Spectral Gaps and Cutoff in Markov Chains

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Outline

- Introduction
- Cut-off Examples
- Spectral gap
- $k$-SAT
- Lumping $k$-SAT
A boy is trying to collect a set of $n$ coupons. He gets a random coupon every day. How long does it take him to get a complete collection?
Coupon Collector’s Problem

- A boy is trying to collect a set of \( n \) coupons. He gets a random coupon every day. How long does it take him to get a complete collection?

- A stochastic process: if at day \( k \) he has \( p \) different coupons (\( p < n \)) then at day \( k + 1 \) he has \( p \) with probability \( \frac{p}{n} \) and \( p + 1 \) with probability \( 1 - \frac{p}{n} \).
**Coupon Collector’s Problem**

- A boy is trying to collect a set of $n$ coupons. He gets a random coupon every day. How long does it take him to get a complete collection?

- A stochastic process: if at day $k$ he has $p$ different coupons ($p < n$) then at day $k + 1$ he has $p$ with probability $p/n$ and $p + 1$ with probability $1 - p/n$.

- Problem has applications in computer science.
Coupon Collector’s problem

\[ A = \frac{1}{n} \begin{bmatrix} 1 & n - 1 \\ 2 & n - 2 \\ \vdots & \vdots \\ n - 1 & 1 \\ n & \end{bmatrix} \]

- \( \sigma(A) = \frac{1}{n}, \frac{2}{n}, \ldots, \frac{n - 1}{n}, 1. \)
- No spectral gap.
- Initial state is \( \pi_0 = \begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}. \)
• As $n$ increases the transition gets sharper.
• We have a cut-off at $k = n \log n$. 
Cut-Off (Diaconis et al., 1982–)

- Let $\mathcal{M} = \{A_n\}$ be transition matrices corresponding to a family of Markov chains with $n$ states, $n = 1, \ldots$.
- Stationary distributions are $\Sigma_n$.
- $f(n) \uparrow$ function of $n$, $\tau_n$ an arbitrary vector.
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- Stationary distributions are $\Sigma_n$.
- $f(n) \uparrow$ function of $n$, $\tau_n$ an arbitrary vector.
- Assume that the limit
  $$g(c) = \lim_{n \to \infty} \|\tau_n A^{cf(n)} - \Sigma_n\|$$
  exists for all $c > 0$.
- If
  $$g(c) = \begin{cases} 
    \alpha 
eq 0 & c < c_* \\
    0 & c > c_*, 
  \end{cases}$$

$\mathcal{M}$ has a cut-off of order $f(n)$ (critical value $c_*$).
Remarks

- Proving there is a cut-off often requires horrendous calculations.
- Use tools from probability theory, combinatorics, group representation theory, asymptotics, ...
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• Diaconis (1996) makes heuristic connections between existence of cut-off, multiplicity of $\lambda_2$ and symmetry.
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- Proving there is a cut-off often requires horrendous calculations.
- Use tools from probability theory, combinatorics, group representation theory, asymptotics, . . .
- For large state spaces, lumping can often be used profitably.
- Diaconis (1996) makes heuristic connections between existence of cut-off, multiplicity of $\lambda_2$ and symmetry.
- Coupon collector’s problem: neither necessary.
- We explore another connection between cut-off and spectrum.
Random Walk on A Hypercube

- In $\mathbb{R}^n$, at each step a particle at a vertex chooses one out of $(n + 1)$ accessible vertices (Markov chain).

- What is the probability of being in state $j$ after $k$ steps if initially we are in state $i$ (initial state random)?
Random Walk on A Hypercube

- In $\mathbb{R}^n$, at each step a particle at a vertex chooses one out of $(n + 1)$ accessible vertices (Markov chain).

- What is the probability of being in state $j$ after $k$ steps if initially we are in state $i$ (initial state random)?

- For large $k$ it should be $2^{-n}$ for any $i$ and $j$.

