Mixturas de Gaussianas[1]

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[1] Para una correcta visualización, se requiere Acrobat Reader v. 7.0 o superior

Índice

1. El corpus MNIST

- MNIST: 60K imágenes de entrenamiento y 10K de test.

mnist_sizes.sh
```
#!/usr/bin/octave
load("train-images-idx3-ubyte.mat.gz"); size(X)
load("train-labels-idx1-ubyte.mat.gz"); size(xl)
load("t10k-images-idx3-ubyte.mat.gz");  size(Y)
load("t10k-labels-idx1-ubyte.mat.gz");  size(yl)
```

```
ans =   60000      784
ans =   60000        1
ans =   10000      784
ans =   10000        1
```

- Visualización:

mnist_show.sh
```
#!/usr/bin/octave
load("train-images-idx3-ubyte.mat.gz");
for n=1:50
  x=reshape(X(n,:),28,28); imshow((255-x)',[]); pause(.5);
end
```

- ***trains:*** primeras N imágenes de entrenamiento.

trains.sh
```
#!/usr/bin/octave
load("train-images-idx3-ubyte.mat.gz"); T=X;
load("train-labels-idx1-ubyte.mat.gz"); Tl=xl;
for N=[2000 20000]
  X=T(1:N,:); save("-z",sprintf("train%d-images.gz",N),"X");
  xl=Tl(1:N); save("-z",sprintf("train%d-labels.gz",N),"xl");
end
```

- Experimento sencillo con el vecino más próximo:

nn.sh
```
#!/usr/bin/octave
if (nargin!=2) printf("%s fX fxl\n",program_name()); exit; end
arg_list=argv(); fX=arg_list{1}; fxl=arg_list{2};
load(sprintf(fX)); load(sprintf(fxl));
N=rows(X); NTr=round(.7*N); NTe=N-NTr; rec=zeros(NTe,1);
for m=1:NTe
  x=X(NTr+m,:)'; nmin=1; min=inf;
  for n=1:NTr
    xn=X(n,:)'; a=x-xn; d=a'*a; if (d<min) min=d; nmin=n; endif
  end
  rec(m)=xl(nmin);
end
[Nerr m]=confus(xl(NTr+1:N),rec);
printf("%s %s %d %d %.1f\n",fX,fxl,Nerr,NTe,100.0*Nerr/NTe);
```

```
./nn.sh train2000-images.gz train2000-labels.gz
train2000-images.gz train2000-labels.gz 64 600 10.7
```

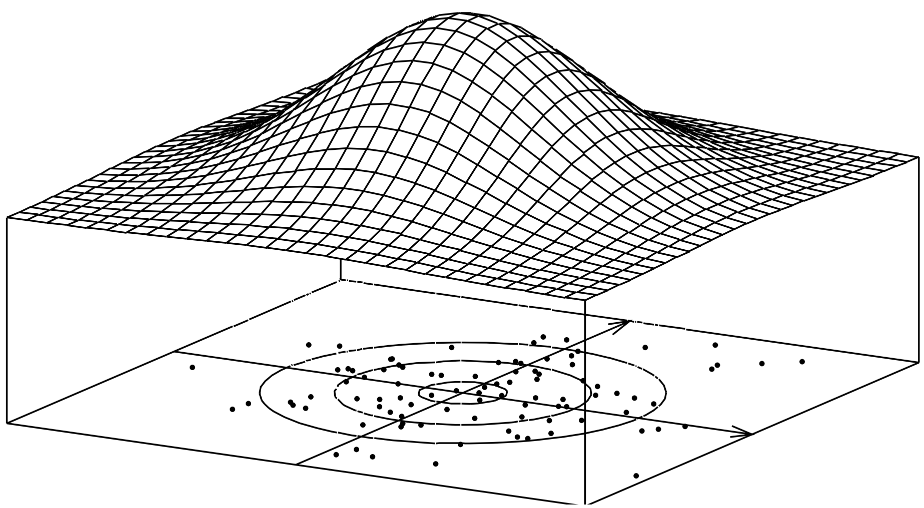
2. El clasificador Gaussiano

2.1. La distribución Gaussiana multivariada

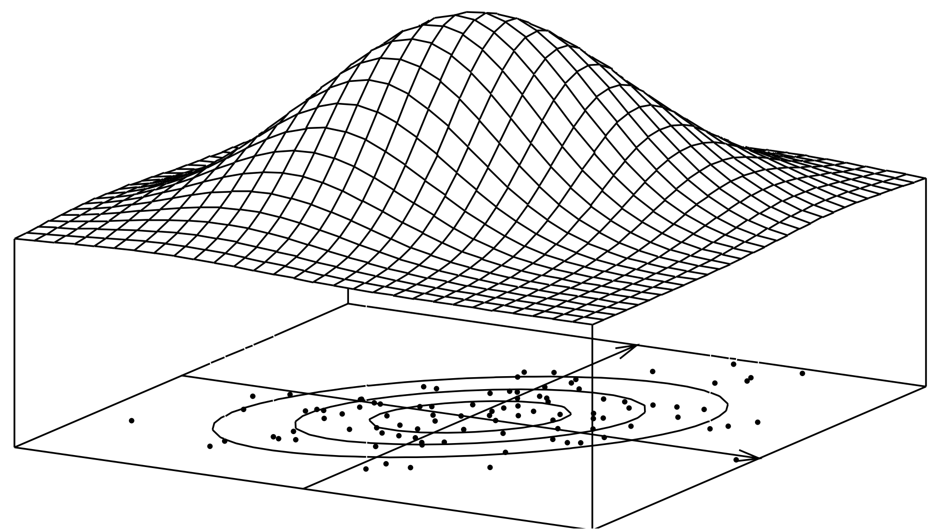
- Sea $\boldsymbol{\mu} \in \mathbb{R}^D$ y sea $\Sigma \in \mathbb{R}^{D \times D}$ simétrica y definida positiva.
- Un vector de características $\boldsymbol{x} \in \mathbb{R}^D$ es $N_D(\boldsymbol{\mu}, \Sigma)$ si su f.d.p. es:

$$p(\boldsymbol{x}) = (2\pi)^{-\frac{D}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^t \Sigma^{-1} (\boldsymbol{x}-\boldsymbol{\mu})\right)$$

