A Simulation-Based Method for Aggregating Markov Chains

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In collaboration with Prashant Mehta and Sean Meyn
Nearly Completely Decomposable Markov Chains (NCDMC)

Phillips and Kokotovic 1981
“Over a longer period the weak interactions become significant, while each group of the coupled states can be replaced by an aggregate state.”
Summary of our previous work

An information-theoretic framework to aggregate MC

- The metric to compare two Markov chains
  - Kullback-Leibler divergence rate

- The optimal aggregated Markov chain
  - Can be found for any fixed partition function

- The optimal partition function
  - 2\textsuperscript{nd} eigenvector $\Rightarrow$ Bi-partition

Assumption (Ergodicity)

- All Markov chains are assumed to be irreducible and aperiodic.
- Unique invariant distribution

\[ \pi_j = \sum_i \pi_i P_{ij}, \quad j \in \mathcal{N}. \]

Definition (Partition function)

\[ \phi : \mathcal{N} \mapsto \mathcal{M} \]

where

\[ \mathcal{N} = \{1, 2, \ldots, n\}, \quad \mathcal{M} = \{1, 2, \ldots, m\}. \]
Kullback-Leibler divergence rate

Markov chains \((\pi, P)\) and \((\varpi, Q)\) on the same state space

\[
R(P \parallel Q) = \sum_{i=1}^{n} \pi_i \sum_{j=1}^{n} P_{ij} \log \left( \frac{P_{ij}}{Q_{ij}} \right).
\]

Markov chains \((\pi, P)\) and \((\varpi, Q)\) on different state spaces

\[
R^{(\phi)}(P \parallel Q) := \min_{\mu \in \mathcal{P}(\mathcal{N})} R(P \parallel \hat{Q}^{(\mu)}(\phi)).
\]
100-state Markov chain

Figure: The colorplot of Markov chain transition probabilities.
Aggregation via spectral partition

100x100 Original Markov Chain

K-L Divergence Rate

Error Bound

I-partition
Aggregation via spectral partition

100x100 Original Markov Chain

K-L Divergence Rate

Error Bound

1-partition
2-partition
Aggregation via spectral partition

100×100 Original Markov Chain

Error Bound

K-L Divergence Rate

1-partition 2-partition 3-partition
Aggregation via spectral partition

100×100
Original Markov Chain

K-L Divergence Rate

1-partition
2-partition
3-partition
4-partition
Aggregation via spectral partition

100×100 Original Markov Chain

Error Bound

K-L Divergence Rate

1-partition 2-partition 3-partition 4-partition 5-partition
Aggregation via spectral partition

100x100 Original Markov Chain

K-L Divergence Rate

Error Bound

1-partition 2-partition 3-partition 4-partition 5-partition
## Roadmap of simulation-based method

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<td>• Kullback-Leibler rate metric as aggregation error</td>
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<td>• Spectral method to find suboptimal partition</td>
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<td>• <em>Not tractable for large-scale Markov chains!</em></td>
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<th>Aggregation via learning (topic of this presentation)</th>
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<td>• K-L metric = Average cost ⇒ Dynamic Programming</td>
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<td>• <em>The dimension of policy space is $m^n$!</em></td>
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<td>• Randomized policy space ⇒ Approximate DP</td>
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<td>• Stochastic-gradient algorithm ⇒ Suboptimal policy</td>
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<td>• <em>Just need a single sample-path of Markov chain!</em></td>
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Average cost representation

One-step cost

The *one-step cost* is defined as

\[
g_i(\phi) = \sum_{j \in \mathcal{N}} P_{ij} \log \left( \frac{P_{ij}}{\hat{Q}_{ij}(\pi)(\phi)} \right), \quad i \in \mathcal{N}.
\]

Average cost

The *average expected cost* is given by

\[
\lambda(x_0; \phi) = \lim_{T \to \infty} \frac{1}{T} \mathbb{E} \left[ \sum_{t=0}^{T-1} g_{X(t)}(\phi) \mid X(0) = x_0 \right],
\]

where \( X(t) \in \mathcal{N} \) denotes the state at time \( t \).
**Dynamic Programming formulation**

**Average cost problem**

- Under the ergodicity assumption, for any $x_0 \in \mathcal{N}$,

$$
\lambda(x_0; \phi) = \lambda(\phi) := \sum_{i \in \mathcal{N}} \pi_i \sum_{j \in \mathcal{N}} P_{ij} \log \left( \frac{P_{ij}}{Q_{ij}^{(\pi)}(\phi)} \right)
$$

- Average cost problem

$$
\lambda^* = \min_{\phi} \left\{ \lim_{T \to \infty} \frac{1}{T} \mathbb{E} \left[ \sum_{t=0}^{T-1} g_X(t)(\phi) \right] \right\}
$$

**Dynamic Programming approach**

$$
\lambda^* + h_i = \min_{\phi \in \Phi} \left\{ g_i(\phi) + \sum_{j \in \mathcal{N}} P_{ij} h_j \right\}, \quad i \in \mathcal{N}
$$
Approximate Dynamic Programming

Complexity of DP approach
For $m$-partition problem, the dimension of policy space is $m^n!$

Randomized and parameterized policy
The *randomized and parameterized* policy:

$$\eta_\phi(\cdot, \theta) : \mathcal{N} \mapsto [0, 1]^{m^n},$$

where $\theta \in \mathbb{R}^K$ is the parameter vector $K \ll m^n$. The quantity $\eta_\phi(i, \theta)$ represents the probability that the partition function $\phi$ is assigned to the state $i$.