- What is the rate of convergence of the probability to this number?
Random Walk on A Hypercube

• **Problem:** State space has size $2^n$. 
Random Walk on A Hypercube

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- **Solution:** Take as our variable $j$, the distance from vertex $i$, which we can take to be at the origin.
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The state space is of size $n + 1$ and the transition matrix is

$$A = \begin{bmatrix}
\frac{1}{n+1} & \frac{n}{n+1} \\
\frac{1}{n+1} & \frac{1}{n+1} & \frac{n-1}{n+1} \\
\frac{1}{n+1} & \frac{n-1}{n+1} & \frac{1}{n+1} \\
\frac{n}{n+1} & \frac{1}{n+1} \\
\frac{n}{n+1} & \frac{1}{n+1} \\
\end{bmatrix}$$
\begin{itemize}
  \item $\lambda_1 = 1$, $\lambda_2 = 1 - 2/n$: no spectral gap.
  \item We have a cut-off at $k = 0.25n \log n$.
\end{itemize}
A Spectral Gap

- Define the $n \times n$ matrix $A$, such that for $i = 1, \ldots, n - 1,$

$$A[i, i] = \frac{bi}{n - 1}, \quad 0 < b < 1,$$


- This is an upper triangular matrix with a spectral gap $1 - b$. 
A Spectral Gap

\[
A = \begin{bmatrix}
\frac{b}{n-1} & 1 - \frac{b}{n-1} \\
\frac{2b}{n-1} & 1 - \frac{2b}{n-1} \\
\vdots & \vdots \\
1 & 1 - b
\end{bmatrix}
\]

- Final state is absorbing.
- If \( b = 1 \), we (almost) have coupon collector’s problem.
- Given that \( \pi_0 = \begin{bmatrix} 1 & 0 & \ldots & 0 \end{bmatrix} \), how long does it take to arrive at the final state?
\[ b = \frac{7}{8} \]
Theorem

- For $0 < b < 1$, this family of matrices exhibits $O(n)$ cut-off.
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- $c_*(b) = -\frac{\log(1 - b)}{b}$.
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- For $0 < b < 1$, this family of matrices exhibits $O(n)$ cut-off.

- $c^*_b(b) = -\frac{\log(1 - b)}{b}$.

- Need to compute $\pi_0 A^k$. 
A Spectral Gap

\[ \pi_0 A^{n+s-1} = p(n, b) \sum_{j=0}^{s} \sum_{k=1}^{n-1} B(s, n, b). \]

\[ B(s, n, b) = \sum_{k=1}^{n-1} \frac{(-1)^{n-1-k}k^{n-2}}{(k-1)!(n-k-1)!} \left( \frac{bk}{n-1} \right)^j. \]

\[ p(n, b) = \prod_{i=1}^{n-1} \left( 1 - \frac{ib}{n-1} \right). \]
A Spectral Gap

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- $p(n, b) = \prod_{i=1}^{n-1} \left( 1 - \frac{ib}{n-1} \right)$.

- $p(n, b)$ is independent of $s$.

- We seek (the unique) $j^* = j^*(b, n)$ that maximizes $B(s, n, b)$.

- Cut-off at $j^* + n - 1$. 
Proof

\[ k^n + j - 2 = \frac{\Gamma(n + j - 1)}{2\pi i} \int_{-\infty}^{(0+)} e^{kz} z^{-n-j+1} dz, \]

from which we obtain after some manipulation

\[ B(j, n, b) = \left( \frac{b}{n-1} \right)^j \frac{\Gamma(n + j - 1)}{\Gamma(n-1)} I(j, n), \]

where

\[ I(j, n) = \frac{1}{2\pi i} \int_{-\infty}^{(0+)} e^{z} (e^{z} - 1)^{n-2} z^{-n-j+1} dz. \]

We write \( j = \alpha n + \beta \), and

\[ I(\alpha n + \beta, n) = \frac{1}{2\pi i} \int_{-\infty}^{(0+)} \frac{e^{\alpha z} z^{1-\beta}}{(e^{z} - 1)^2} e^{-n f(z)} dz, \]

where \( f(z) = (1 + \alpha) \ln z - \ln(e^{z} - 1) \). The saddle points satisfy

\[ f'(z) = \frac{1 + \alpha}{z} - \frac{1}{1 - e^{-z}} = 0. \]

Hence, \( f(z) \) has a unique saddle point \( z_\alpha > 0 \). The previous line can be written as \( \frac{z_\alpha}{1 - e^{-z_\alpha}} = 1 + \alpha \). (1)
Proof, ctd.

We let $n \to \infty$ and obtain from the method of steepest descents

$$I(\alpha n + \beta, n) \sim \frac{1}{\sqrt{2\pi n}} e^{-n(\alpha \ln z \alpha - z \alpha + \ln(1+\alpha))} e^{-z \alpha z^{-\beta}} (1 + \alpha)^{3/2} (z \alpha - \alpha)^{-1/2}.$$

Hence,

$$B(\alpha n + \beta, n, b) \sim \left( \frac{b}{n-1} \right)^{\alpha n + \beta} \frac{\Gamma(n(1+\alpha) + \beta - 1)}{\Gamma(n-1)} \frac{1}{\sqrt{2\pi n}} e^{-n(\alpha \ln z \alpha - z \alpha + \ln(1+\alpha))}$$

$$\times e^{-z \alpha} z^{-\beta} (1 + \alpha)^{3/2} (z \alpha - \alpha)^{-1/2}.$$

