ML_homework3

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Colab link: https://bit.ly/2XyhEO7

1 [SVM; 40p] 선형적으로 분리가 가능한 경우, 다음을 증명하세요.

1.1 A. SVM의 원시 형태 (primal form) 해를 구하는 방법

linear disciminant function $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$
$g(\mathbf{x})$ is proportional to signed distance from $\mathbf{x}$ to hyperplane
scale $\mathbf{w}$ and $\mathbf{b}$ to get following hold:

$$g(\mathbf{x}_+) = +1$$

$$g(\mathbf{x}\_) = -1$$

support vector : $\mathbf{x}\_$, $\mathbf{x}_+$
the constraints are then

$$g(\mathbf{x}_t) = \mathbf{w}^T\mathbf{x}_t + b \geq +1 \quad for \quad y_t = +1$$
$$g(\mathbf{x}_t) = \mathbf{w}^T\mathbf{x}_t + b \leq -1 \quad for \quad y_t = -1$$

these can be combined into

$$y_t(\mathbf{w}^T\mathbf{x}_t + b) \geq +1$$

support vectors

$$\{\mathbf{x}_t | \mathbf{w}^T\mathbf{x}_t + b = \pm 1\}$$

distance(r) from support vector to $H(\mathbf{w}, b)$

$$r = \frac{\mathbf{w}^T\mathbf{x}_t + b}{||\mathbf{w}||} = \frac{\pm 1}{||\mathbf{w}||}$$

then, the margin is

$$\left| \frac{+1}{||\mathbf{w}||} - \frac{-1}{||\mathbf{w}||} \right| = \frac{2}{||\mathbf{w}||}$$

therefore, we want to minimize: $||\mathbf{w}||$

So, we can re-define SVM optimization problem below:

SVM(primal) optimization problem

$$minimize_{\mathbf{w}} \ \ \frac{1}{2}||\mathbf{w}||^2$$

$$subject\ to\ \ y_t(\mathbf{w}^T\mathbf{x}_t + b) \geq 1,\ \forall t \in [1, N]$$

this is a constrained optimization problem:

- convex quadratic programming
- linear inequality constraints
- $d+1$ parameters, N constraints

note: $\mathbf{x} \in \mathbb{R}^d, \mathbf{w} \in \mathbb{R}^d, y \in \mathbb{R}, b \in \mathbb{R}$, and N training examples

To use QP solver, we need to change SVM optimization problem to Quadratic programming form

$$\mathbf{z} = \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} \in \mathbb{R}^{d+1}$$

$$\frac{1}{2}\mathbf{w}^T\mathbf{w} = \begin{bmatrix} b & \mathbf{w}^T \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} b \\ \mathbf{w}^T \end{bmatrix} = \mathbf{z}^T \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix} \mathbf{z}$$

$$\therefore Q = \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix},\ c = 0$$

$$y_t(\mathbf{w}^T\mathbf{x}_t + b) \geq 1 \equiv \begin{bmatrix} y_n & y_n\mathbf{x}_n^T \end{bmatrix} \mathbf{z} \geq 1$$

$$\Rightarrow \begin{bmatrix} y_1 & y_1\mathbf{x}_1^T \\ \vdots & \vdots \\ y_n & y_n\mathbf{x}_n^T \end{bmatrix} \mathbf{z} \geq \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

$$\therefore A = \begin{bmatrix} y_1 & y_1\mathbf{x}_1^T \\ \vdots & \vdots \\ y_n & y_n\mathbf{x}_n^T \end{bmatrix},\ a = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Using QP solver to get result

$$\mathbf{z}^* \leftarrow QP(Q, c, A, a)$$

1.2 B. SVM의 이중 형태 (dual form) 해를 구하는 방법

1.2.1 Step1: compute Lagrangian function

Given SVM(primal) optimization problem is

$$minimize_{\mathbf{w}} \ \ \frac{1}{2}||\mathbf{w}||^2$$

$ $

$$subject\ to\ \ y_t(\mathbf{w}^T\mathbf{x}_t + b) \geq 1,\ \forall t \in [1, N]$$

this is a constrained optimization problem:

- convex quadratic programming
- linear inequality constraints
- $d+1$ parameters, N constraints

note: $\mathbf{x} \in \mathbb{R}^d, \mathbf{w} \in \mathbb{R}^d, y \in \mathbb{R}, b \in \mathbb{R}$, and N training examples
formulate uncontrained optimization using Lagrange multipliers
Lagrangian function is

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}||\mathbf{w}||^2 - \sum_{t=1}^{N} \alpha_t [y_t(\mathbf{w}^T \mathbf{x}_t + b) - 1]$$

where $\alpha_t \leq 0$ are Lagrange multipliers (aka dual variables)
The solution is determined by saddle point of Lagrangian $\mathcal{L}$
This solution is based on saddle point theorem:

