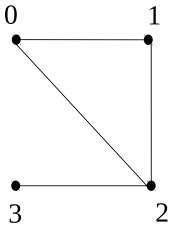
Graphs

DS 2020/2021

Content

Graphs

- $G = (V, E)$
  - V a set of vertices
  - E a set of edges; an edge = a non-ordered pair of distinct vertices



$V = \{0, 1, 2, 3\}$
$E = \{\{0, 1\}, \{0, 2\}, \{1, 2\}, \{2, 3\}\}$
$u = \{0, 1\} = \{1, 0\}$

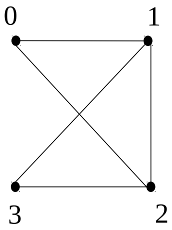
0,1 - the ends of u

u is incident with 0 and 1

0 and 1 are adjacent (neighbors)

Graphs

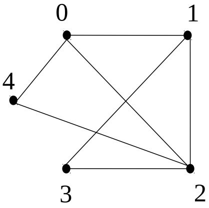
- Walk from u to v: $u = i_0, \{i_0, i_1\}, i_1, \cdots, \{i_{k-1}, i_k\}, i_k = v$
  3, {3,2}, 2, {2,0}, 0, {0,1}, 1, {1,3},3, {3,2},2
- Trail: a walk where any two edges are distinct
- Circuit = a closed trail where any two intermediate edges are distinct
- Path: a walk where any two vertices are distinct
- Cycle: closed path ($i_0 = i_k$)



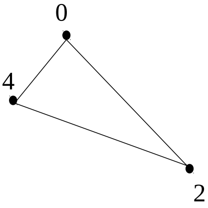
Induced subgraph

- $G = (V, E)$ – a graph, W – a subset of V
- Induced subgraph: $G'(W, E')$, where
  $E' = \{\{i,j\} | \{i,j\} \in E \text{ și } i \in W, j \in W\}$

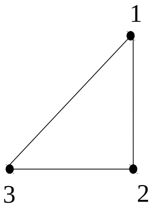
V = {0,1,2,3,4}



W = {0,2,4}

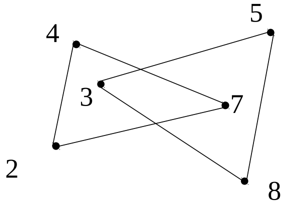


W = {1,2,3}



Any graph can be expressed as the disjoint union of induced, connected and maximal subgraphs (connected components).

- $i\ R\ j$ if and only if there is a path from i to j
- R is an equivalence relation
- $V_1, \cdots, V_p$ equivalence classes
- $G_1, \cdots, G_p$ connected components, where $G_i = (V_i, E_i)$ a subgraph induced by V_i



$V_1 = \{2, 4, 7\}$

$E_1 = \{\{2, 4\}, \{4, 7\}, \{2, 7\}\}$

$V_2 = \{3, 5, 8\}$

$E_2 = \{\{3, 5\}, \{5, 8\}, \{8, 3\}\}$

- connected graph = a graph with a single connected component

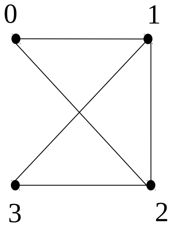
Abstract data type **Graph**

- objects:
  - graphs $G = (V, E)$, $V = \{0, 1, \cdots, n-1\}$
- operations:
  - emptyGraph()
    - input: nothing
    - output: the empty graph $(\emptyset, \emptyset)$
  - isEmptyGraph()
    - input: $G = (V, E)$,
    - output: true if $G = (\emptyset, \emptyset)$, false other way
  - insertEdge()
    - input: $G = (V, E)$, $i, j \in V$
    - output: $G = (V, E \cup \{i, j\})$
  - insertVertex()
    - input: $G = (V, E)$, $V = \{0, 1, \cdots, n-1\}$
    - output: $G = (V', E)$, $V' = \{0, 1, \cdots, n-1, n\}$