Consequently,

$$\frac{B(\alpha n + 1, n, b)}{B(\alpha n + 0, n, b)} \sim \frac{b}{(n-1)z \alpha} \sim \frac{(1+\alpha)b}{z \alpha},$$

as $n \to \infty$. By definition of $j^*$, we are looking for $\alpha$ such that

$$\frac{B(\alpha n + 1, n, b)}{B(\alpha n + 0, n, b)} \sim 1.$$

Hence, we need $\alpha$ such that $z \alpha = (1 + \alpha)b$. We substitute this result into (1) and deduce that

$$\alpha = -\frac{\ln(1-b)}{b} - 1.$$
Alternative Derivation

- Write $A_n = \begin{bmatrix} Q_n & r_n \\ 0 & 1 \end{bmatrix}$.

- Let $\tau^{(n)} = (I - Q_n)^{-1}e$. Mean arrival time is $\tau^{(n)}_1$. 
Alternative Derivation

- Write \( A_n = \begin{bmatrix} Q_n & r_n \\ 0 & 1 \end{bmatrix} \).

- Let \( \tau^{(n)} = (I - Q_n)^{-1}e \). Mean arrival time is \( \tau_1^{(n)} \).

\[
\tau_1^{(n)} = \sum_{i=1}^{n} \frac{n}{n - ib} = \sum_{i=1}^{n} \sum_{j=0}^{\infty} \left( \frac{ib}{n} \right)^j
\]
\[
= \frac{n}{b} \sum_{j=0}^{\infty} \frac{b^{j+1}}{j + 1} + o(n) = -n \frac{\log(1 - b)}{b} + o(n).
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\textbf{\textit{k-SAT} Problem}

- Assume we are given a set of \( n \) literals (Boolean variables) \( \{s_1, \ldots, s_n\} \).
- Create \( m \) clauses (conjunctions) each involving \( k \) literals.
**k-SAT Problem**

- Assume we are given a set of \( n \) literals (Boolean variables) \( \{s_1, \ldots, s_n\} \).
- Create \( m \) clauses (conjunctions) each involving \( k \) literals.
- Can we find an assignment of these variables such that the disjunction of all the clauses is true?
Remarks

- Applications in areas such as AI (e.g., theorem proving) and scheduling (e.g., airlines, cars).
- NP-complete.
- Solve by “back-tracking” (Davis-Putnam).
- There appears to be a phase change.
- 1-SAT: trivial, 2-SAT: ok, 3-SAT: hard!
Phase Transition

Define $P(n, k, m)$ to be the probability that a $k$-SAT problem in $n$ literals having $m$ clauses has a solution.
Phase Transition

Define $\mathcal{P}(n, k, m)$ to be the probability that a $k$-SAT problem in $n$ literals having $m$ clauses has a solution.

- There is numerical evidence that the limit

$$f(c, k) = \lim_{n \to \infty} \mathcal{P}(n, k, nc)$$

exists for all $c > 0$.

- $f(c, k) = 1$ if $c < c_*(k)$, $f(c, k) = 0$, $c > c_*$.
Define $\mathcal{P}(n, k, m)$ to be the probability that a $k$-SAT problem in $n$ literals having $m$ clauses has a solution.

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  $$f(c, k) = \lim_{n \to \infty} \mathcal{P}(n, k, nc)$$
  exists for all $c > 0$.
- $f(c, k) = 1$ if $c < c_*(k)$, $f(c, k) = 0$, $c > c_*$.
- Goerdt: for $k = 2$, $c_*(2) = 1$.
- Numerically, $c_*(3) \approx 4.25$. 
Phase Transition

Define $\mathcal{P}(n, k, m)$ to be the probability that a $k$-SAT problem in $n$ literals having $m$ clauses has a solution.

- There is numerical evidence that the limit
  
  $$f(c, k) = \lim_{n \to \infty} \mathcal{P}(n, k, nc)$$

  exists for all $c > 0$.

- $f(c, k) = 1$ if $c < c_*(k)$, $f(c, k) = 0$, $c > c_*$.

- Goerdt: for $k = 2$, $c_*(2) = 1$.

- Numerically, $c_*(3) \approx 4.25$.

- $k$-SAT is hardest to solve when the probability that the problem has precisely one solution is at a max.
An assignment of literals can be thought as an integer in \( \{0, \ldots, 2^n - 1\} \) or a vertex on the unit cube \( I_n \).