Ejemplos:



$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



$$\Sigma = \begin{pmatrix} 1 & 0{,}5 \\ 0{,}5 & 1 \end{pmatrix}$$

2.2. El clasificador Gaussiano

- El clasificador de Bayes para un vector D-dimensional $\boldsymbol{x}$ es:

$$c^*(\boldsymbol{x}) = \arg\max_c \; p(c \mid \boldsymbol{x}) = \arg\max_c \; p(c)\, p(\boldsymbol{x} \mid c)$$

- Suponemos que las densidades condicionales son Gaussianas:

$$p(\boldsymbol{x} \mid c) \sim N_D(\boldsymbol{\mu}_c, \Sigma_c) \qquad \text{(para todo } c\text{)}$$

- El clasificador de Bayes se reduce al ***clasificador Gaussiano:***

$$c^*(\boldsymbol{x}) = \arg\max_c \; \ln p(c) + \ln p(\boldsymbol{x} \mid c)$$

donde, omitiendo la constante aditiva $-\frac{D}{2}\ln(2\pi)$:

$$\ln p(\boldsymbol{x} \mid c) = -\frac{1}{2}\ln|\Sigma_c| - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_c)^t \Sigma_c^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_c)$$

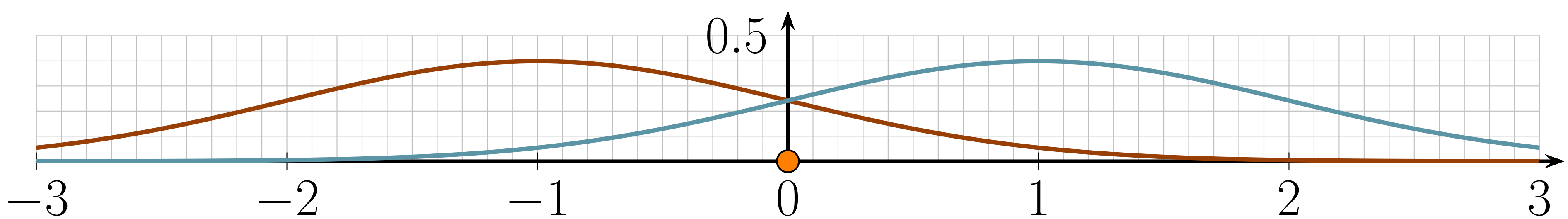
- El clasificador Gaussiano es ***cuadrático*** con $\boldsymbol{x}$:

$$c^*(\boldsymbol{x}) = \arg\max_c \; g_c(\boldsymbol{x}) \quad \text{con} \quad g_c(\boldsymbol{x}) = \boldsymbol{x}^t\, W_c\, \boldsymbol{x} + \boldsymbol{w}_c^t\, \boldsymbol{x} + w_{c0}$$

donde

$$W_c = -\frac{1}{2}\Sigma_c^{-1}$$
$$\boldsymbol{w}_c = \Sigma_c^{-1}\boldsymbol{\mu}_c$$
$$w_{c0} = \ln p(c) - \frac{1}{2}\ln|\Sigma_c| - \frac{1}{2}\boldsymbol{\mu}_c^t\Sigma_c^{-1}\boldsymbol{\mu}_c$$

- **Ejemplo:** $C=2 \;\; D=1 \;\; p(1)=p(2)=\frac{1}{2} \quad \mu_1=-1 \;\; \mu_2=1 \quad \sigma_1^2=\sigma_2^2=1$



$$g_c(x) = -\frac{1}{2\sigma_c^2}x^2 + \frac{\mu_c}{\sigma_c^2}x + \ln p(c) - \frac{1}{2}\ln\sigma_c^2 - \frac{\mu_c^2}{2\sigma_c^2}$$

$$\left.\begin{array}{l} g_1(x) = -x \\ g_2(x) = x \end{array}\right\} \rightarrow \quad c^*(x) = \begin{cases} \mathbf{1} & \text{si } x < 0 \\ \mathbf{2} & \text{si } x \geq 0 \end{cases}$$

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- $\ln|\Sigma|$: $|\Sigma| = \prod_d \lambda_d \;\Rightarrow\; \ln|\Sigma| = \sum_d \ln\lambda_d$

logdet.m

```
function v=logdet(S)
  L=eig(S); if any(L<=0) v=log(realmin); else v=sum(log(L)); end
end
```