Abstract data type **Graph**

- removeEdge()
  - input: $G = (V, E)$, $i, j \in V$
  - output: $G = (V, E \setminus \{i, j\})$
- removeVertex()
  - input: $G = (V, E)$, $V = \{0, 1, \cdots, n-1\}$, k
  - output: $G = (V', E')$, $V' = \{0, 1, \cdots, n-2\}$

$$\begin{aligned} \{i', j'\} \in E' \Leftrightarrow (\exists \{i, j\} \in E)\ & i \neq k, j \neq k, \\ & i' = \mathit{if}\ (i < k)\ \mathit{then}\ i\ \mathit{else}\ i-1, \\ & j' = \mathit{if}\ (j < k)\ \mathit{then}\ j\ \mathit{else}\ j-1 \end{aligned}$$



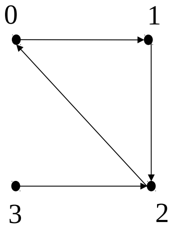
Abstract data type **Graph**

- adjacencyList()
  - input: $G = (V, E)$, $i \in V$
  - output: the list of vertices adjacent with i
- listOfReachableVertices()
  - input: $G = (V, E)$, $i \in V$
  - output: the list of vertices reachable from i

Content

Digraph (directed graph)

- $D = (V, A)$
  - V a set of vertices
  - A a set of arcs (directed edges); an arc = an ordered pair of distinct vertices



$V = \{0, 1, 2, 3\}$
$A = \{(0, 1), (2, 0), (1, 2), (3, 2)\}$
$a = (0, 1) \neq (1, 0)$

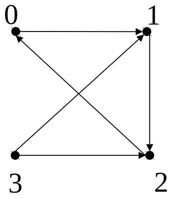
0 – the tail of a

1 – the head of a

Digraph

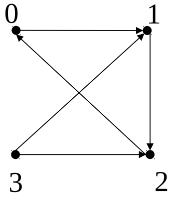
- Walk: $i_0, (i_0, i_1), i_1, \cdots, (i_{k-1}, i_k), i_k$
  3, (3,2), 2, (2,0), 0, (0,1), 1, (1,2), 2, (2,0), 0
- Trail: a walk where any two arcs are distinct
- Circuit = a closed trail where any two intermediate arcs are distinct

- Path: a walk where any two vertices are distinct
- Cycle: closed path ($i_0 = i_k$)



Digraph - Connectivity

- $i\ R\ j$ if and only if there is a path from i to j and a path from j to i
- R is an equivalence relation
- $V_1, \cdots, V_p$ the equivalence classes
- $G_1, \cdots, G_p$ strongly connected components, where $G_i = (V_i, A_i)$ the subdigraph induced by V_i



$$V1 = \{0, 1, 2\}$$
$$A1 = \{(0, 1), (1, 2), (2, 0)\}$$

$$V2 = \{3\}$$
$$A2 = \emptyset$$

- strongly connected digraph $=$ digraph with a single strongly connected component
- connected digraph

Abstract data type **Digraph**

- objects: digraphs $D = (V, A)$
- operations:
  - emptyDigraph()
    - input: nothing
    - output: the empty digraph $(\emptyset, \emptyset)$
  - isEmptyDigraph()
    - input: $D = (V, A)$,
    - output: true if $D = (\emptyset, \emptyset)$, false other way
  - insertArc()
    - input: $D = (V, A)$, $i, j \in V$
    - output: $D = (V, A \cup (i, j))$
  - insertVertex()
    - input: $D = (V, A)$, $V = \{0, 1, \cdots, n-1\}$
    - output: $D = (V', A)$, $V' = \{0, 1, \cdots, n-1, n\}$

