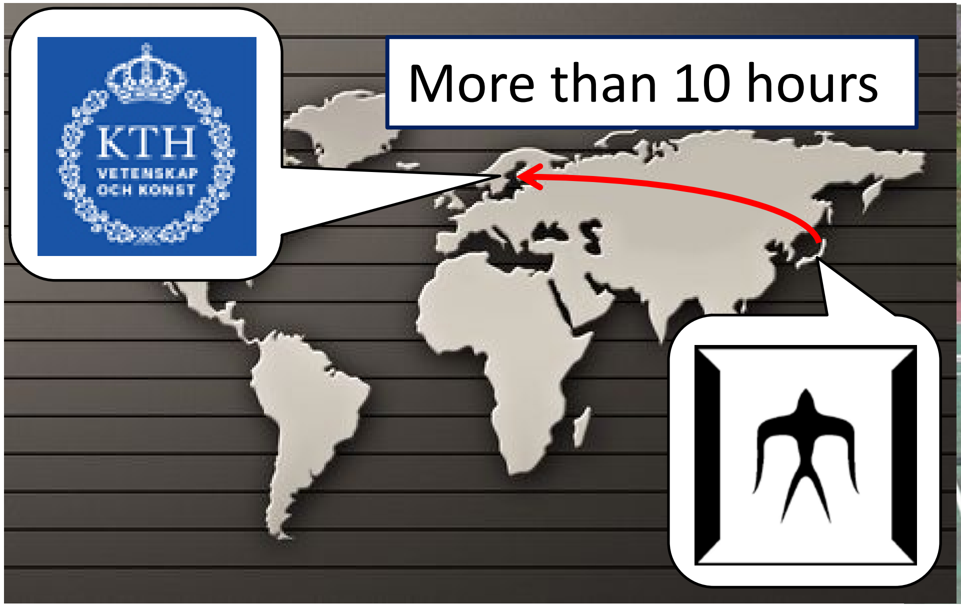
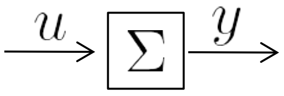


From Tokyo to Stockholm

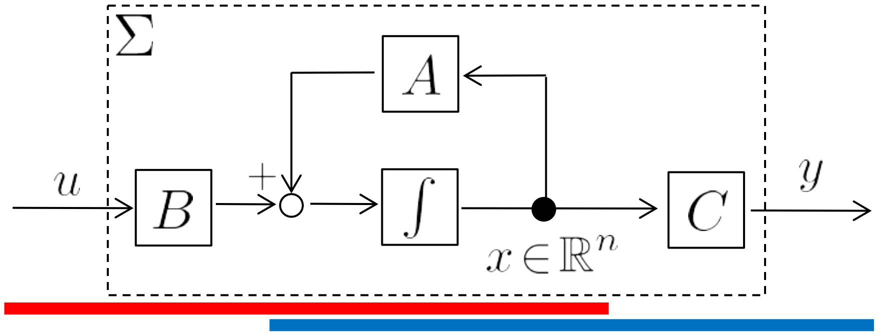
I am (was?) tennis man

Model Reduction via Projection

Given stable system



$$\Sigma : \begin{cases} \dot{x} = Ax + Bu \\ y = Cx \end{cases}$$



input-to-state map

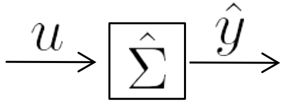
(A, B)

state-to-output map

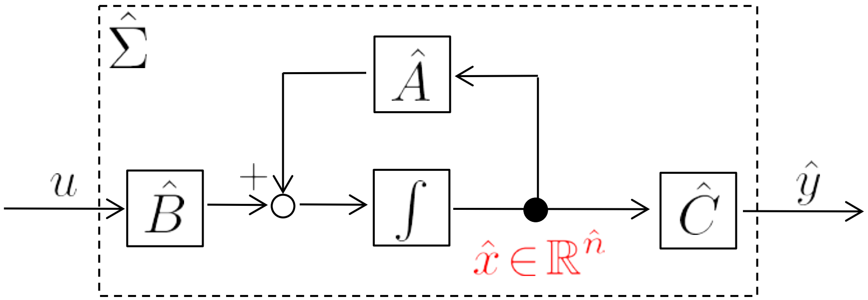
(A, C)

Find

Stable reduced model



$$\hat{\Sigma} : \begin{cases} \dot{\hat{x}} = \hat{A}\hat{x} + \hat{B}u \\ \hat{y} = \hat{C}\hat{x} \end{cases}$$



Dim. of state: $\hat{n} < n$

$Px = \hat{x},\ \ P \in \mathbb{R}^{\hat{n} \times n}$

✓ $PP^\dagger = I_{\hat{n}}$

$$(A, B, C) \longrightarrow (\hat{A}, \hat{B}, \hat{C}) = (PAP^\dagger, PB, CP^\dagger)$$

Find P such that $\|\Sigma - \hat{\Sigma}\|$ is small enough

Typical System Norms

✓ $\mathscr{L}[\cdot]$: Laplace transform
$\|\cdot\|_F$: Frobenius norm

Stable system $\Sigma : \begin{cases} \dot{x} = Ax + Bu \\ y = Cx \end{cases}$

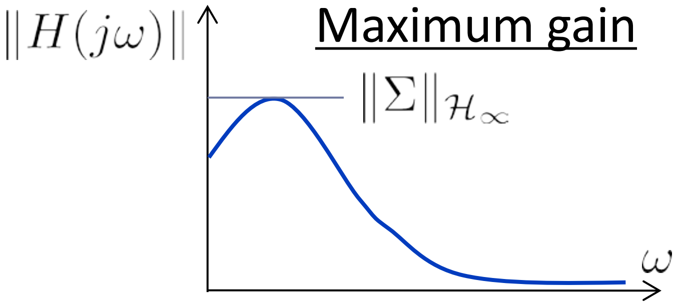
Solution $y(t) = \int_0^t h(t-\tau)u(\tau)d\tau$

Impulse response $h(t) := Ce^{At}B$

Transfer function $H(s) := \mathscr{L}[h] = C(sI_n - A)^{-1}B$

$\mathcal{H}_\infty$-norm

$$\|\Sigma\|_{\mathcal{H}_\infty} = \sup_{u \neq 0} \frac{\|y(t)\|_{\mathcal{L}_2}}{\|u(t)\|_{\mathcal{L}_2}} = \sup_{\omega \in \mathbb{R}} \|H(j\omega)\|$$



Maximum gain

$\mathcal{H}_2$ -norm

$$\|\Sigma\|_{\mathcal{H}_2} = \|h\|_{\mathcal{L}_2} = \left(\int_{-\infty}^{\infty} \|H(j\omega)\|_F^2 \frac{d\omega}{2\pi}\right)^{\frac{1}{2}}$$