- $g_c(\boldsymbol{x}) - \ln p(c) = -\frac{1}{2}\left(\boldsymbol{x}^t\Sigma_c^{-1}\boldsymbol{x} + \ln|\Sigma_c| + \boldsymbol{\mu}_c^t\Sigma_c^{-1}\boldsymbol{\mu}_c\right) + \boldsymbol{x}^t\Sigma_c^{-1}\boldsymbol{\mu}_c$

$$\boldsymbol{g}_c(\boldsymbol{X}) - \ln p(c) = -\frac{1}{2}\left(\boldsymbol{X}\Sigma_c^{-1} \odot \boldsymbol{X}\mathbf{1}_D + \ln|\Sigma_c| + \boldsymbol{\mu}_c^t\Sigma_c^{-1}\boldsymbol{\mu}_c\right) + \boldsymbol{X}\Sigma_c^{-1}\boldsymbol{\mu}_c$$

compute_pxGc.m

```
function [pxGc]=compute_pxGc(m,S,X)
  I=pinv(S); pxGc=-.5*(sum((X*I).*X,2)+logdet(S)+m'*I*m)+X*I*m;
end
```

octave

```
X=[-3:3]'; [X compute_pxGc(-1,1,X) compute_pxGc(1,1,X)]
ans = -3.00000  -2.00000  -8.00000
      -2.00000  -0.50000  -4.50000
      -1.00000   0.00000  -2.00000
       0.00000  -0.50000  -0.50000
       1.00000  -2.00000   0.00000
       2.00000  -4.50000  -0.50000
       3.00000  -8.00000  -2.00000
```


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2.3. Estimación máximo-verosímil

▸ ***Log-verosimilitud*** de $\boldsymbol{\Theta} = \{(p(c), \boldsymbol{\mu}_c, \Sigma_c)\}$ respecto a $\{(\boldsymbol{x}_n, c_n)\}$:

$$L(\boldsymbol{\Theta}) = \sum_c \sum_{n:c_n=c} \ln p(c) - \frac{1}{2} \ln |\Sigma_c| - \frac{1}{2} (\boldsymbol{x}_n - \boldsymbol{\mu}_c)^t \Sigma_c^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_c)$$

▸ ***Estimador máximo-verosímil*** de $\boldsymbol{\Theta}$,$\hat{\boldsymbol{\Theta}}$: para todo c:

$$\hat{p}(c) = \frac{N_c}{N}$$

$$\hat{\boldsymbol{\mu}}_c = \frac{1}{N_c} \sum_{n:c_n=c} \boldsymbol{x}_n$$

$$\hat{\Sigma}_c = \frac{1}{N_c} \sum_{n:c_n=c} (\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_c)(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_c)^t$$

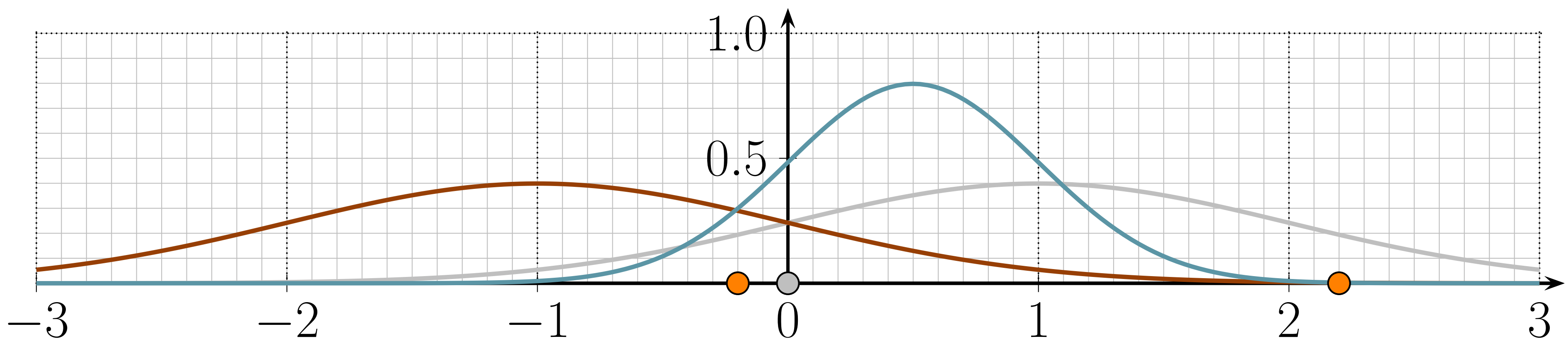
▸ ***Suavizado*** de matrices de covarianzas: $0 \leq \alpha \leq 1$

$$\tilde{\Sigma}_c = \alpha\, \hat{\Sigma}_c + (1 - \alpha)\, I_D$$

Ej. (cont.): $C=2\;\; D=1\;\; p(1)=p(2)=\frac{1}{2}\;\; \mu_1=-1\;\; \mu_2=1\;\; \sigma_1^2=\sigma_2^2=1$

$$\{(-2,1),(0,2),(0,1),(1,2)\}\rightarrow\begin{cases}\hat{p}(1)=\hat{p}(2)=\frac{2}{4}\\ \hat{\mu}_1=-1 \quad \hat{\mu}_2=0{,}5\\ \hat{\sigma}_1^2=1 \quad \hat{\sigma}_2^2=0{,}25\end{cases}$$

$$\rightarrow\begin{cases}\hat{g}_1(x)=-\frac{1}{2}\,x^2-x\\ \hat{g}_2(x)=-2\,x^2+2\,x+\ln 2\end{cases}\xrightarrow{\hat{g}_1(x)=\hat{g}_2(x)} x=\begin{cases}-0{,}2\\ 2{,}2\end{cases}$$



$$\hat{c}(x)=\begin{cases}\mathbf{1} & x\notin[-0{,}2,\,2{,}2]\\ \mathbf{2} & x\in[-0{,}2,\,2{,}2]\end{cases}\;\approx\; c^*(x)$$