Clauses \( C_i \), can be seen as maps \( C_i : I_n \mapsto \{0, 1\} \).

For each \( i = 1, \ldots, m \), define

\[
S_i = \{x \in I_n | C_i(x) = 0\}.
\]

\( S_i \) is the set of the vertices on which \( C_i \) is false.
**k-SAT and Vertex Painting**

- An assignment of literals can be thought as an integer in \( \{0, \ldots, 2^n - 1\} \) or a vertex on the unit cube \( I_n \).

- Clauses \( C_i \), can be seen as maps \( C_i : I_n \mapsto \{0, 1\} \).

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\[
S_i = \{x \in I_n | C_i(x) = 0\}.
\]

\( S_i \) is the set of the vertices on which \( C_i \) is false.

- E.g., if \( n = 4 \), \( C_1 = s_1 \lor s_2 \lor \neg s_3 \), \( S_1 \) can be seen as either the set \( \{2, 3\} \) or the set of vertices \((0010, 0011)\).
Each set $S_i$ is an $(n - k)$-face of the cube $I_n$.

Solving a $k$-SAT problem in $n$ literals having $m$ clauses is the same as taking an $n$-cube with white vertices, $m$ times choosing at random an $(n - k)$-face and applying, say, black paint to the set of its vertices.

The number of solutions of a $k$-SAT problem is the size of the set of unpainted vertices.
The Transition Matrix for \((n - k, n)\)

- We can formulate a Markov chain on the power set of \((n - k)\) faces of \(I_n\).
- This has dimension \(2^{2^k \binom{n}{k}} = N\).
- Matrix is upper-triangular and sparse.
- Diagonal entries are monotone increasing.
- \(P(N, N) = 1, P(N - 1, N - 1) = 1 - 2^{-k}\): a spectral gap.
- The transition matrix can be lumped into one of dimension \((2^k - 1)\binom{n}{k} + 1\).
Weak Lumpability

- Lumping is not as straightforward as for random walk.
- It is dependent on the initial condition for the system.
- We make use of the notion of weak lumping (Kemeny and Snell, 1960).
- Define \( R_m \) to be the set of all states having exactly \( m \) painted \( n - k \) faces, \( R_A \) the absorbing state.
- We can weakly lump using states \( R_1, R_2, \ldots, R_M, R_A \) where \( M = (2^k - 1)\binom{n}{k} \).
- Weak lumpability in this case seems to come from upper-triangularity: severe restrictions are placed on the itineraries.
The $(1,3)$-problem

- Paint a $3$-cube by picking random edges.
- The state space has $4096$ elements.
- Using weak lumpability we can condense the problem to $10$ states.
The \((1, 3)\)-problem

- Paint a 3-cube by picking random edges.
- The state space has 4096 elements.
- Using weak lumpability we can condense the problem to 10 states.

\[
\begin{bmatrix}
\frac{1}{12} & \frac{11}{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{6} & \frac{5}{6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{4} & \frac{81}{110} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{3} & \frac{95}{162} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{5}{12} & \frac{143}{342} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & \frac{161}{572} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{7}{12} & \frac{4}{23} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{2}{3} & \frac{1}{12} & \frac{1}{4} & \frac{3}{4} & \frac{1}{4} & \frac{1}{4} \\
0 & 0 & 0 & 0 & \frac{3}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4}
\end{bmatrix}
\]
Remarks

- This procedure can be generalised.
- The simplified model

\[
\begin{pmatrix}
\frac{b}{N} & 1 - \frac{b}{N} \\
\vdots & \vdots \\
\frac{(m-1)b}{N} & 1 - \frac{(m-1)b}{N} \\
\frac{mb}{N} & b - \frac{mb}{N} \\
\vdots & \vdots \\
\frac{(N-1)b}{N} & \frac{b}{N} & 1-b \\
\frac{b}{N} & b & 1-b \\
\end{pmatrix}
\]

has an $O(n)$ cut-off.
**Automated Lumping**

- We can automate the process for weak lumping.
- First determine all the appropriate symmetry classes.
- In the $(1, 3)$ case we get a $77 \times 77$ matrix:

  ![Matrix Diagram](image)

- Then classify into $R_1, \ldots, R_9$. 

Conclusions

• Apparent connection between spectral gap and nature of cut-off.

• $k$-SAT is a Markov chain.

• It can be lumped.

• Certain processes in the lumping can be automated, and matrices can be explicitly computed for modest values of $n$.

• To locate $c_* (3)$ using this process is hard! (but since a cut-off exists . . . )