Genetic Code A Matrix and Combinatoric Approach

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Introduction

Genetic and Gray Code Matrices Relating to Genetic Code

Eigenstructure of D_n

Eigenvalues Eigenvectors

The Genetic Code Matrix C_n

Basic Structures of C_n Hypercube Structure

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Acknowledgments

Thanks to Dr. Chi-Kwong Li, for advising me on my honors thesis and his dedication to this work.

I would also like to thank the Professors at William and Mary that have made CSUMS possible.

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Genetic and Gray Code Matrices Relating to Genetic Code

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Genetic code

 Genetic Code is the set of rules by which information is encoded in DNA/RNA that is translated into amino acid sequences by living cells.

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- ► Nucleotides are the basis for encoding which are labeled {*C*, *U*, *A*, *G*}
- ▶ A genetic code map is $g : C' \to A'$, where $C' = (\{x_1x_2x_3\}) : x_i \in R = \{A, C, G, U\}$, where C' is the set of codons, and A' are the amino acids and termination codons.

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- The focus of this study is building matrices for different length nucleotide sequences, and how to represent the sequences more efficiently

Genetic and Gray Code Matrices Relating to Genetic Code

- A Gray-code representation of the nucleotides was proposed by Swanson (Swanson, 1984)
- Gray code is a set of binary sequences with the property that two consecutive number only differ by one position

Genetic and Gray Code Matrices Relating to Genetic Code

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- Example: In classical binary three and four are 011 and 100 respectively. In Gray Code, the 3 bit representations for three and four are 011 and 010, respectively.

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- Example: In classical binary three and four are 011 and 100 respectively. In Gray Code, the 3 bit representations for three and four are 011 and 010, respectively.
- In genetic transcription a mismatch in genetic coding segments will reduce the degree of mutation

Genetic and Gray Code Matrices Relating to Genetic Code

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Gray Code

• Let G_n , be all the Gray code sequences of length n; G_n can be generated by a recursive algorithm.

Genetic and Gray Code Matrices Relating to Genetic Code

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- Let G_n , be all the Gray code sequences of length n; G_n can be generated by a recursive algorithm.
- $G_n = \{0||a_0, 0||a_1, \dots, 0||a_{n-1}, 1||a_{n-1}, 1||a_{n-1}, \dots, 1||a_0\},$ where $a_i \in G_{n-1}$
- Example: $G_1 = \{0, 1\}$, then $G_2 = \{0||0, 0||1, 1||1, 1||0\} = \{00, 01, 11, 10\}$

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- ► Clearly since $|G_n|$ doubles in size from $|G_{n-1}|$ and G_1 only has 2 entries, $|G_n| = 2^n$
- ▶ Using two bit Gray code construction $C \sim \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, $U \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $G \sim \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and $A \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

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Genetic Code Matrix

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$$\blacktriangleright \ C_1 \sim \begin{array}{c} 0 & 1 \\ \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \end{pmatrix} \\ \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ \end{pmatrix}$$

Genetic and Gray Code Matrices Relating to Genetic Code

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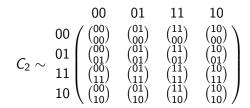
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Genetic Code Matrix

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$$C_1 \sim \begin{array}{c} 0 & 1 \\ C_1 \sim \begin{array}{c} 0 & \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ C_1 = \begin{pmatrix} C & U \\ A & G \end{pmatrix}$$

Outline Introduction	Genetic and Gray Code
Eigenstructure of D_n The Genetic Code Matrix C_n	Matrices Relating to Genetic Code



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$$C_{2} \sim \begin{array}{c} 00 & 01 & 11 & 10 \\ 00 & \begin{pmatrix} 00 \\ 00 \end{pmatrix} & \begin{pmatrix} 01 \\ 00 \end{pmatrix} & \begin{pmatrix} 11 \\ 00 \end{pmatrix} & \begin{pmatrix} 10 \\ 00 \end{pmatrix} & \begin{pmatrix} 10 \\ 00 \end{pmatrix} \\ \begin{pmatrix} 00 \\ 01 \end{pmatrix} & \begin{pmatrix} 01 \\ 01 \end{pmatrix} & \begin{pmatrix} 11 \\ 01 \end{pmatrix} & \begin{pmatrix} 10 \\ 01 \end{pmatrix} \\ \begin{pmatrix} 00 \\ 11 \end{pmatrix} & \begin{pmatrix} 11 \\ 11 \end{pmatrix} & \begin{pmatrix} 10 \\ 11 \end{pmatrix} \\ \begin{pmatrix} 00 \\ 10 \end{pmatrix} & \begin{pmatrix} 01 \\ 11 \end{pmatrix} & \begin{pmatrix} 11 \\ 11 \end{pmatrix} & \begin{pmatrix} 10 \\ 11 \end{pmatrix} \\ \begin{pmatrix} 00 \\ 10 \end{pmatrix} & \begin{pmatrix} 01 \\ 10 \end{pmatrix} & \begin{pmatrix} 11 \\ 11 \end{pmatrix} & \begin{pmatrix} 10 \\ 10 \end{pmatrix} \end{array} \right)$$