- let P be a constrained optimization problem over $\mathcal{W} = \mathbb{R}^d$
- if $(\mathbf{w}^*, \boldsymbol{\alpha}^*)$ is saddle point of the associated Lagrangian: i.e., $\forall \mathbf{w} \in \mathbb{R}^d,\ \forall \boldsymbol{\alpha} \geq 0,\ \mathcal{L}(\mathbf{w}^*, \boldsymbol{\alpha}) \leq \mathcal{L}(\mathbf{w}^*, \boldsymbol{\alpha}^*) \leq \mathcal{L}(\mathbf{w}, \boldsymbol{\alpha}^*)$
- then $(\mathbf{w}^*, \boldsymbol{\alpha}^*)$ is a solution of the problem P

thus, Lagrangian $\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha})$ should be

- minimized with respect to $\mathbf{w}$ and b $\quad [\mathcal{L}(\mathbf{w}^*, \boldsymbol{\alpha}^*) \leq \mathcal{L}(\mathbf{w}, \boldsymbol{\alpha}^*)]$
- maximized with respect to $\boldsymbol{\alpha}$ $\quad [\mathcal{L}(\mathbf{w}^*, \boldsymbol{\alpha}) \leq \mathcal{L}(\mathbf{w}^*, \boldsymbol{\alpha}^*)]$

1.2.2 Step2: apply the Karush-Kuhn-Tucker (KKT) conditions

Using KKT condition on Lagrangian function becomes the dual problem
The dual problem requires only maximization with respect to $\boldsymbol{\alpha}$ subject to $\boldsymbol{\alpha} \geq 0$
KKT condition: express primal variables $\mathbf{w}$ and b in terms of dual variable $\boldsymbol{\alpha}$

$$\textit{condition } 1: \quad \frac{\partial \mathcal{L}(\mathbf{w}^*, b^*, \boldsymbol{\alpha}^*)}{\partial \mathbf{w}} = 0 \tag{1}$$

$$\textit{condition } 2: \quad \frac{\partial \mathcal{L}(\mathbf{w}^*, b^*, \boldsymbol{\alpha}^*)}{\partial b} = 0 \tag{2}$$

$$\textit{condition } 3: \quad \alpha_t^* [y_t(\mathbf{w}^{*T} \mathbf{x}_t + b^*) - 1] = 0,\ \forall t \in [1, N] \tag{3}$$

$$\tag{4}$$

Given Lagrangian function is

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}||\mathbf{w}||^2 - \sum_{t=1}^{N} \alpha_t [y_t(\mathbf{w}^T \mathbf{x}_t + b) - 1]$$

From condition 1 & 2 :

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \mathbf{w} - \sum_{t=1}^{N} \alpha_t y_t \mathbf{x}_t = 0 \qquad \Rightarrow \quad \mathbf{w} = \sum_{t=1}^{N} \alpha_t y_t \mathbf{x}_t \tag{5}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}} = -\sum_{t=1}^{N} \alpha_t y_t = 0 \qquad \Rightarrow \quad \sum_{t=1}^{N} \alpha_t y_t = 0 \tag{6}$$

$$\tag{7}$$

From condition 3:

$$\alpha_t > 0 \Rightarrow y_t(\mathbf{w}^T \mathbf{x}_t + b^) = 1 \tag{8}$$

$$y_t(\mathbf{w}^T \mathbf{x}_t + b) > 1 \Rightarrow \alpha_t = 0 \tag{9}$$

$$\tag{10}$$

$$\tag{11}$$

$$\therefore \mathbf{w} = \sum_{t=1}^{N} \alpha_t y_t \mathbf{x}_t = \sum_{t=1}^{N_s \ll N} \alpha_t y_t \mathbf{x}_t$$

$$cf. N_s: \ number\ of\ vectors\ associated\ with\ \alpha_t > 0$$

1.2.3 Step3: formulate dual problem

Expand Lagrangian function:

$$\mathcal{L} = \frac{1}{2}||\mathbf{w}||^2 - \sum_{t=1}^{N} \alpha_t y_t \mathbf{w}^T \mathbf{x}_t + b \sum_{t=1}^{N} \alpha_t y_t + \sum_{t=1}^{N} \alpha_t$$

$$\mathcal{L} = \frac{1}{2}||\mathbf{w}||^2 - \sum_{t=1}^{N} \alpha_t y_t \mathbf{w}^T \mathbf{x}_t + \sum_{t=1}^{N} \alpha_t$$

$$(\because \sum_{t=1}^{N} \alpha_t y_t = 0)$$

$$\mathcal{L} = \frac{1}{2}||\sum_{t=1}^{N} \alpha_t y_t \mathbf{x}_t||^2 - \sum_{t=1}^{N} \alpha_t y_t \left(\sum_{s=1}^{N} \alpha_s y_s \mathbf{x}_s \right)^T \mathbf{x}_t + \sum_{t=1}^{N} \alpha_t \tag{12}$$

$$= -\frac{1}{2} \sum_{s=1}^{N} \sum_{t=1}^{N} \alpha_s \alpha_t y_s y_t \mathbf{x}_s^T \mathbf{x}_t + \sum_{t=1}^{N} \alpha_t \tag{13}$$