Abstract data type **Digraph**

- removeArc()
  - input: $D = (V, A),\ i, j \in V$
  - output: $D = (V, A \setminus (i, j))$
- removeVertex()
  - input: $D = (V, A),\ V = \{0, 1, \cdots, n-1\},\ k$
  - output: $D = (V', A'),\ V' = \{0, 1, \cdots, n-2\}$

$$\begin{aligned}\{i', j'\} \in A' \Leftrightarrow (\exists \{i, j\} \in A)\ & i \neq k, j \neq k,\\ & i' = \mathit{if}\ (i < k)\ \mathit{then}\ i\ \mathit{else}\ i-1,\\ & j' = \mathit{if}\ (j < k)\ \mathit{then}\ j\ \mathit{else}\ j-1\end{aligned}$$

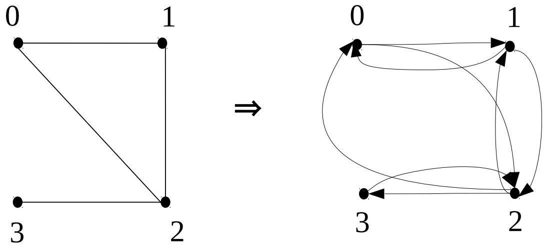
Abstract data type **Digraph**

- outAdjacencyList()
  - input: $D = (V, A),\ i \in V$
  - output: the list of direct successors of i
- inAdjacencyList()
  - input: $D = (V, A),\ i \in V$
  - output: the list of direct predecessors of i
- listOfReachableVertices()
  - input: $D = (V, A),\ i \in V$
  - output: the list of vertices reachable from i

The representation of graphs as digraphs

$G = (V, E) \implies D(G) = (V, A)$
$\{i, j\} \in E \implies (i, j),\ (j, i) \in A$

- the topology is preserved
  - the adjacency list of i in G = the out (=in) adjacency list of i in D



Content

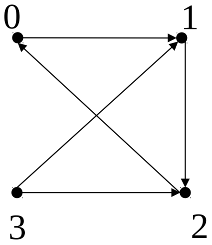
The implementation of digraphs with adjaceny matrices

- the representation of digraphs
  - n the number of vertices
  - m the number of arcs (optional)
  - a matrix $(a[i,j] | \ 1 \leq i, \ j \leq n)$
    $a[i,j] = \mathit{if} \ (i,j) \in A \ \mathit{then} \ 1 \ \mathit{else} \ 0$

  - if the digraph is a graph, then $a[i,j]$ is symmetric
  - the out adjacency list of $i \subseteq$ line i
  - the in adjacency list of $i \subseteq$ column i

The implementation with adjacency matrices

	0	1	2	3
0	0	1	0	0
1	0	0	1	0
2	1	0	0	0
3	0	1	1	0



The implementation with adjacency matrices

- operations
  - emptyDigraph
    $n \leftarrow 0;\ \ m \leftarrow 0$
  - insertVertex: $O(n)$
  - insertArc: $O(1)$
  - removeArc: $O(1)$

- removeVertex()

Procedure *removeVertex(a, n, k)*
begin
    for $i \leftarrow 0$ **to** $n-1$ **do**
        for $j \leftarrow 0$ **to** $n-1$ **do**
            if $(i > k)$ **then**
                $a[i-1, j] \leftarrow a[i, j]$
            if $(j > k)$ **then**
                $a[i, j-1] \leftarrow a[i, j]$
    $n \leftarrow n-1$
end

the execution time: $O(n^2)$

- listOfReachableVertices()
  - If $i = j$ then j is reachable from i
    If $i \neq j$ then there is a path $i \rightsquigarrow j$ if there is the arc $i \rightarrow j$ or there is k: $\exists i \rightsquigarrow k, k \rightsquigarrow j$

The implementation with adjacency matrices

- listOfReachableVertices()

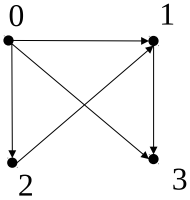
Procedure *reflTransClosure(a, n, b) // (Warshall, 1962)*
begin
    for $i \leftarrow 0$ **to** $n-1$ **do**
        for $j \leftarrow 0$ **to** $n-1$ **do**
            $b[i,j] \leftarrow a[i,j]$
            if $(i = j)$ **then**
                $b[i,j] \leftarrow 1$
    for $k \leftarrow 0$ **to** $n-1$ **do**
        for $i \leftarrow 0$ **to** $n-1$ **do**
            if $(b[i,k] = 1)$ **then**
                for $j \leftarrow 0$ **to** $n-1$ **do**
                    if $(b[k,j] = 1)$ **then**
                        $b[i,j] \leftarrow 1$
end