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gaussian.m

```
function [eY]=gaussian(X,xl,Y,yl,a)
  ll=unique(xl); N=rows(X); M=rows(Y); D=columns(X);
  for c=ll'; ic=find(c==ll);
    Xc=X(find(xl==c),:); Nc=rows(Xc); pc(ic)=Nc/N;
    mc=mean(Xc); m(:,ic)=mc'; S{ic}=((Xc-mc)'*(Xc-mc))/Nc; end
  for i=1:length(a)
    for c=ll'; ic=find(c==ll); sS=a(i)*S{ic}+(1-a(i))*eye(D);
      gY(:,ic)=log(pc(ic))+compute_pxGc(m(:,ic),sS,Y); end
    [~,idY]=max(gY'); eY(i)=mean(ll(idY)!=yl)*100; end
end
```

ge.sh

```
#!/usr/bin/octave
if (nargin!=5) printf("ge.sh X xl as tr%% dev%%\n"); exit(1); end
arg_list=argv(); fX=arg_list{1}; load(fX);
fxl=arg_list{2}; load(fxl); a=str2num(arg_list{3});
tp=str2num(arg_list{4}); dp=str2num(arg_list{5});
N=rows(X); rand("seed",23); p=randperm(N); X=X(p,:); xl=xl(p,:);
Nt=round(tp/100*N); Nd=round(dp/100*N);
Xt=X(1:Nt,:); xlt=xl(1:Nt); Xd=X(N-Nd+1:N,:); xld=xl(N-Nd+1:N);
[ed]=gaussian(Xt,xlt,Xd,xld,a);
printf("\n  alpha dv-err\n------- ------\n");
for i=1:length(a); printf("%.1e %6.3f\n",a(i),ed(i)); end
```

```
time ./ge.sh train-images-idx3-ubyte.mat.gz
↪ train-labels-idx1-ubyte.mat.gz "[1e-5 1e-4 1e-3]" 90 10
  alpha dv-err
------- ------
1.0e-05  6.317
1.0e-04  4.267
1.0e-03  6.383
real   1m15,827s
user   2m14,806s
sys    0m17,510s
```

- ***Experimento final:*** fijamos el hiperparámetro $\alpha \triangleq 10^{-4}$ y usamos t10k por primera y única vez para estimar el error del Gaussiano

ge2.sh

```
#!/usr/bin/octave
if (nargin!=5) printf("ge2.sh X xl Y yl a\n"); exit(1); end;
arg_list=argv(); a=str2num(arg_list{5});
fX=arg_list{1}; load(fX); fxl=arg_list{2}; load(fxl);
fY=arg_list{3}; load(fY); fyl=arg_list{4}; load(fyl);
[e]=gaussian(X,xl,Y,yl,a);
printf("\n alpha te-err\n------- ------\n");
printf("%.1e %6.3f\n",a,e);
```

```
time ./ge2.sh train-images-idx3-ubyte.mat.gz
↪ train-labels-idx1-ubyte.mat.gz t10k-images-idx3-ubyte.mat.gz
↪ t10k-labels-idx1-ubyte.mat.gz 1e-4
 alpha te-err
------- ------
1.0e-04  4.180
real   0m38,028s
user   1m8,171s
sys    0m8,949s
```

3. Mixturas finitas

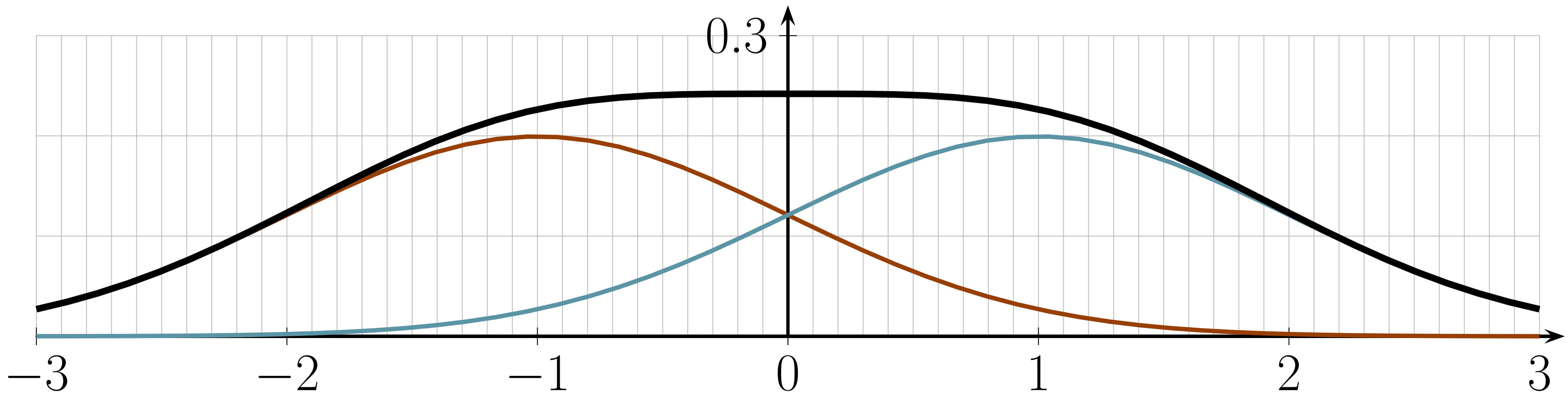
3.1. Modelo de mixtura finita

- Un modelo de ***mixtura finita*** de K componentes es:

$$p_{\boldsymbol{\Theta}}(\boldsymbol{x}) = \sum_{k=1}^{K} p_k \, p_{\boldsymbol{\Theta}'}(\boldsymbol{x} \mid k) \qquad (p_k > 0,\; p_1 + \cdots + p_K = 1)$$

siendo p_k y $p_{\boldsymbol{\Theta}'}(\boldsymbol{x} \mid k)$ los k-ésimos ***coeficiente*** y ***componente***.