$$\tag{14}$$

SVM (dual) optimization problem

$$maximize_{\alpha} \quad \sum_{t=1}^{N} \alpha_t - \frac{1}{2} \sum_{s=1}^{N} \sum_{t=1}^{N} \alpha_s \alpha_t y_s y_t \mathbf{x}_s^T \mathbf{x}_t \tag{15}$$

$$subject\ to \quad \sum_{t=1}^{N} \alpha_t y_t = 0 \tag{16}$$

$$\alpha_t \geq 0, \ \forall t \in [1, N] \tag{17}$$

1.2.4 Step4: solve dual problem

conversion of dual form for QP solver:

$$\begin{aligned}
&\mathit{minimize}_{\alpha} \quad \frac{1}{2}\boldsymbol{\alpha}^T Q\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha} &(18)\\
&\mathit{subject\ to} \quad -\boldsymbol{\alpha} \le 0 &(19)\\
&\mathbf{y}^T\boldsymbol{\alpha} = 0 &(20)
\end{aligned}$$

where

$$Q = \begin{bmatrix} y_1y_1\mathbf{x}_1^T\mathbf{x}_1 & y_1y_2\mathbf{x}_1^T\mathbf{x}_2 & \cdots & y_1y_N\mathbf{x}_1^T\mathbf{x}_N \\ y_2y_1\mathbf{x}_2^T\mathbf{x}_1 & y_2y_2\mathbf{x}_2^T\mathbf{x}_2 & \cdots & y_2y_N\mathbf{x}_2^T\mathbf{x}_N \\ \cdots & \cdots & \cdots & \cdots \\ y_Ny_1\mathbf{x}_N^T\mathbf{x}_1 & y_Ny_2\mathbf{x}_N^T\mathbf{x}_2 & \cdots & y_Ny_N\mathbf{x}_N^T\mathbf{x}_N \end{bmatrix}$$

final form

$$\begin{aligned}
&\mathit{minimize}_{\alpha} \quad \frac{1}{2}\boldsymbol{\alpha}^T \begin{bmatrix} y_1y_1\mathbf{x}_1^T\mathbf{x}_1 & y_1y_2\mathbf{x}_1^T\mathbf{x}_2 & \cdots & y_1y_N\mathbf{x}_1^T\mathbf{x}_N \\ y_2y_1\mathbf{x}_2^T\mathbf{x}_1 & y_2y_2\mathbf{x}_2^T\mathbf{x}_2 & \cdots & y_2y_N\mathbf{x}_2^T\mathbf{x}_N \\ \cdots & \cdots & \cdots & \cdots \\ y_Ny_1\mathbf{x}_N^T\mathbf{x}_1 & y_Ny_2\mathbf{x}_N^T\mathbf{x}_2 & \cdots & y_Ny_N\mathbf{x}_N^T\mathbf{x}_N \end{bmatrix} \boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha} &(21)\\
&\mathit{subject\ to} \quad \mathbf{y}^T\boldsymbol{\alpha} = 0 \quad (\mathit{linear\ constraint}) &(22)\\
&0 \le \boldsymbol{\alpha} \le \infty \quad (\mathit{lower\ and\ upper\ bounds}) &(23)\\
& &(24)
\end{aligned}$$

QP solver will return one α per input point

$$\boldsymbol{\alpha} = [\alpha_1 \ \alpha_2 \ \cdots \ \alpha_N]^T$$

1.2.5 Step5: complete the picture

final solutions

$\boldsymbol{\alpha}^*$: obtained by solving final form using QP solver

$\mathbf{w}^*$: linear combination of input vectors in training data

$$\mathbf{w}^* = \sum_{t=1}^{N} \alpha_t^* y_t \mathbf{x}_t$$

b^*: for any positive and negative support vector (x_+ and x_-) :

$$\mathbf{w}^{*T}\mathbf{x}_+ + b = +1$$

$$\mathbf{w}^{*T}\mathbf{x}_- + b = -1$$

solving these equations gives

$$b^* = -\frac{1}{2}(\mathbf{w}^{*T}\mathbf{x}_+ + \mathbf{w}^{*T}\mathbf{x}_-)$$

2 [kernel; 20p] 다음의 함수가 valid kernel 임을 보이세요.

2.1 A. 임의의 행렬 A 에 대한 $K(x,z) = x^T A^T A z$

2.1.1 풀이

Kernal algebra에 의해서

$$K(\mathbf{x},\mathbf{v}) = \mathbf{x}^T B \mathbf{v},$$

When B is positive semi-definite

따라서 $A^T A$ 가 positive semi-definite 라면 주어진 커널은 valid 한 커널이다. eigenvalue 의 정의에 의해

$$Ax = \lambda x$$

$$\begin{aligned} A\lambda x &= \lambda(Ax) && (25)\\ &= \lambda^2 x && (26)\\ &= A^2 x && (27) \end{aligned}$$

positive semi-definite 는 eigenvalue 의 모든값이 음수가 아닌경우이므로 $A^T A$ 의 모든 고유값은 음수가 아닌 값을 가지게된다.

$$\because A^2 x = \lambda^2 x$$

따라서 주어진 $K(x,z) = x^T A^T A z$ 은 valid kernel이다.