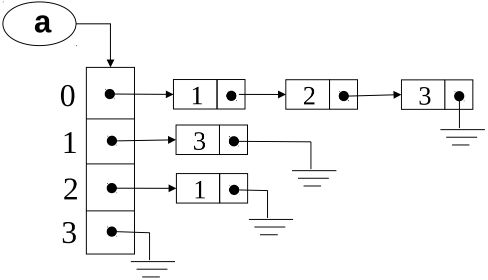
the execution time: $O(n^3)$

Content

The implementation with adjacency lists

- the representation of digraphs with (out) adjacency lists

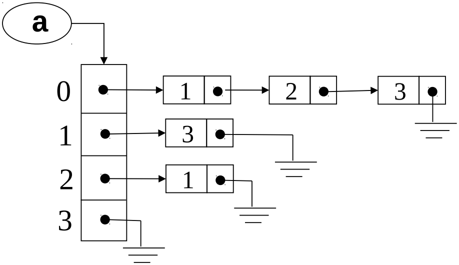




  - a vector $a[0..n-1]$ of linked lists (pointers)
  - $a[i]$ is the out adjacency list corresponding to i

The implementation with adjacency lists

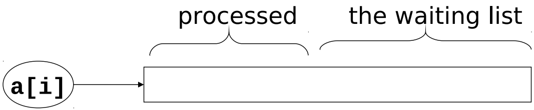
- operations
  - emptyDigraph
  - insertVertex: $O(1)$
  - insertArc: $O(1)$
  - removeVertex: $O(n+m)$
  - removeArc: $O(m)$



Content

Digraphs: systematic exploration

- it manages two sets
  - S = the set of already visited vertices
  - $SB \subseteq S$ the subset of vertices for which there are chances to find neighbors not visited yet
- the adjacency list of i is divided in:



Digraphs: systematic exploration

- the current step
  - read a vertex i from SB
  - extract j from the "waiting" list of i (if it is nonempty)
  - if j isn't in S, then add it to S and to SB
  - if the "waiting" list of i is empty, then remove i from SB
- initially
  - $S = SB = \{i_0\}$
  - the "waiting" list of i = the adjacency list of i
- termination $SB = \emptyset$

Digraphs: systematic exploration

```
Procedure exploration(a, n, i0, S)
begin
    for i ← 0 to n − 1 do
        p[i] ← a[i]
    SB ← (i0)
    visit(i0); S ← (i0)
    while (SB ≠ ∅) do
        i ← read(SB)
        if (p[i] = NULL) then
            SB ← SB − {i}
        else
            j ← p[i] → varf
            p[i] ← p[i] → succ
            if (j ∉ S) then
                SB ← SB ∪ {j}
                visit(j); S ← S ∪ {j}
end
```

Systematic exploration: complexity

Theorem

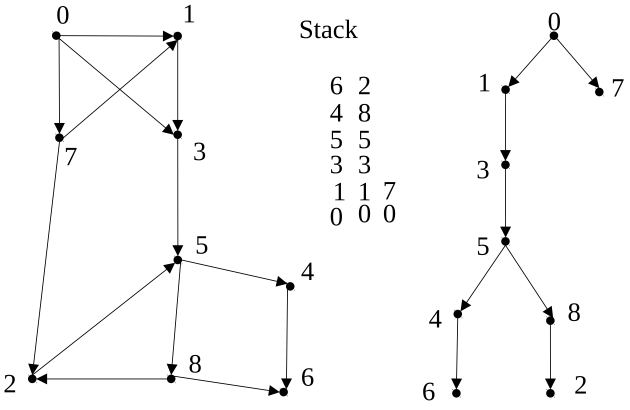
Assuming that the operations over S and SB as well as visit() are achieved in $O(1)$, the time complexity, in the worst case, of the exploration algorithm is $O(n+m)$.