Ejemplo: $p(x) = \frac{1}{2} N(\mu_2 = -1, \sigma_2^2 = 1) + \frac{1}{2} N(\mu_1 = 1, \sigma_1^2 = 1)$



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3.2. Estimación máximo-verosímil

- ***Log-verosimilitud*** de $\boldsymbol{\Theta} = (\{p_k\}, \boldsymbol{\Theta}')$ respecto a un conjunto $\{\boldsymbol{x}_n\}$:

$$L(\boldsymbol{\Theta}) = \sum_n \ln \sum_{k=1}^{K} p_k \, p_{\boldsymbol{\Theta}'}(\boldsymbol{x}_n \mid k)$$

- ***Estimador máximo-verosímil*** de $\boldsymbol{\Theta}$: ***EM:*** $\boldsymbol{\Theta}^{(0)} \rightarrow \boldsymbol{\Theta}^{(1)} \rightarrow \cdots \rightarrow \hat{\boldsymbol{\Theta}}$

$$\boldsymbol{\Theta}^{(t+1)} = \arg\max_{\boldsymbol{\Theta}} \; Q(\boldsymbol{\Theta}, \boldsymbol{\Theta}^{(t)}) \quad \text{sujeto a } \sum_k p_k = 1$$

donde

$$Q(\boldsymbol{\Theta}, \boldsymbol{\Theta}^{(t)}) = \sum_n \sum_k z_{nk}^{(t)} \left(\ln p_k + \ln p_{\boldsymbol{\Theta}'}(\boldsymbol{x}_n \mid k)\right)$$

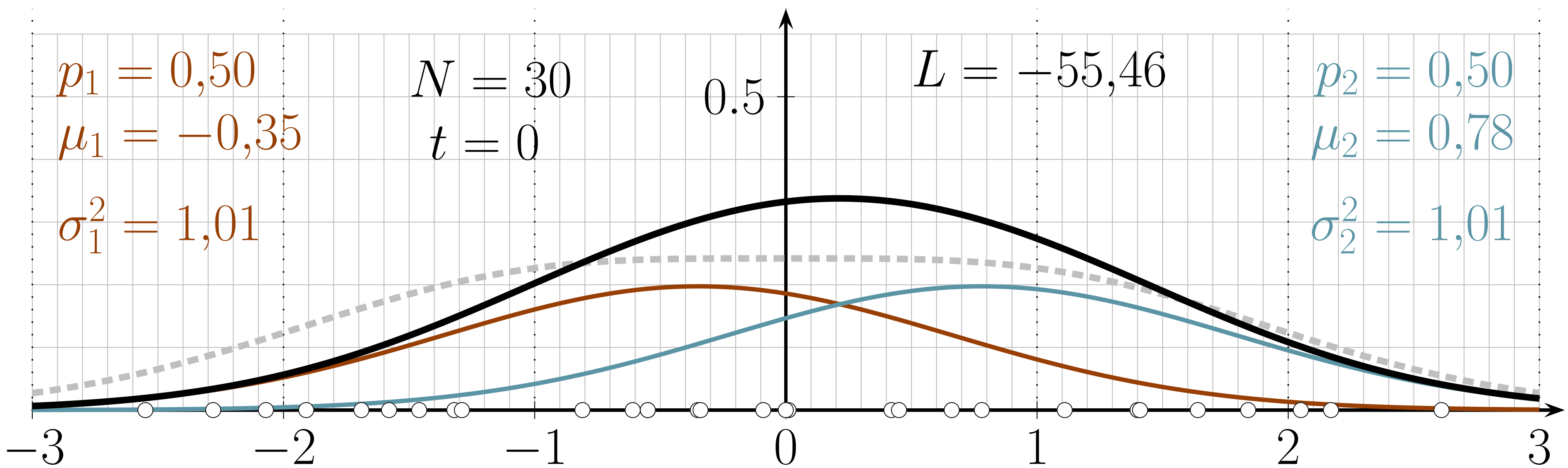
con

$$z_{nk}^{(t)} = \frac{p_k^{(t)} \, p_{\boldsymbol{\Theta}'^{(t)}}(\boldsymbol{x}_n \mid k)}{\sum_{k'} p_{k'}^{(t)} \, p_{\boldsymbol{\Theta}'^{(t)}}(\boldsymbol{x}_n \mid k')}$$

Ejemplo (cont.): $p(x) = \frac{1}{2}\,N(\mu_1{=}{-1}, \sigma_1^2{=}1) + \frac{1}{2}\,N(\mu_2{=}1, \sigma_2^2{=}1)$

$$Q(\boldsymbol{\Theta}, \boldsymbol{\Theta}^{(t)}) = \sum_n \sum_k z_{nk}^{(t)} \left(\ln p_k + \ln \mathcal{N}(\mu_k, \sigma_k^2; x_n)\right)$$

$$\boldsymbol{\Theta}^{(t+1)} = \left\{ \begin{array}{l} p_k^{(t+1)} = \frac{N_k}{N} \quad \text{con} \quad N_k = \sum_n z_{nk}^{(t)} \\ \mu_k^{(t+1)} = \frac{1}{N_k} \sum_n z_{nk}^{(t)} x_n \\ \sigma_k^{2\,(t+1)} = \frac{1}{N_k} \sum_n z_{nk}^{(t)} \left(x_n - \mu_k^{(t+1)}\right)^2 \end{array} \right\}$$



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4. Clasificador con mixturas de Gaussianas

4.1. Clasificador con mixturas de Gaussianas

- Suponemos que las condicionales son mixturas de K Gaussianas:

$$p(\boldsymbol{x} \mid c) = \sum_{k=1}^{K} p(\boldsymbol{x}, k \mid c) = \sum_{k=1}^{K} p(k \mid c)\, p(\boldsymbol{x} \mid c, k)$$

  con

$$p(\boldsymbol{x} \mid c, k) \sim N_D(\boldsymbol{\mu}_{ck}, \Sigma_{ck}) \qquad \text{(para todo } c \text{ y } k\text{)}$$