2.2 B. $K(x,z) = (x^T z + c)^2$

2.2.1 풀이

$$\begin{aligned} K(\mathbf{x},\mathbf{z}) &= \left(\sum_{j=1}^{n} x^{(j)} z^{(j)} + c\right)\left(\sum_{l=1}^{n} x^{(l)} z^{(l)} + c\right) && (28)\\ &= \sum_{j=1}^{n}\sum_{l=1}^{n} x^{(j)} x^{(l)} z^{(j)} z^{(l)} + 2c\sum_{j=1}^{n} x^{(j)} z^{(j)} + c^2 && (29)\\ &= \sum_{j,l=1}^{n} (x^{(j)} x^{(l)})(z^{(j)} z^{(l)}) + \sum_{j=1}^{n} (\sqrt{2c}\,x^{(j)})(\sqrt{2c}\,z^{(j)}) + c^2 && (30)\\ &= \Phi(\mathbf{x}) \cdot \Phi(\mathbf{z}) && (31) \end{aligned}$$

$$\Phi(\mathbf{x}) = [x^{(1)2}, x^{(1)}x^{(2)},\ \ldots, x^{(3)2}, \sqrt{2c}\,x^{(1)}, \sqrt{2c}\,x^{(2)}, \sqrt{2c}\,x^{(3)}, c]$$

3 [HMM; 40p]

3.1 It is well known that a DNA sequence is a series of components from A, C, G, T. Now let's assume there is one hidden variable S that controls the generation of DNA sequence. S takes 2 possible states $\{S1, S2\}$. Assume the following transition probabilities for HMM M

$$P(S1|S1) = 0.8, P(S2|S1) = 0.2, P(S1|S2) = 0.2, P(S2|S2) = 0.8$$

emission probabilities as following

$$P(A|S1) = 0.4, P(C|S1) = 0.1, P(G|S1) = 0.4, P(T|S1) = 0.1$$

$$P(A|S2) = 0.1, P(C|S2) = 0.4, P(G|S2) = 0.1, P(T|S2) = 0.4$$

and start probabilities as following

$$P(S1) = 0.5, P(S2) = 0.5$$

Assume the observed sequence is $x = CGTCAG$, calculate:

3.2 A. Draw the state diagram of this HMM M and mark the transition probabilities.

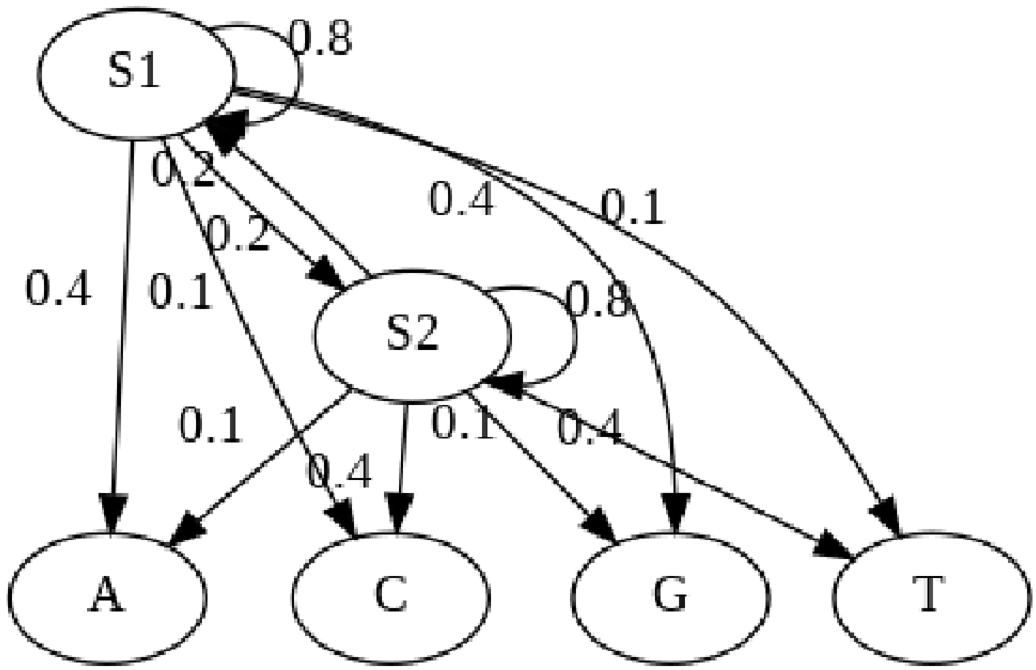
In [0]:
```
# Install library
!sudo apt-get install python-dev graphviz libgraphviz-dev pkg-config
!pip install pygraphviz
```

```
Reading package lists… Done
Building dependency tree
Reading state information… Done
pkg-config is already the newest version (0.29.1-0ubuntu2).
python-dev is already the newest version (2.7.15~rc1-1).
graphviz is already the newest version (2.40.1-2).
The following package was automatically installed and is no longer required:
  libnvidia-common-410
Use 'sudo apt autoremove' to remove it.
The following additional packages will be installed:
  libgail-common libgail18 libgtk2.0-0 libgtk2.0-bin libgtk2.0-common
  libgvc6-plugins-gtk libxdot4
Suggested packages:
  gvfs
The following NEW packages will be installed:
  libgail-common libgail18 libgraphviz-dev libgtk2.0-0 libgtk2.0-bin
  libgtk2.0-common libgvc6-plugins-gtk libxdot4
0 upgraded, 8 newly installed, 0 to remove and 8 not upgraded.
Need to get 2,120 kB of archives.
After this operation, 7,128 kB of additional disk space will be used.
Get:1 http://archive.ubuntu.com/ubuntu bionic/main amd64 libgtk2.0-common all 2.24.32-1ubuntu1
Get:2 http://archive.ubuntu.com/ubuntu bionic/main amd64 libgtk2.0-0 amd64 2.24.32-1ubuntu1 [1
Get:3 http://archive.ubuntu.com/ubuntu bionic/main amd64 libgail18 amd64 2.24.32-1ubuntu1 [14.
Get:4 http://archive.ubuntu.com/ubuntu bionic/main amd64 libgail-common amd64 2.24.32-1ubuntu1
Get:5 http://archive.ubuntu.com/ubuntu bionic/universe amd64 libxdot4 amd64 2.40.1-2 [15.7 kB]
Get:6 http://archive.ubuntu.com/ubuntu bionic/universe amd64 libgvc6-plugins-gtk amd64 2.40.1-
Get:7 http://archive.ubuntu.com/ubuntu bionic/universe amd64 libgraphviz-dev amd64 2.40.1-2 [5
Get:8 http://archive.ubuntu.com/ubuntu bionic/main amd64 libgtk2.0-bin amd64 2.24.32-1ubuntu1
Fetched 2,120 kB in 6s (366 kB/s)
debconf: unable to initialize frontend: Dialog
debconf: (No usable dialog-like program is installed, so the dialog based frontend cannot be us
debconf: falling back to frontend: Readline
```

```
debconf: unable to initialize frontend: Readline
debconf: (This frontend requires a controlling tty.)
debconf: falling back to frontend: Teletype
dpkg-preconfigure: unable to re-open stdin:
Selecting previously unselected package libgtk2.0-common.
(Reading database ··· 130912 files and directories currently installed.)
Preparing to unpack ···/0-libgtk2.0-common_2.24.32-1ubuntu1_all.deb ···
Unpacking libgtk2.0-common (2.24.32-1ubuntu1) ···
Selecting previously unselected package libgtk2.0-0:amd64.
Preparing to unpack ···/1-libgtk2.0-0_2.24.32-1ubuntu1_amd64.deb ···
Unpacking libgtk2.0-0:amd64 (2.24.32-1ubuntu1) ···
Selecting previously unselected package libgail18:amd64.
Preparing to unpack ···/2-libgail18_2.24.32-1ubuntu1_amd64.deb ···
Unpacking libgail18:amd64 (2.24.32-1ubuntu1) ···
Selecting previously unselected package libgail-common:amd64.
Preparing to unpack ···/3-libgail-common_2.24.32-1ubuntu1_amd64.deb ···
Unpacking libgail-common:amd64 (2.24.32-1ubuntu1) ···
Selecting previously unselected package libxdot4.
Preparing to unpack ···/4-libxdot4_2.40.1-2_amd64.deb ···
Unpacking libxdot4 (2.40.1-2) ···
Selecting previously unselected package libgvc6-plugins-gtk.
Preparing to unpack ···/5-libgvc6-plugins-gtk_2.40.1-2_amd64.deb ···
Unpacking libgvc6-plugins-gtk (2.40.1-2) ···
Selecting previously unselected package libgraphviz-dev.
Preparing to unpack ···/6-libgraphviz-dev_2.40.1-2_amd64.deb ···
Unpacking libgraphviz-dev (2.40.1-2) ···
Selecting previously unselected package libgtk2.0-bin.
Preparing to unpack ···/7-libgtk2.0-bin_2.24.32-1ubuntu1_amd64.deb ···
Unpacking libgtk2.0-bin (2.24.32-1ubuntu1) ···
Setting up libgtk2.0-common (2.24.32-1ubuntu1) ···
Setting up libxdot4 (2.40.1-2) ···
Processing triggers for libc-bin (2.27-3ubuntu1) ···
Processing triggers for man-db (2.8.3-2ubuntu0.1) ···
Setting up libgtk2.0-0:amd64 (2.24.32-1ubuntu1) ···
Setting up libgail18:amd64 (2.24.32-1ubuntu1) ···
Setting up libgail-common:amd64 (2.24.32-1ubuntu1) ···
Setting up libgvc6-plugins-gtk (2.40.1-2) ···
Setting up libgraphviz-dev (2.40.1-2) ···
Setting up libgtk2.0-bin (2.24.32-1ubuntu1) ···
Processing triggers for libc-bin (2.27-3ubuntu1) ···
Collecting pygraphviz
  Downloading https://files.pythonhosted.org/packages/7e/b1/d6d849ddaf6f11036f9980d433f383d4c1
     |                  | 122kB 5.1MB/s
Building wheels for collected packages: pygraphviz
  Building wheel for pygraphviz (setup.py) ··· done
  Stored in directory: /root/.cache/pip/wheels/65/54/69/1aee9e66ab19916293208d4c9de0d3898adebe
Successfully built pygraphviz
Installing collected packages: pygraphviz
```

```
Successfully installed pygraphviz-1.5
```

```
In [0]: import matplotlib.pyplot as plt
        from PIL import Image
        from networkx.drawing.nx_agraph import to_agraph

        import networkx as nx

        G = nx.MultiDiGraph()

        G.add_edge('S1', 'S1', 1, weight=0.8)
        G.add_edge('S1', 'S2', 2, weight=0.2)

        G.add_edge('S2', 'S1', 3, weight=0.2)
        G.add_edge('S2', 'S2', 4, weight=0.8)

        G.add_edge('S1', 'A', weight=0.4)
        G.add_edge('S1', 'C', weight=0.1)
        G.add_edge('S1', 'G', weight=0.4)
        G.add_edge('S1', 'T', weight=0.1)

        G.add_edge('S2', 'A', weight=0.1)
        G.add_edge('S2', 'C', weight=0.4)
        G.add_edge('S2', 'G', weight=0.1)
        G.add_edge('S2', 'T', weight=0.4)

        A = to_agraph(G)
        A.layout('dot')

        edge_lbs = nx.get_edge_attributes(G,'weight')
        graph = dict(((u, v), edge_lbs[u,v,k]) for u, v, k in edge_lbs)

        for pair in graph:
            edge = A.get_edge(pair[0], pair[1])
            edge.attr['label'] = str(graph[pair]) + "  "

        A.draw('HMM.png')
        img = Image.open('HMM.png')
        plt.figure(figsize=(10,10))
        plt.axis('off')
        plt.imshow(img)

Out[0]: <matplotlib.image.AxesImage at 0x7f4f1d95f748>
```