Energy of $h(t) = Ce^{At}B$

✓ $\mathcal{L}_2$-norm of $f : \mathbb{R}_+ \to \mathbb{R}^{p \times m}$ $\quad \|f\|_{\mathcal{L}_2} := \left(\int_0^\infty \|f(t)\|_F^2 \, dt\right)^{\frac{1}{2}}$

Contents

- Clustering-based State Aggregation in terms of $\mathcal{H}_\infty$-norm
  - How to reduce systems while preserving network topology?
  - Use of positive tri-diagonalization
  - Application to diffusion process over complex network

- $\mathcal{H}_2$-aggregation of Positive Networks
  - Preservation of network topology as well as positivity
  - Use of controllability gramian
  - Application to Chemical Master Equation

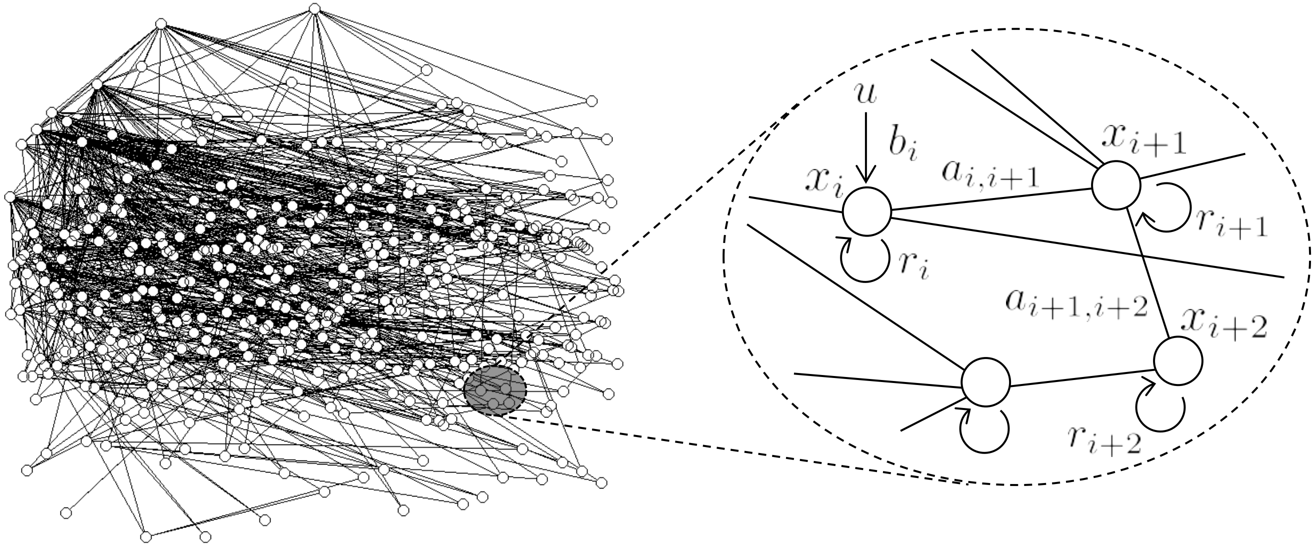
System Description

[Definition] **Bidirectional Network** (A, b)

$\dot{x} = Ax + bu$ with $A = \{a_{i,j}\} \in \mathbb{R}^{n \times n}$ and $b = \{b_i\} \in \mathbb{R}^n$

is said to be *bidirectional network* (A, b) if A is symmetric and stable.

Including reaction-diffusion systems: $\dot{x}_i = -r_i x_i + \sum_{j=1, j \neq i}^{n} a_{i,j} (x_j - x_i) + b_i u$

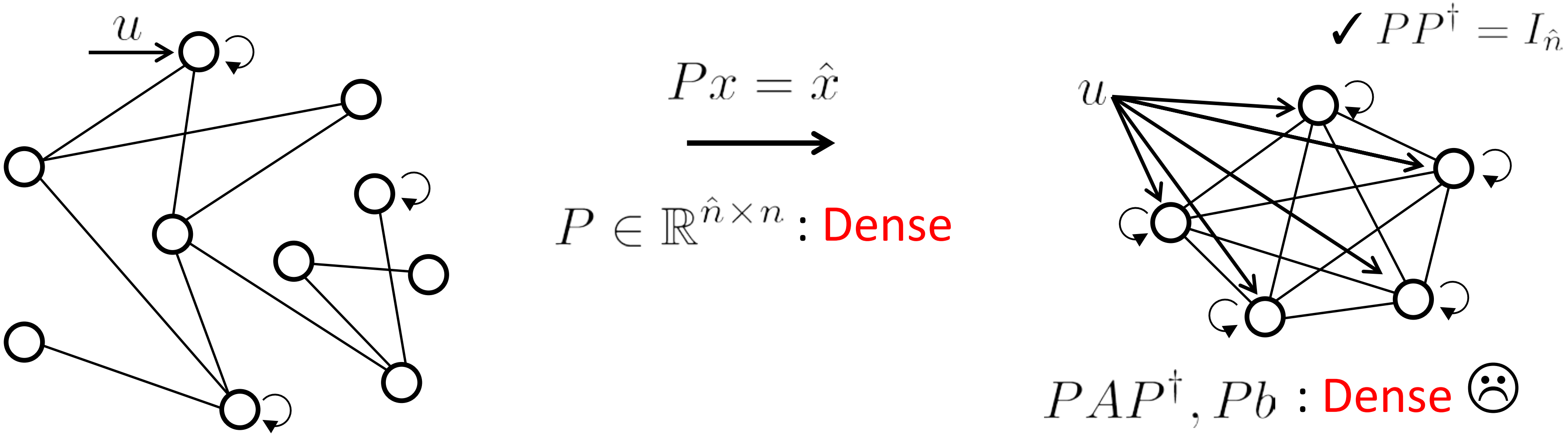


r_i : **reaction** of x_i $a_{i,j} = a_{j,i}$: **diffusion** between x_i and x_j

Traditional Model Reduction

- Traditional model reduction methods
  - Balanced truncation, Krylov projection, Hankel norm approximation
  - No specific structure in transformation matrix P