The DFS (*Depth First Search*) exploration

- SB is implemented as a stack

$$
\begin{aligned}
SB \leftarrow (i0) &\Leftrightarrow SB \leftarrow emptyStack() \\
& push(SB, i0) \\
i \leftarrow read(SB) &\Leftrightarrow i \leftarrow top(SB) \\
SB \leftarrow SB - \{i\} &\Leftrightarrow pop(SB) \\
SB \leftarrow SB \cup \{j\} &\Leftrightarrow push(SB, j)
\end{aligned}
$$

The DFS exploration: example



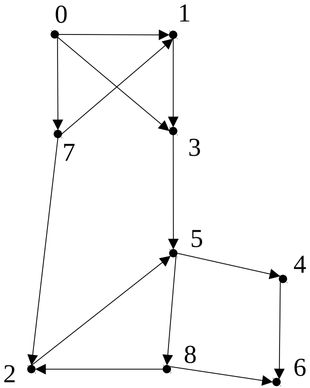
DFS Tree

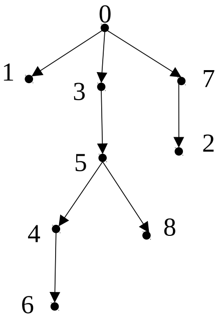
The BFS (*Breadth First Search*) exploration

- SB is implemented as a queue

$$\begin{aligned}
SB \leftarrow (i0) &\Leftrightarrow SB \leftarrow emptyQueue(); \\
&\quad\; insert(SB, i0) \\
i \leftarrow read(SB) &\Leftrightarrow read(SB, i) \\
SB \leftarrow SB - \{i\} &\Leftrightarrow remove(SB) \\
SB \leftarrow SB \cup \{j\} &\Leftrightarrow insert(SB, j)
\end{aligned}$$

The BFS exploration: example





BFS Tree

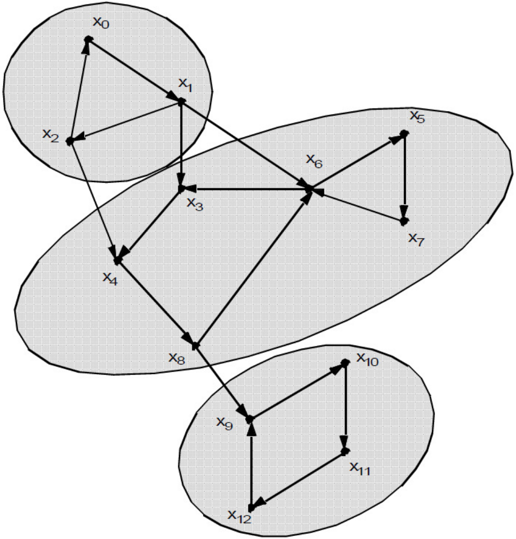
Content

```
Function ConnectedCompDFS(D)
begin
    for i ← 0 to n − 1 do
        color[i] ← 0
    k ← 0
    for i ← 0 to n − 1 do
        if (color[i] = 0) then
            k ← k + 1
            DfsRecConnectedComp(i, k)
    return k
end
```

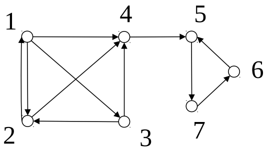
Finding the connected components (undirected graphs)

```
Procedure DfsRecConnectedComp(i, k)
begin
    color[i] ← k
    for (each vertex j in listaDeAdiac(i)) do
        if (color[j] = 0) then
            DfsRecConnectedComp(j, k)
end
```

The strongly connected components (digraphs)

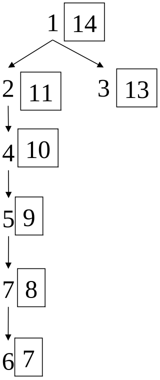


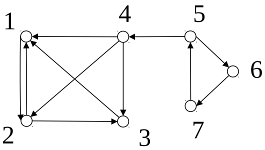
The strongly connected components: example