3.3 B. P(x|M) using the forward algorithm. Show your work to get full credit.

```
In [0]: # Setup data for processing forward backward algorithm
        import numpy as np
        import pandas as pd
        import networkx as nx

        hidden_states = ['S1', 'S2']
        pi = [0.5, 0.5]
        state_space = pd.Series(pi, index=hidden_states, name='states')
        print(state_space)
        print('\n', state_space.sum())
```

```
S1    0.5
S2    0.5
Name: states, dtype: float64

 1.0
```

```
In [0]: # create hidden transition matrix
        # a or alpha
        #   = transition probability matrix of changing states given a state
        # matrix is size (M x M) where M is number of states
```

```python
a_df = pd.DataFrame(columns=hidden_states, index=hidden_states)
a_df.loc[hidden_states[0]] = [0.8, 0.2]
a_df.loc[hidden_states[1]] = [0.2, 0.8]

print(a_df)

a = a_df.values
print('\n', a, a.shape, '\n')
print(a_df.sum(axis=1))
```

```
     S1   S2
S1  0.8  0.2
S2  0.2  0.8

 [[0.8 0.2]
 [0.2 0.8]] (2, 2)

S1    1.0
S2    1.0
dtype: float64
```

In [0]:
```python
states = ['A', 'C', 'G', 'T']
observable_states = states

b_df = pd.DataFrame(columns=observable_states, index=hidden_states)
b_df.loc[hidden_states[0]] = [0.4, 0.1, 0.4, 0.1]
b_df.loc[hidden_states[1]] = [0.1, 0.4, 0.1, 0.4]

print(b_df)

b = b_df.values
print('\n', b, b.shape, '\n')
print(b_df.sum(axis=1))
```

```
      A    C    G    T
S1  0.4  0.1  0.4  0.1
S2  0.1  0.4  0.1  0.4

 [[0.4 0.1 0.4 0.1]
 [0.1 0.4 0.1 0.4]] (2, 4)

S1    1.0
S2    1.0
dtype: float64
```