Drawback: Network structure (spatial information) is destroyed



Given (A, b) A, b : Sparse ☺

Reduced model $(PAP^\dagger, Pb)$

✓ $PP^\dagger = I_{\hat{n}}$

$$Px = \hat{x}$$

$$\longrightarrow$$

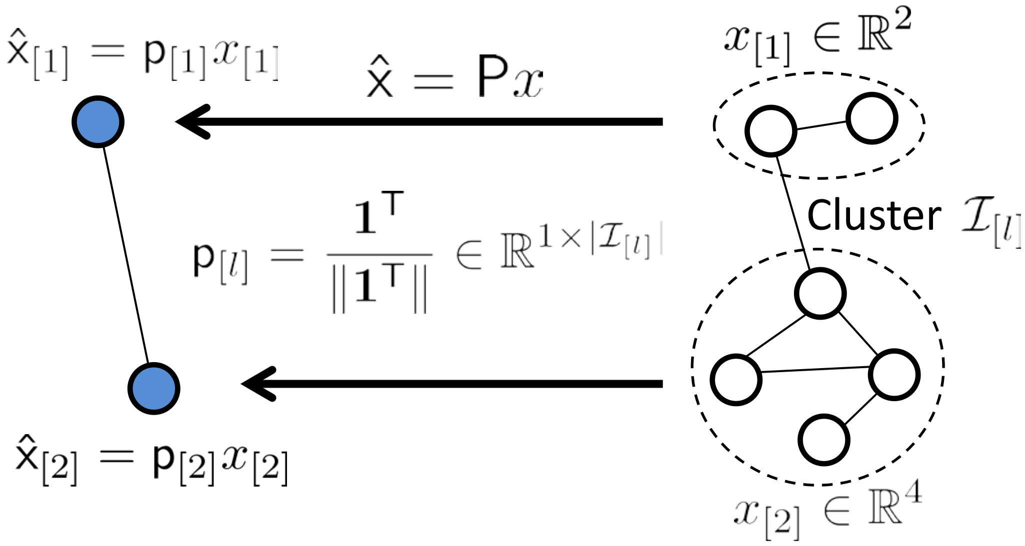
$P \in \mathbb{R}^{\hat{n} \times n}$: Dense

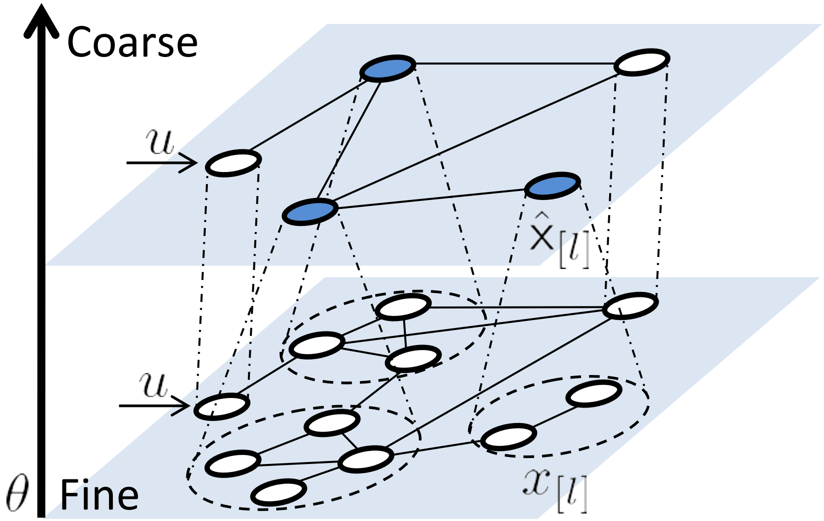
$PAP^\dagger, Pb$: Dense ☹

Need to impose suitable sparse structure on P

Clustering-based State Aggregation

- Aggregation of disjoint sets of states (clusters) $\{x_{[1]}, \ldots, x_{[L]}\}$
  - Block-diagonally structured aggregation matrix $\mathsf{P} = \mathrm{Diag}\left(\mathsf{p}_{[1]}, \ldots, \mathsf{p}_{[L]}\right)$
  - Interconnection topology among clusters is preserved ☺





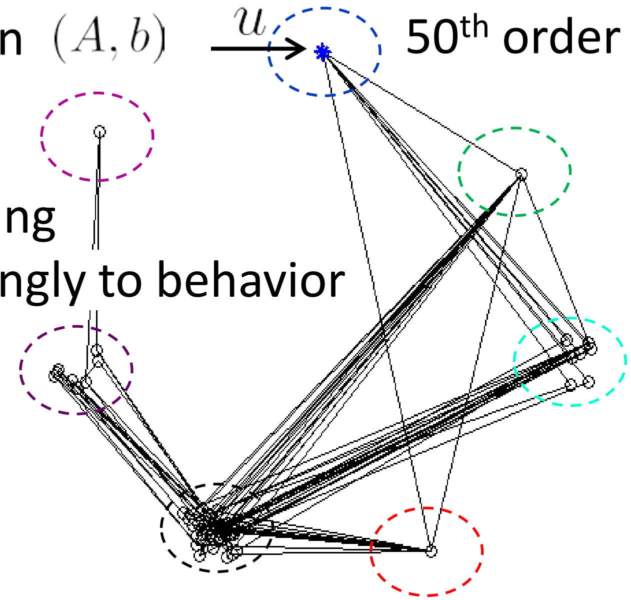
$$\hat{\mathsf{x}} = \mathsf{P} x \quad \Leftrightarrow \quad \begin{bmatrix} \hat{\mathsf{x}}_{[1]} \\ \hat{\mathsf{x}}_{[2]} \end{bmatrix} = \begin{bmatrix} \mathsf{p}_{[1]} & \\ & \mathsf{p}_{[2]} \end{bmatrix} \begin{bmatrix} x_{[1]} \\ x_{[2]} \end{bmatrix}$$

How to find reducible clusters?

✓ For simplicity, Aggregation = Averaging: $\mathbf{1}^\mathsf{T} = [1, \ldots, 1]$

Key Observation to Construct Reducible Clusters

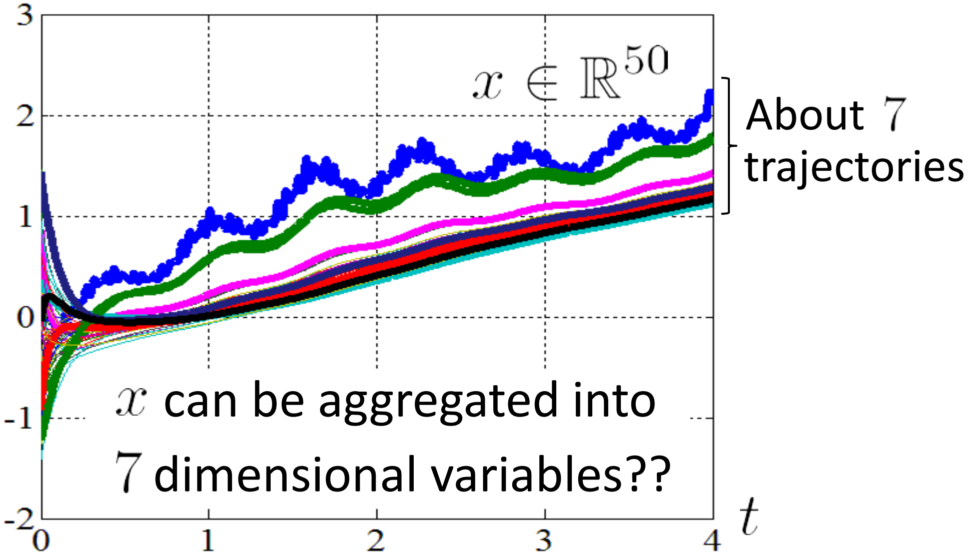
Given (A, b)