- Bayes se reduce al ***clasificador con mixturas de Gaussianas:***

$$c^*(\boldsymbol{x}) = \arg\max_{c} \; \ln p(c) + \ln p(\boldsymbol{x} \mid c)$$

  donde, omitiendo la constante aditiva $-\frac{D}{2}\ln(2\pi)$:

$$\ln p(\boldsymbol{x} \mid c) = \ln \sum_{k=1}^{K} p(k \mid c)\, |\Sigma_{ck}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_{ck})^t \Sigma_{ck}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_{ck})\right)$$

- Consideremos priors y condicionales integrados en la conjunta:

$$\begin{aligned} p(\boldsymbol{x}, c) &= p(c)\, p(\boldsymbol{x} \mid c) \\ &= p(c) \sum_{k=1}^{K} p(k \mid c)\, p(\boldsymbol{x} \mid c, k) \\ &= \sum_{k=1}^{K} p(c, k)\, p(\boldsymbol{x} \mid c, k) \end{aligned}$$

- Así, Bayes se puede expresar como:

$$c^*(\boldsymbol{x}) = \arg\max_{c} \; \ln p(\boldsymbol{x}, c)$$

donde, omitiendo la constante aditiva $-\frac{D}{2}\ln(2\pi)$:

$$\ln p(\boldsymbol{x}, c) = \ln \sum_{k=1}^{K} p(c, k)\, |\Sigma_{ck}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_{ck})^t \Sigma_{ck}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_{ck})\right)$$

4.2. Estimación máximo-verosímil

- Modelo de K Gaussianas por clase, con $\boldsymbol{\Theta} = \{(p_{ck}, \boldsymbol{\mu}_{ck}, \Sigma_{ck})\}$:

$$
\begin{aligned}
p_{\boldsymbol{\Theta}}(\boldsymbol{x}) &= \sum_{c=1}^{C} p_{\boldsymbol{\Theta}}(\boldsymbol{x}, c) \\
&= \sum_{c=1}^{C} \sum_{k=1}^{K} p_{ck} \mathcal{N}(\boldsymbol{\mu}_{ck}, \Sigma_{ck}; \boldsymbol{x}) \qquad (p_{ck} > 0, \ \textstyle\sum_c \sum_k p_{ck} = 1)
\end{aligned}
$$

- ***Log-verosimilitud*** de $\boldsymbol{\Theta}$ respecto a $\{(\boldsymbol{x}_n, c_n)\}$:

$$
\begin{aligned}
L(\boldsymbol{\Theta}) &= \sum_{n} \ln p_{\boldsymbol{\Theta}}(\boldsymbol{x}_n, c_n) \\
&= \sum_{c} \sum_{n:c_n=c} \ln \sum_{k=1}^{K} p_{ck} \mathcal{N}(\boldsymbol{\mu}_{ck}, \Sigma_{ck}; \boldsymbol{x}_n)
\end{aligned}
$$

▸ **Algoritmo EM:** $\boldsymbol{\Theta}^{(0)} \rightarrow \boldsymbol{\Theta}^{(1)} \rightarrow \cdots \rightarrow \hat{\boldsymbol{\Theta}}$

$$\boldsymbol{\Theta}^{(t+1)} = \arg\max_{\boldsymbol{\Theta}} \; Q(\boldsymbol{\Theta}, \boldsymbol{\Theta}^{(t)}) \quad \text{sujeto a } \textstyle\sum_c \sum_k p_{ck} = 1$$

con
$$Q(\boldsymbol{\Theta}, \boldsymbol{\Theta}^{(t)}) = \sum_c \sum_{n:c_n=c} \sum_k z_{nck}^{(t)} \left(\ln p_{ck} + \ln \mathcal{N}(\boldsymbol{\mu}_{ck}, \Sigma_{ck}; \boldsymbol{x}_n)\right)$$

y
$$z_{nck}^{(t)} = \frac{p_{ck}^{(t)} \mathcal{N}(\boldsymbol{\mu}_{ck}^{(t)}, \Sigma_{ck}^{(t)}; \boldsymbol{x}_n)}{\sum_{k'} p_{ck'}^{(t)} \mathcal{N}(\boldsymbol{\mu}_{ck'}^{(t)}, \Sigma_{ck'}^{(t)}; \boldsymbol{x}_n)}$$

El paso M maximiza Q como sigue:

$$p_{ck}^{(t+1)} = \frac{1}{N_c} \sum_{n:c_n=c} z_{nck}^{(t)}$$

$$\boldsymbol{\mu}_{ck}^{(t+1)} = \frac{1}{\sum_{n:c_n=c} z_{nck}^{(t)}} \sum_{n:c_n=c} z_{nck}^{(t)} \boldsymbol{x}_n$$

$$\Sigma_{ck}^{(t+1)} = \frac{1}{\sum_{n:c_n=c} z_{nck}^{(t)}} \sum_{n:c_n=c} z_{nck}^{(t)} (\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_{ck}^{(t+1)})(\boldsymbol{x}_n - \hat{\boldsymbol{\mu}}_{ck}^{(t+1)})^t$$

- ***Suavizado*** de matrices de covarianzas: $0 \leq \alpha \leq 1$

$$p(\boldsymbol{x} \mid c, k) \sim N_D(\boldsymbol{\mu}_{ck}, \alpha\,\Sigma_{ck} + (1-\alpha)\,I_D) \quad \text{(para todo } c \text{ y } k\text{)}$$