In [0]:
```python
obs_map = {'A':0, 'C':1, 'G':2, "T":3}
obs = np.array([1,2,3,1,0,2])
```

```
        inv_obs_map = dict((v,k) for k, v in obs_map.items())
        obs_seq = [inv_obs_map[v] for v in list(obs)]

        print( pd.DataFrame(np.column_stack([obs, obs_seq]),
                        columns=['Obs_code', 'Obs_seq']) )
```

```
  Obs_code Obs_seq
0        1       C
1        2       G
2        3       T
3        1       C
4        0       A
5        2       G
```

```
In [0]: def forward(pi, a, b, obs):

            nStates = np.shape(b)[0]
            T = np.shape(obs)[0]

            # alpha --> highest probability of any path that reaches state i
            alpha = np.zeros((nStates, T))

            # init alpha and phi
            alpha[:, 0] = pi * b[:, obs[0]]

            print('\nForward Algorithm Process\n')

            print('s={s} and t={t}: alpha[{s}, {t}] = {alpha}'.format(s=0, t=0, alpha=alpha[0,
            print('s={s} and t={t}: alpha[{s}, {t}] = {alpha}'.format(s=1, t=0, alpha=alpha[1,

            for t in range(1, T):
                for s in range(nStates):
                    alpha[s, t] = np.sum(alpha[:, t-1]* a[:, s]) * b[s, obs[t]]
                    print('s={s} and t={t}: alpha[{s}, {t}] = {alpha}'.format(s=s, t=t, alpha=a

            return alpha
        alpha = forward(pi, a, b, obs)
        print('\n')
        df = (pd.DataFrame()
         .assign(alpha = ['t=1','t=2','t=3','t=4','t=5','t=6'])
         .assign(S1 = alpha[0])
         .assign(S2 = alpha[1]))
        display(df)
        print('\tcf. P(x|M) = alpha')
```

```
Forward Algorithm Process
```

```
s=0 and t=0: alpha[0, 0] = 0.05
s=1 and t=0: alpha[1, 0] = 0.2
s=0 and t=1: alpha[0, 1] = 0.03200000000000001
s=1 and t=1: alpha[1, 1] = 0.017000000000000005
s=0 and t=2: alpha[0, 2] = 0.002900000000000001
s=1 and t=2: alpha[1, 2] = 0.008000000000000004
s=0 and t=3: alpha[0, 3] = 0.0003920000000000002
s=1 and t=3: alpha[1, 3] = 0.0027920000000000015
s=0 and t=4: alpha[0, 4] = 0.00034880000000000024
s=1 and t=4: alpha[1, 4] = 0.00023120000000000017
s=0 and t=5: alpha[0, 5] = 0.0001301120000000001
s=1 and t=5: alpha[1, 5] = 2.5472000000000023e-05
```

	alpha	S1	S2
0	t=1	0.050000	0.200000
1	t=2	0.032000	0.017000
2	t=3	0.002900	0.008000
3	t=4	0.000392	0.002792
4	t=5	0.000349	0.000231
5	t=6	0.000130	0.000025

```
cf. P(x|M) = alpha
```

3.4 C. The posterior probabilities $P(\pi_i = S1|x, M)$ for $i = 1, ..., 6$. Show your work to get full credit.

```
In [0]: def backward(pi, a, b, obs):

            nStates = np.shape(b)[0]
            T = np.shape(obs)[0]

            # alpha --> highest probability of any path that reaches state i
            alpha = np.zeros((nStates, T))

            # init alpha and phi
            alpha[:, 0] = pi * b[:, obs[0]]

            # Forward Algorithm Process
            for t in range(1, T):
                for s in range(nStates):
                    alpha[s, t] = np.sum(alpha[:, t-1]* a[:, s]) * b[s, obs[t]]
```

```
    # Backward Algorithm Process
    beta = np.ones((nStates, T))
    print('s={s} and t={t}: beta[{s}, {t}] = {beta}'.format(s=0, t=5, beta=beta[s, t]))
    print('s={s} and t={t}: beta[{s}, {t}] = {beta}'.format(s=1, t=5, beta=beta[s, t]))

    for i, t in enumerate(range(T-2, -1, -1)):
        for s in range(nStates):
            beta[s,t] = np.sum(beta[:, t+1]* a[:, s] * b[:, obs[t+1]])
            print('s={s} and t={t}: beta[{s}, {t}] = {beta}'.format(s=s, t=t, beta=beta

    total = np.sum(alpha[:, 0]*beta[:, 0])
    P = alpha[0,:]*beta[0,:]/total
    return beta, P

beta, P = backward(pi, a, b, obs)

print('\n\n')
df = (pd.DataFrame()
 .assign(beta=['t=1','t=2','t=3','t=4','t=5','t=6'])
 .assign(S1=beta[0])
 .assign(S2=beta[1]))
display(df)
print('\tcf. beta = P(O_t+1,...,O_T|S_i)')
print('\n Posterior')
df = (pd.DataFrame()
 .assign(P_S1=['t=1','t=2','t=3','t=4','t=5','t=6'])
 .assign(S1=P))
display(df)
print('\tcf. P_S1= P(pi_1 = S1| x,M)')
```

```
s=0 and t=5: beta[0, 5] = 1.0
s=1 and t=5: beta[1, 5] = 1.0
s=0 and t=4: beta[0, 4] = 0.3400000000000001
s=1 and t=4: beta[1, 4] = 0.16000000000000003
s=0 and t=3: beta[0, 3] = 0.11200000000000003
s=1 and t=3: beta[1, 3] = 0.040000000000000015
s=0 and t=2: beta[0, 2] = 0.012160000000000004
s=1 and t=2: beta[1, 2] = 0.015040000000000006
s=0 and t=1: beta[0, 1] = 0.002176000000000001
s=1 and t=1: beta[1, 1] = 0.005056000000000002
s=0 and t=0: beta[0, 0] = 0.0007974400000000004
s=1 and t=0: beta[1, 0] = 0.0005785600000000003
```