50th order

Clustering accordingly to behavior

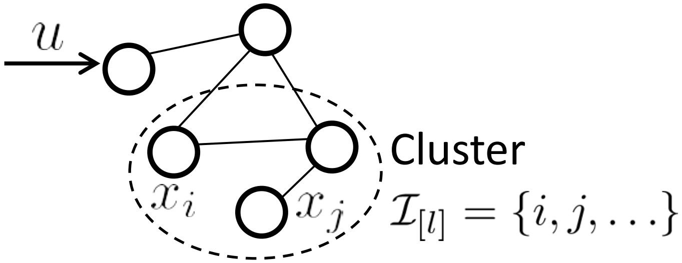
[State trajectory under random input]



About 7 trajectories

x can be aggregated into 7 dimensional variables??

[Definition] **Reducible Cluster**



A cluster $\mathcal{I}_{[l]}$ is said to be *reducible* if

$\forall i, j \in \mathcal{I}_{[l]}$ s.t. $x_i(t) \equiv x_j(t)$ under any input signal $u(t)$.

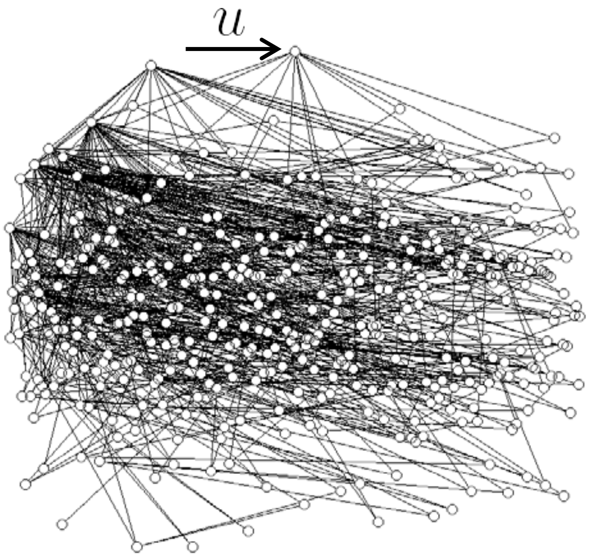
Positive Tri-diagonalization

[Lemma] For every bidirectional network (A, b), there exists a unitary $H \in \mathbb{R}^{n \times n}$ such that $(\tilde{A}, \tilde{b}) = (H^\mathsf{T} A H, H^\mathsf{T} b)$ has the structure below.

Bidirectional network (A, b)

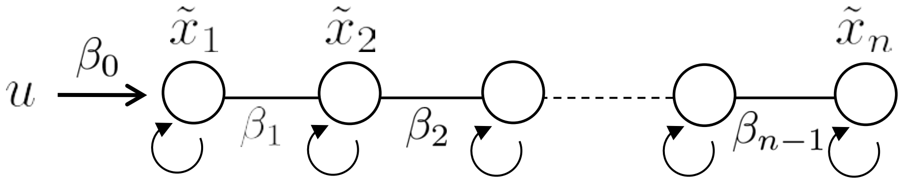
$$\dot{x} = Ax + bu, \quad A = A^\mathsf{T}$$

(not necessarily positive)



$$\overset{x = H\tilde{x}}{\longleftrightarrow}$$

Positive tri-diagonal realization $(\tilde{A}, \tilde{b})$



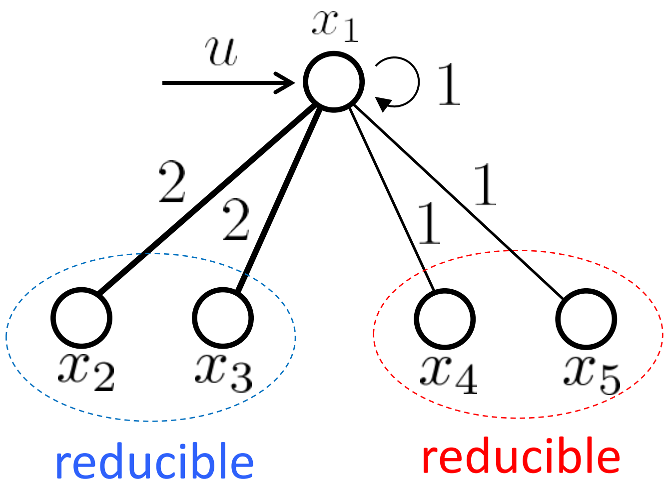
Metzler

$$\tilde{A} = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix} \quad \tilde{b} = \begin{bmatrix} \beta_0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$\beta_i \geq 0$ for all $i \in \{0, \ldots, n-1\}$

Reducibility Characterization

Bidirectional network (A, b)



$(\tilde{A}, \tilde{b})$: positive tri-diagonal realization
H : transformation matrix

Index matrix

$$\Phi := H\mathrm{diag}(-\tilde{A}^{-1}\tilde{b})$$

$-\tilde{A}^{-1}\tilde{b}$: DC-gain ⇔ Maximal gain
due to positivity

$$\Phi = \left[\begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1.20 & -0.20 & 0 & 0 \\ \hline 0 & 1.20 & -0.20 & 0 & 0 \\ \hline 0 & 0.60 & 0.40 & 0 & 0 \\ \hline 0 & 0.60 & 0.40 & 0 & 0 \end{array}\right] \begin{array}{l} \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} \text{identical} \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} \text{identical} \end{array}$$