Jump to bi-partition case

---

DP and ADP

Average cost for DP ($|\phi| = m^n$)

$$\lambda(\phi) = \lim_{T \to \infty} \frac{1}{T} \mathbb{E} \left[ \sum_{t=0}^{T-1} g_X(t)(\phi) \right] = \sum_i \pi_i g_i(\phi).$$

Randomized average cost for ADP ($\theta \in \mathbb{R}^K$)

$$\lambda(\theta) = \lim_{T \to \infty} \frac{1}{T} \mathbb{E} \left[ \sum_{t=0}^{T-1} \mathbb{E}_{\eta_\phi} \left[ g_X(t)(\phi) \right] \right] = \sum_i \pi_i g_i(\theta),$$

where

$$g_i(\theta) := \mathbb{E}_{\eta_\phi} [g_i(\phi)] = \sum_{\phi} \eta_\phi(i, \theta) g_i(\phi), \quad i \in \mathcal{N}.$$
Gradient-descent algorithm to minimize $\lambda(\theta) = \sum_i \pi_i g_i(\theta)$

- **Idealized gradient-descent algorithm:**
  \[
  \theta(t+1) = \theta(t) - \gamma_t \nabla \lambda(\theta(t)).
  \]

- **Simulation-based gradient-descent algorithm:**
  \[
  \theta(t+1) = \theta(t) - \gamma_t \nabla g_{X(t)}(\theta(t)).
  \]
Bi-partition of a 4-state Markov chain

Original model

The partition function $\phi^* = [1, 1, 2, 2]$ is optimal for

$$P = \begin{bmatrix}
0.5 & 0.4 & 0.0 & 0.1 \\
0.4 & 0.5 & 0.1 & 0.0 \\
0.0 & 0.1 & 0.5 & 0.4 \\
0.1 & 0.0 & 0.4 & 0.5
\end{bmatrix}.$$ 

Aggregation using Dynamic Programming

- The optimal aggregated Markov chain is

$$Q^* = \begin{bmatrix}
0.9 & 0.1 \\
0.1 & 0.9
\end{bmatrix}.$$ 

- Policy Iteration Algorithm of DP shows the optimal average cost $\lambda^* = 0.0749.$
Bi-partition of a 4-state Markov chain

- Idealized gradient-descent algorithm:

- Simulation-based gradient-descent algorithm
Bi-partition of an 100-state Markov chain

Figure: Colorplot (left) and 2nd eigenvector (right) of transition matrix.
Bi-partition of an 100-state Markov chain

- Simulation-based gradient-descent algorithm:

- Global optimum v.s. local optimum
Conclusions

- K-L minimization as an average cost problem
- Randomization and parameterization to obtain ADP
- Stochastic-gradient method to search for the optimum

Thank you!
Objectives

Markov model reduction via state aggregation

- How to compare two Markov chains?
- What’s the optimal aggregation?
- Can we find the optimal solution?

Figure: Original and Aggregated Markov Chain
### Partial Literature

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<td>- HMM model reduction: Kotsalis 2006.</td>
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Modeling error as K-L rate

Modeling error in terms of uncertainty

The modeling error between $P$ and $Q$ is defined as

$$\Delta \mathcal{H} := \hat{\mathcal{H}}(x) - \mathcal{H}(x),$$

where

$$\mathcal{H}(x) = \lim_{t \to \infty} \mathbb{E}_{p(x_0^t)}[-\ln p(x_t|x_0^{t-1})],$$

$$\hat{\mathcal{H}}(x) = \lim_{t \to \infty} \mathbb{E}_{p(x_0^t)}[-\ln q(x_t|x_0^{t-1})].$$

Modeling error for Markov chains

$$\Delta \mathcal{H} = R(P \parallel Q) = \sum_{i=1}^{n} \pi_i \sum_{j=1}^{n} P_{ij} \log \left( \frac{P_{ij}}{Q_{ij}} \right).$$
Model reduction error as K-L rate