Sustituimos Σ_{ck} por $\alpha\,\Sigma_{ck} + (1-\alpha)\,I_D$ en $c^*(\boldsymbol{x})$, $L(\boldsymbol{\Theta})$ y EM, donde:

$$Q(\boldsymbol{\Theta}, \boldsymbol{\Theta}^{(t)}) = \sum_c \sum_{n:c_n=c} \sum_k z_{nck}^{(t)} (\ln p_{ck} + \ln \mathcal{N}(\boldsymbol{\mu}_{ck}, \alpha\,\Sigma_{ck} + (1-\alpha)\,I_D; \boldsymbol{x}_n))$$

con

$$z_{nck}^{(t)} = \frac{p_{ck}^{(t)}\,\mathcal{N}(\boldsymbol{\mu}_{ck}^{(t)}, \alpha\,\Sigma_{ck}^{(t)} + (1-\alpha)\,I_D; \boldsymbol{x}_n)}{\sum_{k'} p_{ck'}^{(t)}\,\mathcal{N}(\boldsymbol{\mu}_{ck'}^{(t)}, \alpha\,\Sigma_{ck'}^{(t)} + (1-\alpha)\,I_D; \boldsymbol{x}_n)}$$

- ***Cálculo robusto:*** sea $\boldsymbol{a} \in \mathbb{R}^K$, a_k dado como $\ln a_k$; ***ln-sum-exp:***

$$\operatorname{lse}(\boldsymbol{a}) \triangleq \ln \sum_k \exp(\ln a_k) = \max_{k'} \ln a_{k'} + \ln \sum_k \exp(\ln a_k - \max_{k'} \ln a_{k'})$$

La lse facilita el cálculo robusto de L; tras el de la $z_{nck}^{(t)}$:

$$\frac{\exp(\ln a_k)}{\sum_{k'} \exp(\ln a_{k'})} = \frac{\exp(\ln a_k - \max_{k''} \ln a_{k''})}{\sum_{k'} \exp(\ln a_{k'} - \max_{k''} \ln a_{k''})}$$

- Log del numerador de z_{nck} para todo n: $\ln p_{ck} + \ln \mathcal{N}(\boldsymbol{\mu}_{ck}, \Sigma_{ck}; \boldsymbol{x}_n)$

compute_zk.m

```
function [zk]=compute_zk(ic,k,pkGc,mu,sigma,X)
  D=columns(X); zk=log(pkGc{ic}(k))-.5*D*log(2*pi);
  m=mu{ic}(:,k); S=sigma{ic,k}; I=pinv(S);
  zk=zk+-.5*(sum((X*I).*X,2)+logdet(S)+m'*I*m)+X*I*m; end
```

- Aprendizaje del clasificador con mixturas de Gaussianas:

mixgaussian.m

```
function [tee]=mixgaussian(X,xl,Y,yl,K,a)
  ll=unique(xl); C=rows(ll); N=rows(X); M=rows(Y); D=columns(X);
  rand('seed',23); pc=histc(xl,ll)/N; S=cell(C,K);
  for c=ll'; ic=find(c==ll); pkGc{ic}(1:K)=1/K; idc=find(xl==c);
    Nc=rows(idc); mu{ic}=X(idc(randperm(Nc,K)),:)';
    S(ic,1:K)=a*cov(X(idc,:),1)/K+(1-a)*eye(D); end
  epsilon=1e-4; L=-inf; it=0;
  printf(" It             oL               L  trerr  teerr\n");
  printf("--- -------------- -------------- ------ ------\n");
  do; oL=L; L=0;
    for c=ll'; ic=find(c==ll); idc=find(xl==c); Nc=rows(idc); Xc=X(idc,:);
      z=[]; for k=1:K; z(:,k)=compute_zk(ic,k,pkGc,mu,S,Xc); end
      mz=max(z,[],2); z=exp(z-mz); sz=sum(z,2); z=z./sz;
      L=L+Nc*log(pc(ic))+sum(mz+log(sz));
      sz=sum(z); pkGc{ic}=sz/Nc; mu{ic}=(Xc'*z)./sz;
      for k=1:K; Sick=Xc-mu{ic}(:,k)';
        S(ic,k)=a*(Sick'*(Sick.*z(:,k)))/sz(k)+(1-a)*eye(D); end; end
    L=L/N;
    for c=ll'; ic=find(c==ll);
      z=[]; for k=1:K; z(:,k)=compute_zk(ic,k,pkGc,mu,S,X); end
      mz=max(z,[],2); z=exp(z-mz); sz=sum(z,2);
      gtr(:,ic)=log(pc(ic))+mz+log(sz);
      z=[]; for k=1:K; z(:,k)=compute_zk(ic,k,pkGc,mu,S,Y); end
      mz=max(z,[],2); z=exp(z-mz); sz=sum(z,2);
      gte(:,ic)=log(pc(ic))+mz+log(sz); end
    [~,idx]=max(gtr'); tre=mean(ll(idx)!=xl)*100;
    [~,idy]=max(gte'); tee=mean(ll(idy)!=yl)*100;
    it=it+1; printf("%3d %14.5f %14.5f %6.3f %6.3f\n",it,oL,L,tre,tee);
  until ((L-oL)/abs(oL) < epsilon); end
```