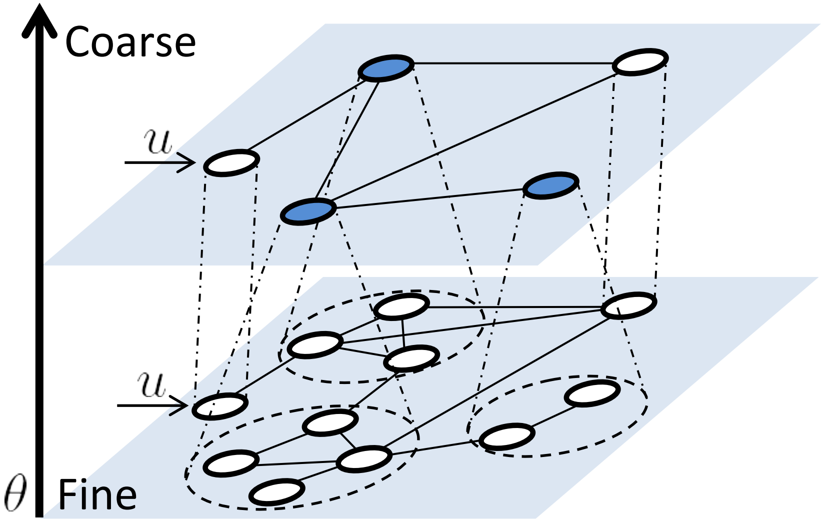
Cluster reducibility is characterized by rows of Φ

Reducible Cluster Aggregation

Reducibility: $\forall i,j \in \mathcal{I}_{[l]}$ s.t. $g_i(s) = g_j(s)$ $\quad\quad$ $\Phi = H\mathrm{diag}(-\tilde{A}^{-1}\tilde{b})$

[Theorem] A cluster $\mathcal{I}_{[l]}$ is reducible iff $\forall i,j \in \mathcal{I}_{[l]}$ s.t. $\mathrm{row}_i[\Phi] = \mathrm{row}_j[\Phi]$.

Furthermore, if all clusters are reducible, then $g(s) = \hat{\mathrm{g}}(s)$ holds.



Aggregated model $(\mathrm{P}A\mathrm{P}^{\mathsf{T}}, \mathrm{P}b)$

$$\hat{\mathrm{g}}(s) = \mathrm{P}^{\mathsf{T}}\left(sI_L - \mathrm{P}A\mathrm{P}^{\mathsf{T}}\right)^{-1}\mathrm{P}b$$

with $\mathrm{P} = \mathrm{Diag}(\mathrm{p}_{[1]}, \ldots, \mathrm{p}_{[L]}) \in \mathbb{R}^{L\times n}$

Dynamical network (A, b)

$$g\left(s\right) = \left(sI_n - A\right)^{-1} b$$

Relaxation to $\|\mathrm{row}_i[\Phi] - \mathrm{row}_j[\Phi]\| \leq \theta$??

Reducibility Relaxation

[Definition] θ**-reducible Cluster** ✓ $\|v\|_{l_\infty} = \|v^\mathsf{T}\|_{l_1}$ for **row** vector v

A cluster $\mathcal{I}_{[l]}$ is said to be *θ-reducible* if

$$\forall j \in \mathcal{I}_{[l]},\ \exists i \in \mathcal{I}_{[l]} \ \text{ s.t. } \ \|\mathrm{row}_i[\Phi] - \mathrm{row}_j[\Phi]\|_{l_\infty} \leq \theta.$$

θ : coarseness parameter

[Theorem] If all clusters are θ-reducible, then

$$\|g(s) - \hat{\mathrm{g}}(s)\|_{\mathcal{H}_\infty} \leq \sqrt{\alpha}\,\|(\mathsf{P}A\mathsf{P}^\mathsf{T})^{-1}\mathsf{P}A\|\theta$$

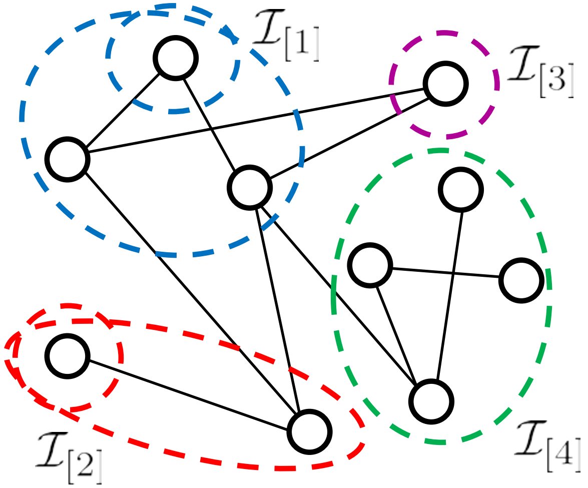
holds where $\alpha := \sum_{l=1}^{L} |\mathcal{I}_{[l]}|(|\mathcal{I}_{[l]}| - 1)$.

linear dependence on θ

Preservation: Stability and Interconnection topology among clusters ☺

In addition, $\hat{\mathrm{x}}_{[l]}$ represents average of original state $x_{[l]}$

Cluster Set Construction



- Give $\theta \in \mathbb{R}_+$, Initialize $\{\mathcal{I}_{[l]}\}_{l\in\mathbb{L}} = \emptyset,\ \mathbb{L} = \emptyset,\ l = 0$
  - While $\{\mathcal{I}_{[l]}\}_{l\in\mathbb{L}} \neq \{1,\ldots,n\}$
    - $l{+}{+},\ \mathbb{L} \leftarrow \{\mathbb{L}, l\}$
    - Choose $i \in \{1,\ldots,n\}\backslash\{\mathcal{I}_{[l]}\}_{l\in\mathbb{L}}$, Set $\mathcal{I}_{[l]} = \{i\}$
    - For all $j \in \{1,\ldots,n\}\backslash\{\mathcal{I}_{[l]}\}_{l\in\mathbb{L}}$,

      if (i,j) satisfies $(*)$, then $\mathcal{I}_{[l]} \leftarrow \{\mathcal{I}_{[l]}, j\}$