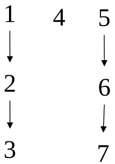
D

$1 \to (2, 3, 4)$
$2 \to (1, 4)$
$3 \to (2, 4)$
$4 \to (5)$
$5 \to (7)$
$6 \to (5)$
$7 \to (6)$





D^T



Finding the strongly connected components

Procedure *DfsStronglyConnectedComp(D)*
begin
    for $i \leftarrow 0$ **to** $n-1$ **do**
        $color[i] \leftarrow 0$
        $parent[i] \leftarrow -1$
    $time \leftarrow 0$
    for $i \leftarrow 0$ **to** $n-1$ **do**
        if $(color[i] = 0)$ **then**
            $DfsRecStronglyConnectedComp(i)$
end

Finding the strongly connected components

Procedure *DfsRecStronglyConnectedComp(i)*
begin
  $time \leftarrow time + 1$
  $color[i] \leftarrow 1$
  for *(each vertex j in adiacList(i))* **do**
    if $(color[j] = 0)$ **then**
      $parent[j] \leftarrow i$
      $DfsRecStronglyConnectedComp(j)$
  $time \leftarrow time + 1$
  $finalTime[i] \leftarrow time$
end

Finding the strongly connected components

Notation: $D^T = (V, A^T)$, $(i,j) \in A \Leftrightarrow (j,i) \in A^T$

Procedure *StronglyConnectedComp(D)*
begin

1. $DFSStronglyConnectedComp(D)$
2. compute D^T
3. $DFSStronglyConnectedComp(D^T)$ but considering in the *for* main loop the vertices in descending order of their final times of visiting $finalTime[i]$
4. return each tree computed at step 3 as being a distinct strongly connected component

end

Finding the strongly connected components: complexity

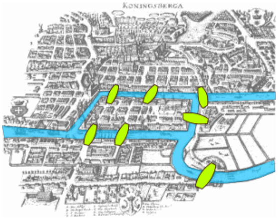
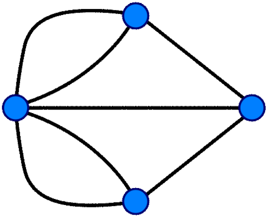
- *DFSStronglyConnectedComp*(D): $O(n+m)$
- compute D^T: $O(m)$
- *DFSStronglyConnectedComp*(D^T): $O(n+m)$
- Total: $O(n+m)$

Applications

- Algorithms, path problems, computer networks (routing), genomics (alignment networks, genome assembly), multi-relational data mining, operations research (scheduling), artificial intelligence (constraint satisfaction), etc.

Applications

The Konigsberg Bridge Problem (1736): starting from one land masses, walk over each of the seven bridges just once

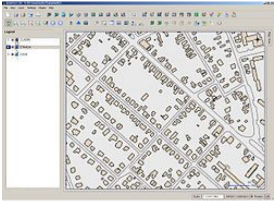



The land masses: vertices, the bridges: edges

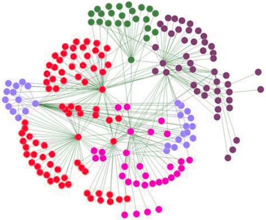
It is possible to choose a vertex, proceed along the edges and return to the chosen vertex, covering each edge once?

Applications

- Google search engine: PageRank algorithm - to determine how important a given web page is
- Geographic Information Systems (GIS): Google Maps, Bing Maps



- Social networks



DNA word design

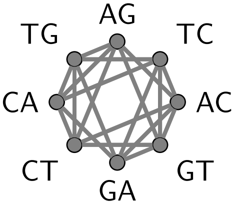
- The design of DNA codes that satisfy combinatorial constraints; use in biomolecular computing to store information, or to manipulate molecules in chemical libraries