mge.sh

```
#!/usr/bin/octave
if (nargin!=6) printf("mge.sh X xl Ks as tr%% dv%%\n"); exit(1);end
arg_list=argv(); fX=arg_list{1}; load(fX); fxl=arg_list{2};
load(fxl); K=str2num(arg_list{3}); a=str2num(arg_list{4});
tp=str2num(arg_list{5}); dp=str2num(arg_list{6});
N=rows(X); rand("seed",23); p=randperm(N); X=X(p,:); xl=xl(p,:);
Nt=round(tp/100*N); Nd=round(dp/100*N);
Xt=X(1:Nt,:); xlt=xl(1:Nt); Xd=X(N-Nd+1:N,:); xld=xl(N-Nd+1:N);
printf("\n  K   alpha dv-err\n--- ------- ------\n");
for i=1:length(a); for k=1:length(K)
  [ed]=mixgaussian(Xt,xlt,Xd,xld,K(k),a(i));
  printf("%3d %.1e %7.2f\n",K(k),a(i),ed);
end; end
```

```
time ./mge.sh train-images-idx3-ubyte.mat.gz
↪  train-labels-idx1-ubyte.mat.gz 1 "[1e-5 1e-4 1e-3]" 90 10
  K   alpha dv-err
--- ------- ------
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf -1504209.90133  5.598  6.317
  2 -1504209.90133  -761413.95958  5.598  6.317
  3  -761413.95958  -761413.95958  5.598  6.317
  1 1.0e-05    6.32
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf  -620842.17812  3.920  4.267
  2  -620842.17812  -313498.91244  3.920  4.267
  3  -313498.91244  -313498.91244  3.920  4.267
  1 1.0e-04    4.27
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf  -179276.08786  5.115  6.383
  2  -179276.08786   -91071.29658  5.115  6.383
  3   -91071.29658   -91071.29658  5.115  6.383
  1 1.0e-03    6.38
real 15m13,494s
user 37m1,656s
sys   3m30,967s
```


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```
time ./mge.sh train-images-idx3-ubyte.mat.gz
↪  train-labels-idx1-ubyte.mat.gz 2 "[1e-5 1e-4 1e-3]" 90 10
  K   alpha dv-err
--- ------- ------
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf -1627893.22128  5.650  6.417
  2 -1627893.22128  -729424.91406  5.467  5.967
  3  -729424.91406  -717833.52284  5.237  5.700
  4  -717833.52284  -709875.25125  5.050  5.433
  5  -709875.25125  -705704.54934  4.811  5.233
  6  -705704.54934  -703298.72854  4.681  5.350
...
 24  -694987.70222  -694939.31105  4.648  5.350
  2 1.0e-05    5.35
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf  -750399.88962  3.581  4.117
  2  -750399.88962  -306572.28986  3.563  4.117
  3  -306572.28986  -302978.08763  3.585  4.183
  4  -302978.08763  -299361.95955  3.507  4.117
  5  -299361.95955  -296546.65211  3.393  3.917
  6  -296546.65211  -294420.18710  3.311  3.867
...
 16  -290455.51334  -290428.93894  3.004  3.683
  2 1.0e-04    3.68
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf  -236394.56423  4.794  6.333
  2  -236394.56423   -89898.71269  4.809  6.317
  3   -89898.71269   -89827.19591  4.806  6.317
  4   -89827.19591   -89704.22590  4.806  6.317
  5   -89704.22590   -89507.31242  4.759  6.350
  6   -89507.31242   -89273.63102  4.709  6.250
...
 24   -87991.54798   -87983.49608  4.533  5.967
  2 1.0e-03    5.97
real  189m17,263s
user  491m51,727s
sys    52m26,086s
```

```
time ./mge.sh train-images-idx3-ubyte.mat.gz
↪  train-labels-idx1-ubyte.mat.gz 5 "[1e-5 1e-4 1e-3]" 90 10
  K   alpha dv-err
--- ------- ------
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf -1600047.21121  4.474  5.183
  2 -1600047.21121  -652960.19574  3.980  4.767
  3  -652960.19574  -639984.48225  3.804  4.617
  4  -639984.48225  -634795.54624  3.672  4.617
  5  -634795.54624  -631617.59815  3.637  4.667
  6  -631617.59815  -629532.79762  3.594  4.617
...
 17  -625925.80963  -625874.52120  3.504  4.317
  5 1.0e-05    4.32
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf  -952521.06166  2.815  3.817
  2  -952521.06166  -280476.43414  2.376  3.100
  3  -280476.43414  -271244.98216  2.028  2.900
  4  -271244.98216  -266263.71107  1.883  2.817
  5  -266263.71107  -263674.49345  1.796  2.800
  6  -263674.49345  -262152.77957  1.780  2.700
...
 17  -259744.70004  -259720.00407  1.787  2.933
  5 1.0e-04    2.93
 It              oL              L  trerr  teerr
--- -------------- -------------- ------ ------
  1           -Inf  -357943.53847  3.765  6.000
  2  -357943.53847   -85598.45886  3.607  6.050
  3   -85598.45886   -84909.98426  3.569  5.900
  4   -84909.98426   -84182.36993  3.619  5.950
  5   -84182.36993   -83274.55876  3.617  5.933
  6   -83274.55876   -82383.34799  3.504  5.800
...
 24   -80278.20523   -80275.20843  2.993  5.217
  5 1.0e-03    5.22
real   393m1,899s
user  1111m30,183s
sys    111m33,235s
```

5. Ejercicios

5.1. Ejercicio 1 (0.5 puntos)

- Estima el error de clasificación en validación, en función de:
  - El número de variables PCA: $D = 1, 2, 5, 10, 20, 50, 100$
  - El número de componentes: $K = 1, 2, 5, 10, 20, 50, 100$
  - El parámetro de suavizado: $\alpha = \ldots$

  Presenta los resultados con una gráfica por cada α probado: error en la vertical, K en la horizontal y una curva por cada D.

5.2. Ejercicio 2 (0.2 puntos)

- Estima el error de clasificación a partir de los conjuntos oficiales, con los mejores valores de D, K y α hallados en el ejercicio 1.

5.3. Ejercicio 3 (0.3 puntos)

- Modifica el código de aprendizaje del clasificador con mixturas de Gaussianas con el fin de mejorar el error en validación. Ideas:
  - Terminación temprana.
  - Número de componentes variable en cada clase.