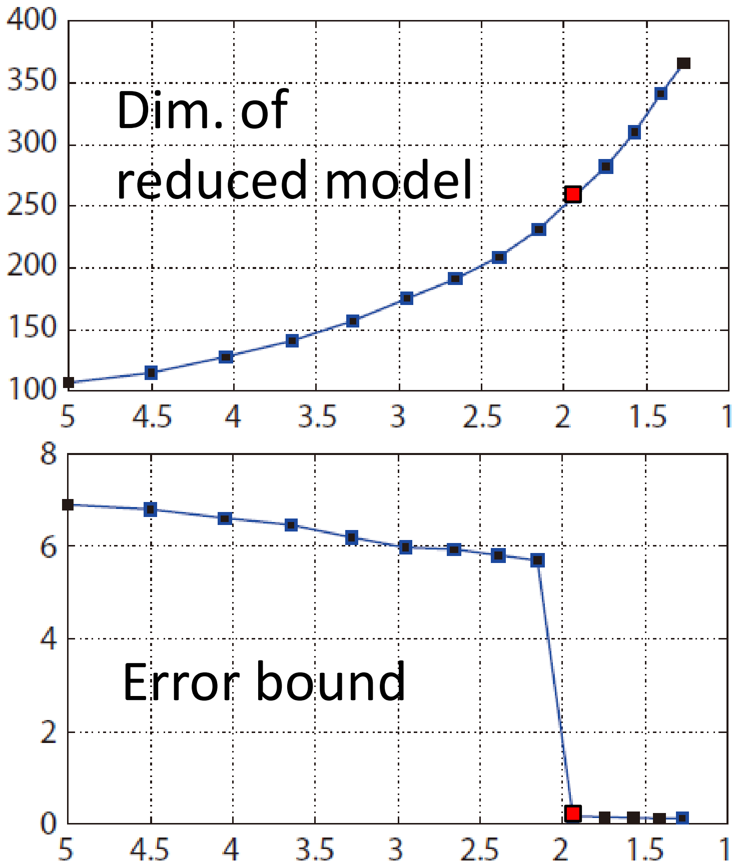
θ- reducibility : $(*)$

$$\|\mathrm{row}_i[\Phi] - \mathrm{row}_j[\Phi]\|_{l_\infty} \leq \theta \quad \text{where} \quad \Phi = H\mathrm{diag}(-\tilde{A}^{-1}\tilde{b})$$

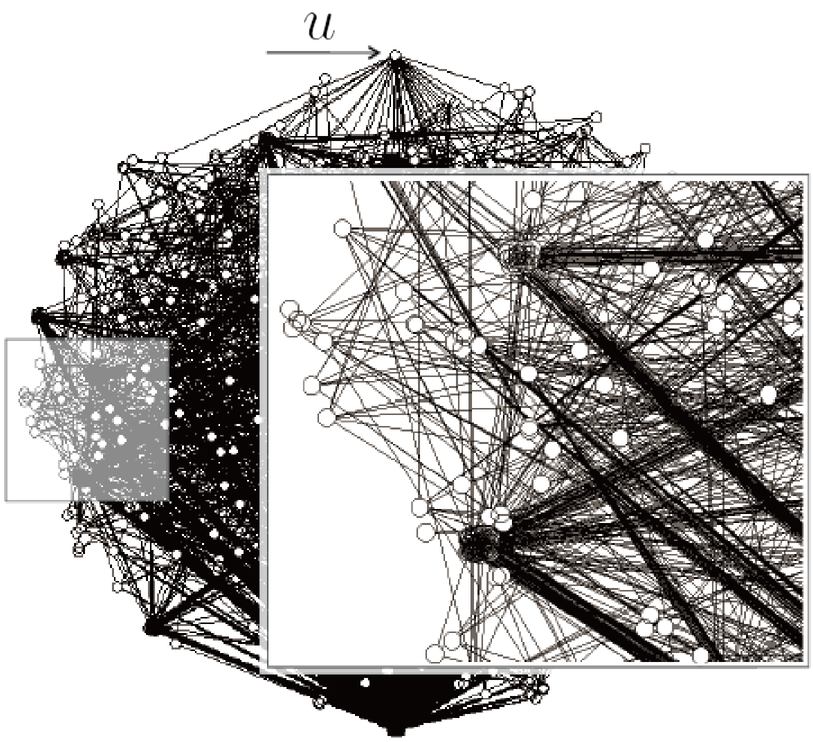
✓ Cluster set to be obtained is not necessarily unique

Numerical Example

- Diffusion process over the Holme-Kim model (3000 th dim.)
  - $\|g(s) - \hat{\mathrm{g}}(s)\|_{\mathcal{H}_\infty} \leq 0.16$ (less than 0.5% error) if $\theta = 1.82$



The value of θ



276 clusters

(276th dimensional model)

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  - Use of controllability gramian
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System Description

[Definition] **Positive Network** (A, b)

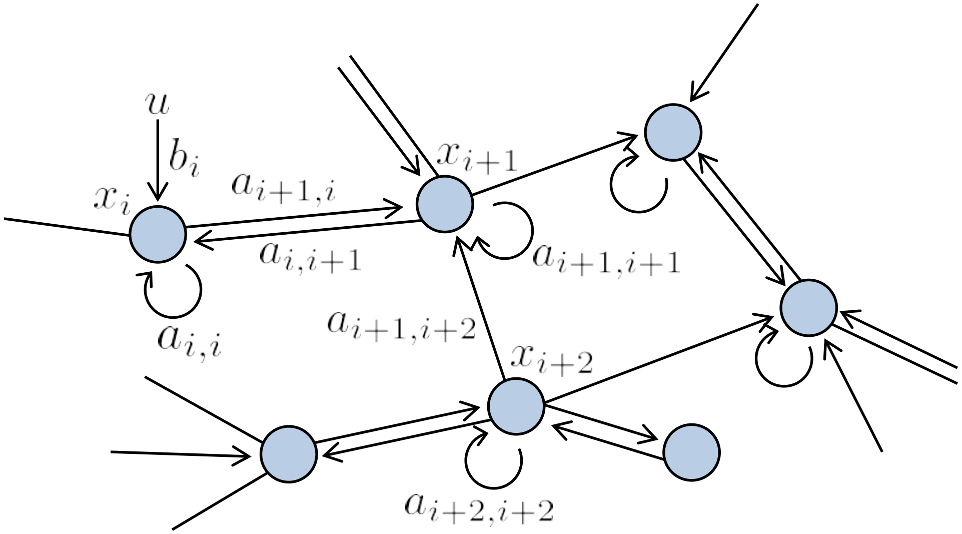
$\dot{x} = Ax + bu$ with $A = \{a_{i,j}\} \in \mathbb{R}^{n \times n}$ and $b = \{b_i\} \in \mathbb{R}^n$ is said to be *positive network* (A, b) if A is Metzler and (marginally) stable, and $b \in \mathbb{R}^n_+$.