$$C_2 = \begin{pmatrix} CC & CU & UU & UC \\ CA & CG & UG & UA \\ AA & AG & GG & GA \\ AC & AU & GU & GC \end{pmatrix}$$

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Genetic and Gray Code Matrices Relating to Genetic Code

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Hamming Distances

The hamming distance is a measure of how different are two strings of the same length

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- ► For example the codon CAG ~ (⁰⁰¹₀₁₁) has a hamming distance of 1, because the second position is different.

Genetic and Gray Code Matrices Relating to Genetic Code

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Hamming Distances

- The hamming distance is a measure of how different are two strings of the same length
- For example the codon $CAG \sim \binom{001}{011}$ has a hamming distance of 1, because the second position is different.
- Define D_n as the hamming distance matrix that computes the hamming distance between the entries of the cells of the genetic code matrix.

Genetic and Gray Code Matrices Relating to Genetic Code

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D_1 and D_2

Recall

 $egin{array}{cccc} 0 & 1 \ C_1 \sim egin{array}{cccc} 0 & (0) & (0) \ 0 & (0) \ (1) & (1) \ 1 \end{pmatrix} & ext{so} \ D_1 = egin{array}{cccc} 0 & 1 \ 1 & 0 \end{pmatrix} \end{array}$

Genetic and Gray Code Matrices Relating to Genetic Code

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Recall

$$C_2 \sim \begin{array}{c} 00 & 01 & 11 & 10 \\ 00 & \begin{pmatrix} 00 \\ 00 \end{pmatrix} & \begin{pmatrix} 01 \\ 00 \end{pmatrix} & \begin{pmatrix} 11 \\ 00 \end{pmatrix} & \begin{pmatrix} 10 \\ 00 \end{pmatrix} & \begin{pmatrix} 00 \\ 00 \end{pmatrix} & \begin{pmatrix} 00 \\ 00 \end{pmatrix} & \begin{pmatrix} 01 \\ 00 \end{pmatrix} & \begin{pmatrix} 10 \\ 00 \end{pmatrix} & \begin{pmatrix} 00 \\ 01 \end{pmatrix} & \begin{pmatrix} 01 \\ 10 \end{pmatrix} & \begin{pmatrix} 10 \\ 00 \end{pmatrix} \\ 10 & \begin{pmatrix} 01 \\ 11 \end{pmatrix} & \begin{pmatrix} 11 \\ 10 \end{pmatrix} & \begin{pmatrix} 10 \\ 10 \end{pmatrix} \end{pmatrix} \quad \text{so } D_2 = \begin{pmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

Genetic and Gray Code Matrices Relating to Genetic Code

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Basic Properties of D_n

Theorem

 (i) The Hamming Distance-based matrix D_n is also a 2ⁿ × 2ⁿ matrix with Hamming distances of 0, 1, 2,...,n. The common row/column sum of the matrix D_n equals n2ⁿ⁻¹ and the total summation of the entries of the matrix D_n is n2²ⁿ⁻¹.

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- (ii) The matrix D_n is doubly stochastic and symmetric.

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- (ii) The matrix D_n is doubly stochastic and symmetric.
- (iii) D_n is centrally embedded in D_{n+1}

Genetic and Gray Code Matrices Relating to Genetic Code

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Recursion in D_n

Theorem Let $D_n = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$ where B_{ij} is a $2^{n-1} \times 2^{n-1}$ sub matrix. Then

$$D_{n+1} = \begin{pmatrix} B_{11} & B_{12} & 2J_{n-1} + B_{11} & B_{12} \\ B_{12} & B_{11} & B_{12} & 2J_{n-1} + B_{12} \\ 2J_{n-1} + B_{11} & B_{12} & B_{11} & B_{12} \\ B_{12} & 2J_{n-1} + B_{11} & B_{12} & B_{11} \end{pmatrix}$$

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► Notice that if D_{n+1} is written in the 4 × 4 block structure, D_n appears centrally embedded as a 2 × 2 block.