K-L rate on different state spaces

Markov chains \((\pi, P)\) on \(\mathcal{N}\) and \((\vartheta, Q)\) on \(\mathcal{M}\)

\[
R^{(\phi)}(P \parallel Q) := \min_{\mu \in \mathcal{P}(\mathcal{N})} R(P \parallel \hat{Q}^{(\mu)}(\phi)),
\]

where \(\mu\) is a probability measure and \(\mu^* = \pi\), and

\[
\hat{Q}^{(\mu)}_{ij}(\phi) = \frac{\mu_j}{\sum_{k \in \phi^{-1} \circ \phi(j)} \mu_k} Q_{\phi(i)\phi(j)}, \quad i, j \in \mathcal{N}.
\]
Optimal partition function

Optimization problem

The $m$-partition problem is equivalent to only finding the optimal partition function $\phi^*$ such that

$$\phi^* \in \arg \min_{\phi: \mathcal{N} \leftrightarrow \mathcal{M}} R(\phi)(P \parallel Q^*(\phi)).$$

Spectral partitioning approach

- 2nd eigenvector $\Rightarrow$ bi-partition
- recursive bi-partition $\Rightarrow$ $m$-partition
Optimal aggregation for a fixed partition

$m$-partition problem

The optimal aggregated chain is found by minimizing K-L rate

\[
\min_{\phi, Q} \quad R(P \parallel Q)
\]

s.t.

\[
Q_{kl} \geq 0, \quad k, l \in \mathcal{M}, \\
\sum_{l \in \mathcal{M}} Q_{kl} = 1, \quad k \in \mathcal{M}.
\]

Optimal solution

For a fixed partition function $\phi$, we obtain

\[
Q_{kl}^*(\phi) = \frac{\sum_{i \in \phi^{-1}(k)} \sum_{j \in \phi^{-1}(l)} \pi_i P_{ij}}{\sum_{i \in \phi^{-1}(k)} \pi_i}, \quad k, l \in \mathcal{M}.
\]

\[
\omega_k^*(\phi) = \sum_{i \in \phi^{-1}(k)} \pi_i, \quad k \in \mathcal{M}.
\]
Optimal partition function

Optimization problem
The $m$-partition problem is equivalent to only finding the optimal partition function $\phi^*$ such that

$$\phi^* \in \arg \min_{\phi \colon \mathcal{N} \leftrightarrow \mathcal{M}} R(\phi)(P \parallel Q^*(\phi)).$$

Two approaches
- Spectral partition: 2nd eigenvector.
- Simulation-based partition: a single sample path.
## Optimal partition function

### Optimization problem

The $m$-partition problem is equivalent to only finding the optimal partition function $\phi^*$ such that

$$\phi^* \in \arg \min_{\phi: \mathcal{N} \mapsto \mathcal{M}} R(\phi)(P \parallel Q^*(\phi)).$$

### Two approaches

- **Spectral partition:** 2nd eigenvector

  *Curse of Dimensionality!*

- **Simulation-based partition:** a single sample path

  *More computable and tractable!*
Parameterized optimization

Optimization problem

The optimization problem is

$$\theta^* \in \arg \min_{\theta \in \mathbb{R}^K} \lambda(\theta),$$

where for ergodic Markov chain,

$$\lambda(\theta) = \sum_i \pi_i g_i(\theta) = \sum_i \pi_i \sum_{\phi \in \Phi} \eta_{\phi}(i, \theta) g_i(\phi).$$
Bi-partition randomized policy

Randomization and Parameterization

- The parameter vector is \( \theta = [\theta_1, \theta_2, \ldots, \theta_n]^T \).
- The probability of group assignment for state \( i \) is

\[
P(\phi(i) = 1) = \frac{1}{1 + \exp(\theta^T i)}, \quad P(\phi(i) = 2) = \frac{\exp(\theta^T i)}{1 + \exp(\theta^T i)}.
\]

Randomized and parameterized policy

\[
\eta_\phi(i, \theta) = \frac{1}{1 + \exp(\theta^T i)} \mathbb{I}_{\phi(i) = 1} + \frac{\exp(\theta^T i)}{1 + \exp(\theta^T i)} \mathbb{I}_{\phi(i) = 2}, \quad i \in \mathcal{N}.
\]
ODE method for convergence analysis

**ODE representation**

- Simulation-based algorithm:
  \[
  \theta(t+1) = \theta(t) - \gamma_t \nabla g_X(t) (\theta(t)), \\
  \tilde{\lambda}(t+1) = \tilde{\lambda}(t) + \gamma_t (g_X(t)(\theta(t)) - \tilde{\lambda}(t)).
  \]

- ODE analogy:
  \[
  \dot{\theta}_t = -\nabla \lambda(\theta_t), \quad \dot{\tilde{\lambda}}_t = \lambda(\theta_t) - \tilde{\lambda}_t.
  \]

**Convergence analysis for ODE**

\[
\lambda(\theta_t) \geq 0, \quad \dot{\lambda}(\theta_t) = -\|\nabla \lambda(\theta_t)\|^2 \leq 0
\]

\[
\Rightarrow \lambda(\theta_t) \to \lambda(\theta_\infty), \quad \tilde{\lambda}_t \to \lambda(\theta_\infty), \quad \text{as } t \to \infty.
\]