beta	S1	S2

```
0  t=1  0.000797  0.000579
1  t=2  0.002176  0.005056
2  t=3  0.012160  0.015040
3  t=4  0.112000  0.040000
4  t=5  0.340000  0.160000
5  t=6  1.000000  1.000000
```

```
        cf. beta = P(O_t+1,⋯,O_T|S_i)
```

```
 Posterior
```

```
  P_S1        S1
0  t=1  0.256273
1  t=2  0.447552
2  t=3  0.226656
3  t=4  0.282188
4  t=5  0.762238
5  t=6  0.836281
```

```
        cf. P_S1= P(pi_1 = S1| x,M)
```

3.5 D. The most likely path of hidden states using the Viterbi algorithm. Show your work to get full credit.

In [38]:
```
def viterbi(pi, a, b, obs):

    nStates = np.shape(b)[0]
    T = np.shape(obs)[0]

    # init blank path
    path = np.zeros(T)
    # delta --> highest probability of any path that reaches state i
    delta = np.zeros((nStates, T))
    # phi --> argmax by time step for each state
    phi = np.zeros((nStates, T))

    # init delta and phi
    delta[:, 0] = pi * b[:, obs[0]]
    phi[:, 0] = 0

    print('\nStart Walk Forward\n')
    # the forward algorithm extension
    for t in range(1, T):
        for s in range(nStates):
            delta[s, t] = np.max(delta[:, t-1] * a[:, s]) * b[s, obs[t]]
```

```
                phi[s, t] = np.argmax(delta[:, t-1] * a[:, s])
                print('s={s} and t={t}: phi[{s}, {t}] = {phi}'.format(s=s, t=t, phi=phi[s

        # find optimal path
        print('-'*50)
        print('Start Backtrace\n')
        path[T-1] = np.argmax(delta[:, T-1])

        for t in range(T-2, -1, -1):
            path[t] = phi[int(path[t+1]), [t+1]]
            print('path[{}] = {}'.format(t, path[t]))

        return path, delta, phi

    path, delta, phi = viterbi(pi, a, b, obs)
    print('\nsingle best state path: \n', path)
    print('delta:\n', delta)
    print('phi:\n', phi)
    df = (pd.DataFrame()
     .assign(delta=['t=1','t=2','t=3','t=4','t=5','t=6'])
     .assign(S1=delta[0])
     .assign(S2=delta[1]))
    display(df)
```

```
Start Walk Forward

s=0 and t=1: phi[0, 1] = 0.0
s=1 and t=1: phi[1, 1] = 1.0
s=0 and t=2: phi[0, 2] = 0.0
s=1 and t=2: phi[1, 2] = 1.0
s=0 and t=3: phi[0, 3] = 0.0
s=1 and t=3: phi[1, 3] = 1.0
s=0 and t=4: phi[0, 4] = 1.0
s=1 and t=4: phi[1, 4] = 1.0
s=0 and t=5: phi[0, 5] = 0.0
s=1 and t=5: phi[1, 5] = 1.0
--------------------------------------------------
Start Backtrace

path[4] = 0.0
path[3] = 1.0
path[2] = 1.0
path[1] = 1.0
path[0] = 1.0

single best state path:
 [1. 1. 1. 1. 0. 0.]
```

```
delta:
 [[5.000000e-02 1.600000e-02 1.280000e-03 1.024000e-04 1.310720e-04
  4.194304e-05]
 [2.000000e-01 1.600000e-02 5.120000e-03 1.638400e-03 1.310720e-04
  1.048576e-05]]
phi:
 [[0. 0. 0. 0. 1. 0.]
 [0. 1. 1. 1. 1. 1.]]
```

```
  delta        S1        S2
0   t=1  0.050000  0.200000
1   t=2  0.016000  0.016000
2   t=3  0.001280  0.005120
3   t=4  0.000102  0.001638
4   t=5  0.000131  0.000131
5   t=6  0.000042  0.000010
```

In [0]:
```python
state_map = {0:'S1', 1:'S2'}
state_path = [state_map[v] for v in path]

(pd.DataFrame()
 .assign(Observation=obs_seq)
 .assign(Best_Path=state_path))
```

Out[0]:
```
  Observation Best_Path
0           C        S2
1           G        S2
2           T        S2
3           C        S2
4           A        S1
5           G        S1
```