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- ► Notice that if D_{n+1} is written in the 4 × 4 block structure, D_n appears centrally embedded as a 2 × 2 block.
- D_n stores information about C_n, however reduces the amount of information stored by a factor of n.

Eigenvalues Eigenvectors

Eigenvalues of D_n

• The matrix $D_n \in M_{2^n}$ has n+1 nonzero eigenvalues equal to

$$n2^{n-1}, \overline{-2^{n-1}, -2^{n-1}, \dots, -2^{n-1}}$$
.

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- ► Notice the first eigenvalue is the column row sum.

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Outline Introduction Eigenstructure of D_n The Genetic Code Matrix C_n

Eigenvalues Eigenvectors

Eigenvectors of D_n

• Recall
$$D_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

▶ It is easy to see that a set of orthonormal eigenvectors are $v_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

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Also recall that
$$D_2 = \begin{pmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

• A set of orthonormal eigenvectors are $v_0 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$,

$$v_1 = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}$$
, $v_2 = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$], and $v_3 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{pmatrix}$

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• There is recursion in the eigenvectors of D_n

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$$\tilde{v}_j = \frac{1}{\sqrt{2}} \begin{pmatrix} v_j \\ v_j \end{pmatrix}$$
 for $j = 0, \dots, n-1$, $\tilde{v}_n = \frac{1}{\sqrt{2}} \begin{pmatrix} v_n \\ -v_n \end{pmatrix}$ and $\tilde{v}_{n+1} = \frac{1}{\sqrt{2}} \begin{pmatrix} v_0 \\ -v_0 \end{pmatrix}$

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These form an orthonormal set of eigenvectors of D_{n+1} corresponding to the nonzero eigenvalues.

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- ► These form an orthonormal set of eigenvectors of D_{n+1} corresponding to the nonzero eigenvalues.
- This lets us write the powers of D^k_n, in terms of the knowing nothing other than D_n, n and k

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Basic Structures of *C_n* Hypercube Structure

The Basics of C_n

- ► The genetic code-base matrix C_n is a 2ⁿ × 2ⁿ matrix with RNA bases of length n. Each two neighboring entries of genetic code, in both directions differs by exactly one base.
- The genetic code matrix can be defined recursively

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- The genetic code matrix can be defined recursively
- If C_n is the genetic code matrix then

$$C_{n+1} = \begin{pmatrix} C || C_n & U || C_n F_n \\ A || F_n C_n & G || F_n C_n F_n \end{pmatrix}$$

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• Note that F_n is a matrix that has 1's on it's off diagonal

Basic Structures of C_n Hypercube Structure

Number of Nucleotides per Cell

This leads to counting the number of nucleotides per cell, which would store double the information of the hamming distance matrix as a 4-tuple

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Basic Structures of C_n Hypercube Structure

Number of Nucleotides per Cell

- This leads to counting the number of nucleotides per cell, which would store double the information of the hamming distance matrix as a 4-tuple
- ► The 4-tuple would be (x_C, x_U, x_A, x_G), where x_i = number of that nucleotide per cell.
- Label the matrix S_n to count the number of nucleotides per cell. Then

$$S_{n+1} = \begin{pmatrix} (1000) + S_n & (0100) + S_n F_n \\ (0010) + F_n S_n & (0001) + F_n S_n F_n \end{pmatrix}$$

Basic Structures of *C_n* **Hypercube Structure**

Decomposition of D_n and Hypercube

Because D_n is doubly stochastic it is decomposable into a convex combination of permutation matrices that have a leading coefficient of {0, 1, ..., n}.

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- There is also a Hamilton circuit between the all nucleotide sequences, where two nucleotide sequences are adjacent if and only if they differ by exactly one position.

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- Each permutation matrix can be as a vertex of a hypercube and within that vertex there is a subcube
- There is also a Hamilton circuit between the all nucleotide sequences, where two nucleotide sequences are adjacent if and only if they differ by exactly one position.
- This may be promising in the study of mutations in genetic code.

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Basic Structures of *C_n* **Hypercube Structure**

Further Research

It would be useful to get the most information of C_n, or S_n and D_n, without having to display an exponential amount of information.

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- It would be useful to get the most information of C_n, or S_n and D_n, without having to display an exponential amount of information.
- ▶ Information is lost with D_n and S_n , i.e. order of nucleotides

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- ▶ Information is lost with D_n and S_n , i.e. order of nucleotides
- Eventually it would be useful to construct matrices that were polynomial in size

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