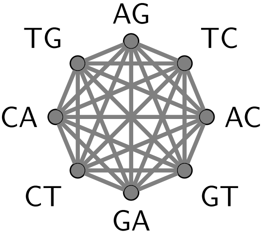
- Find the largest set S of strings of length n over the alphabet $\{A, C, G, T\}$ s.t.:
  - *GC Content Constraint*: each word has 50% symbols from $\{C, G\}$
  - *Hamming Distance Constraint*: each pair of words, $w_1 \neq w_2$ differ in at least d positions: $H(w_1, w_2) \geq d$
  - *Reverse Complement Hamming Distance Constraint*: $H(R(w_1), C(w_2)) \geq d$; $R(w)$: the reversed of word w and $C(w)$ the complement of w ($C \leftrightarrow G$, $A \leftrightarrow T$)

Graph modeling

- every DNA word has an assigned vertex v_i
- $E = E_{HD} \cup E_{RC}$ (E_{HD} pairs of words with a HD conflict, E_{RC} pairs of words with a RC conflict)
- a solution: a maximum independent set

Figura: Graphs for words of size 2 and Hamming distance $d = 2$ (left) and $d = 3$ (right)





Solution of 136 words for $n = 8, d = 4$ instance

AAACCACC	ACCAGTGT	ACCCAAGA	ACGTAGTG	ACTGACGT	AGGAAGCT
AGTCCTCT	AGTTGGCA	ATCCCGTT	ATGGGCTT	CAAACCTC	CAAGAGAC
CAAGCAGT	CACAGTTG	CACCAATC	CAGATGGT	CAGGATCT	CATCGTGT
CATGACTG	CATTCGCT	CCAGTCTT	CCCTGATT	CCGACTTT	CCTCAGTT
CGAAGGTT	CGACACAT	CGATTTGG	CGCACAAT	CGCCTTTT	CGCTAGTA
CGGTGTAT	CGTAAAGG	CGTGTGAT	CTATGCCT	CTCGTACT	CTGAAGAG
CTGCAAGT	CTTACCGT	CTTCCTAG	GAAAGCGT	GAACAGCT	GAACGTAG
GAAGGATC	GACATGAG	GACCTAGT	GACTGTCT	GAGAAGTC	GAGACACT
GAGTACAG	GATGCAAG	GATGTCCT	GCAATAGG	GCAGCTAT	GCCTAGAT
GCGATCAT	GCGGAATT	GCTCGAAT	GCTTATGG	GGAAATGC	GGACCATT
GGATAACG	GGCAACTT	GGGTTGTT	GGTATTCG	GGTTCCAT	GGTTTAGC
GTAACCAG	GTAGAGTG	GTATCGGT	GTCAGTAC	GTCCAAAG	GTCGATGT
GTGAGATG	GTGCTTCT	GTTAGGCT	GTTCTCTG	GTTGACAC	TAACACGC
TAAGCTCG	TACACAGC	TACCGCTT	TAGATCCG	TAGGAAGG	TAGGCGTT
TAGTGTGC	TATCGACG	TATGTGGC	TCAACGTG	TCACGTCT	TCAGACAG
TCATGCTC	TCCATGCT	TCCCATTG	TCCGTATC	TCCTCAAG	TCGAAGGA
TCGAGTAG	TCGCAAAC	TCGGTTGT	TCGTACCT	TCTACCAC	TCTCCTGA
TCTCTGAG	TCTGCACT	TGAACCCT	TGACCTAC	TGAGAGGT	TGATGGAG
TGCAGTCA	TGCGTTAG	TGCTACAC	TGCTCTGT	TGGAGAGT	TGGATGAC
TGGCTATG	TGGGATTC	TGTAGCTG	TGTCTCGT	TGTGACCA	TGTGGAAC
TGTTCGTC	TTAAGGGC	TTACCAGG	TTAGTCCC	TTCAACGG	TTCCTTGC
TTCGCCAT	TTCGGGTA	TTCTGACC	TTGACTCC	TTGCCCTA	TTGCGGAT
TTGTTGGG	TTTCAGCC	TTTGGTGG	TTTTCCCG		