Metzler matrix : having non-negative off-diagonal entries

$\mathbb{R}_+$: non-negative $\mathbb{R}$

non-negative property

$x(t) \in \mathbb{R}^n_+, \quad \forall u \in \mathbb{R}_+, \ \forall t \in [0, \infty)$

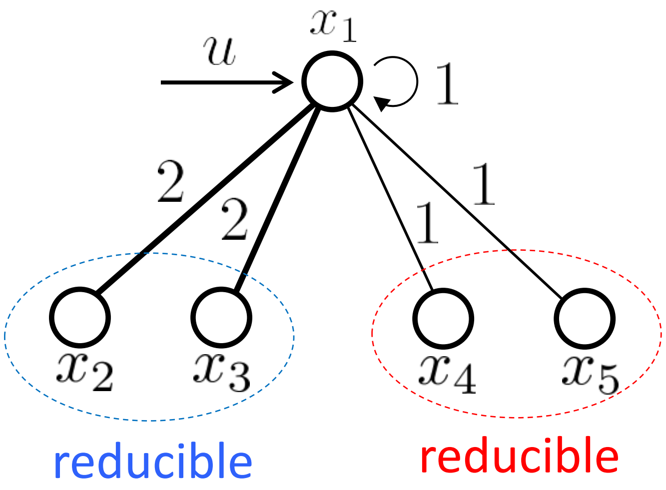


e.g., Heat diffusion systems, Electric circuit systems, Markovian processes

Model reduction while preserving positivity, stability and network

Reducibility Characterization ($\mathcal{H}_2$-case)

Given (A, b) with stable A



Controllability gramian

$$\Phi := \int_0^\infty e^{At} b \, (e^{At} b)^{\mathsf{T}} dt$$

✓ Lyapunov equation $A\Phi + \Phi A^{\mathsf{T}} + bb^{\mathsf{T}} = 0$

Cholesky factorization $\Phi_c \Phi_c^{\mathsf{T}} = \Phi$

$$\Phi_c = \left[\begin{array}{ccccc} 0.39 & 0 & 0 & 0 & 0 \\ \hline 0.21 & 0.19 & 0 & 0 & 0 \\ \hline 0.21 & 0.19 & 0 & 0 & 0 \\ \hline 0.24 & 0.18 & 0.05 & 0.00 & 0 \\ \hline 0.24 & 0.18 & 0.05 & 0.00 & 0 \end{array}\right] \begin{array}{l} \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} \text{identical} \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} \text{identical} \end{array}$$

Cluster reducibility is characterized by rows of Φ_c

$\mathcal{H}_2$-State Aggregation

[Definition] **θ-reducible Cluster** ✓ $\Phi_c\Phi_c^{\mathsf{T}} = \int_0^\infty e^{At}b\,(e^{At}b)^{\mathsf{T}}dt$

The cluster $\mathcal{I}_{[l]}$ is said to be *θ-weakly reducible* if

$$\forall j \in \mathcal{I}_{[l]},\ \ \exists i \in \mathcal{I}_{[l]}\ \ \text{s.t.}\ \ \|\mathrm{row}_i[\Phi_c] - \mathrm{row}_j[\Phi_c]\| \leq \theta.$$

θ : coarseness parameter

[Theorem] If all clusters are θ-weakly reducible, then

$$\|g(s) - \hat{\mathsf{g}}(s)\|_{\mathcal{H}_2} \leq \sqrt{\alpha}\,\|(sI_L - \mathsf{P}A\mathsf{P}^{\mathsf{T}})^{-1}\mathsf{P}A\|_{\mathcal{H}_\infty}\theta$$

holds where $\alpha := \sum_{l=1}^{L}|\mathcal{I}_{[l]}|(|\mathcal{I}_{[l]}| - 1)$.

linearly bounded by θ

Preservation: Stability, Positivity, Interconnection topology among clusters

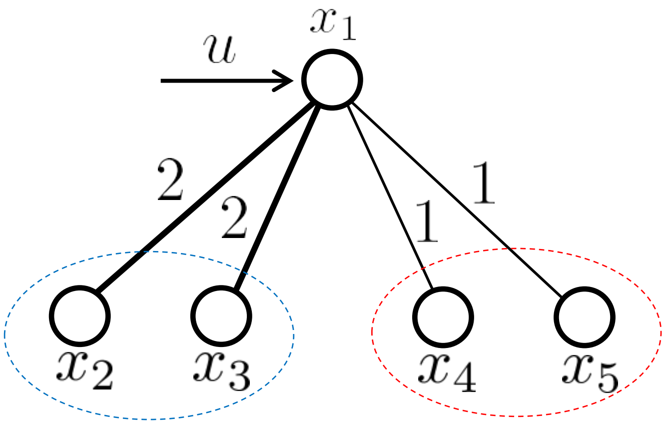
Generalization to Marginally Stable Positive Networks

Gramian is **not defined** if A has zero-eigenvalue ☹

Projected gramian $\Phi = \int_0^\infty W^\top e^{WAW^\top t} Wb\,(W^\top e^{WAW^\top t} Wb)^\top dt$

where $W \in \mathbb{R}^{(n-1)\times n}$ is orthogonal complement of v_l such that $v_l^\top A = 0$.

✓
- Controllability gramian of stable projected system $(WAW^\top, Wb)$
- Unique positive semi-definite matrix for (A, b)



$-A$: Graph Laplacian

Cholesky factorization $\Phi_c \Phi_c^\top = \Phi$

$$\Phi_c = \left[\begin{array}{cccc} -0.18 & -0.05 & 0 & 0 \\ \hline \color{blue}{0.07} & \color{blue}{-0.01} & \color{blue}{0} & \color{blue}{0} \\ \hline \color{blue}{0.07} & \color{blue}{-0.01} & \color{blue}{0} & \color{blue}{0} \\ \hline \color{red}{0.02} & \color{red}{0.04} & \color{red}{0} & \color{red}{0} \\ \hline \color{red}{0.02} & \color{red}{0.04} & \color{red}{0} & \color{red}{0} \end{array}\right] \begin{array}{l} \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} \color{blue}{\text{identical}} \\ \left.\begin{array}{l} \\ \\ \end{array}\right\} \color{red}{\text{identical}} \end{array}$$

Application to Chemical Master Equation（CME）

Michaelis-Menten system

$$S_1 + S_2 \underset{c_2}{\overset{c_1}{\rightleftarrows}} S_3$$

$$S_3 \xrightarrow{c_3} S_4 + S_2$$

c_i : reaction rate constant

ex) Initial number of S_1, S_2 are both $K = 2$

[Realizable distributions]

Realization probability

$$\begin{tikzcd} x_1(t)\begin{bmatrix}2\\2\\0\\0\end{bmatrix} \arrow[r, shift left] & x_2(t)\begin{bmatrix}1\\1\\1\\0\end{bmatrix} \arrow[l, shift left] \arrow[r, shift left] \arrow[d] & x_3(t)\begin{bmatrix}0\\0\\2\\0\end{bmatrix} \arrow[l, shift left] \arrow[d] \\ & x_4(t)\begin{bmatrix}1\\2\\0\\1\end{bmatrix} \arrow[r, shift left] & x_5(t)\begin{bmatrix}0\\1\\1\\1\end{bmatrix} \arrow[l, shift left] \arrow[d] \\ & & x_6(t)\begin{bmatrix}0\\2\\0\\2\end{bmatrix} \end{tikzcd}$$

State $x := [x_1, \ldots, x_n]^\mathsf{T}$ with $x_1(0) = 1$

CME expression: $\dot{x} = Ax, \quad x(0) = [1, 0, \ldots, 0]^\mathsf{T}$

- Continuous-time Markovian process
  - off-diagonal entries of A are non-negative
  - column sums of A are zero $\Leftrightarrow$ $\sum_{i=1}^{n} x_i(t) \equiv 1$ (zero-eigenvalue)
- $n = (K+1)(K+2)/2$ th dimensional

Numerical Example

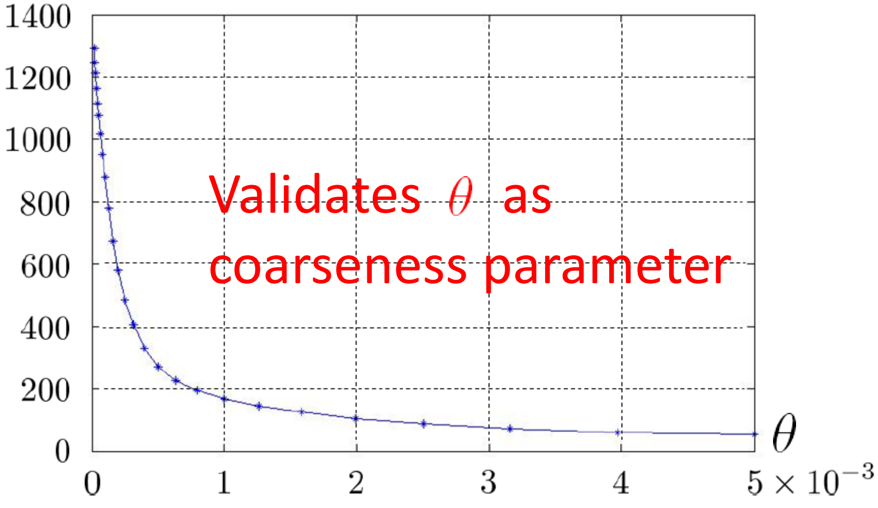
$$\dot{x} = Ax, \quad x(0) = [1, 0, \ldots, 0]^{\mathsf{T}} \xrightarrow{\mathsf{P}x = \hat{\mathsf{x}}} \dot{\hat{\mathsf{x}}} = \mathsf{P}A\mathsf{P}^{\mathsf{T}}\hat{\mathsf{x}}, \quad \hat{\mathsf{x}}(0) = \mathsf{P}x(0)$$

$n = 10011$ th order

if $\theta = 5 \times 10^{-5}$

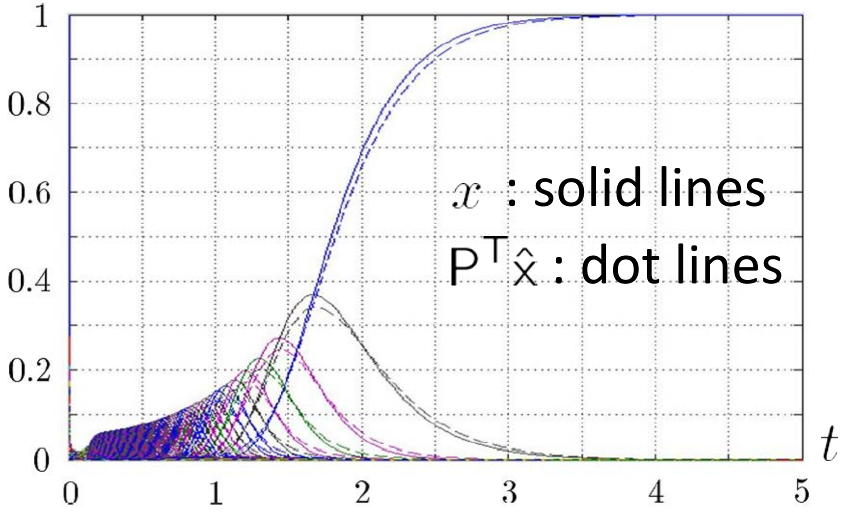
$L = 1077$ th order

[Reduced order versus θ]



Validates θ as coarseness parameter

[Trajectories of x and $\mathsf{P}^{\mathsf{T}}\hat{\mathsf{x}}$]



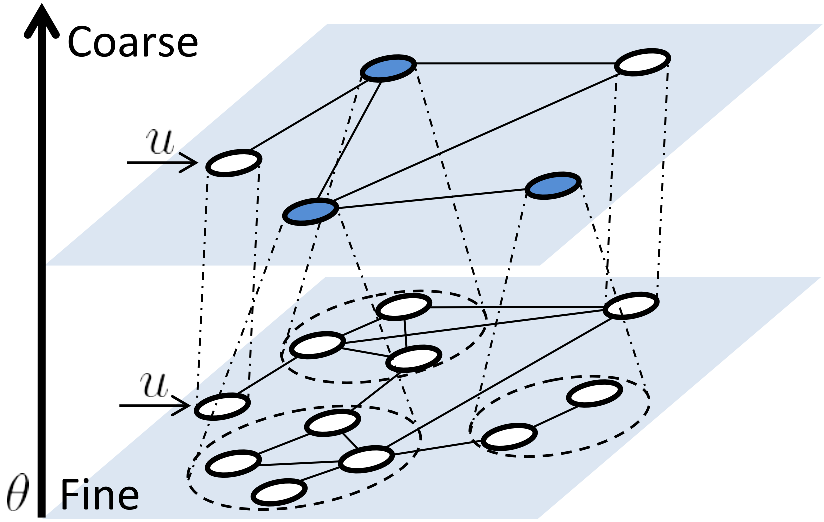
x : solid lines

$\mathsf{P}^{\mathsf{T}}\hat{\mathsf{x}}$: dot lines

Relative error of $x - \mathsf{P}^{\mathsf{T}}\hat{\mathsf{x}}$ in $\mathcal{H}_2$-norm: 2.4%

Summary

- Clustering-based State Aggregation
  - positive tri-diagonalization leads to $\mathcal{H}_\infty$-aggregation
  - controllability graman leads to $\mathcal{H}_2$-aggregation
- Preserving interconnection topology as well as stability, positivity
- Application to diffusion process over complex networks and CMEs



Aggregated model $(\mathsf{P}A\mathsf{P}^\mathsf{T}, \mathsf{P}b)$

$$\hat{\mathsf{g}}(s) = \mathsf{P}^\mathsf{T}\left(sI_L - \mathsf{P}A\mathsf{P}^\mathsf{T}\right)^{-1}\mathsf{P}b$$

with $\mathsf{P} = \mathrm{Diag}(\mathsf{p}_{[1]}, \ldots, \mathsf{p}_{[L]}) \in \mathbb{R}^{L \times n}$

Dynamical network (A, b)

$$g\left(s\right) = \left(sI_n - A\right)^{-1} b$$