Bir Coklu Ikisel Dagilim (Multivar. Binary Distribution) ve Boltzmann Dagilimi

$$P(x;W) = \frac{1}{Z(W)} \exp\left[\frac{1}{2} x^T W x\right] \tag{3}$$

ki W simetrik ve caprazinda (diagonal) sifir iceren bir matristir.

Olurluk (likelihood)

$$\prod_{n=1}^{N} P(x^{(n)};W) = \frac{1}{Z(W)} \exp\left[\frac{1}{2} x^{(n)^T} W x^{(n)}\right]$$

Log olurluk

$$\mathcal{L} = \ln\Big(\prod_{n=1}^{N} P(x^{(n)};W)\Big) = \sum_{n=1}^{N}\left[\frac{1}{2} x^{(n)^T} W x^{(n)} - \ln Z(W)\right] \tag{1}$$

Birazdan $\frac{\partial \mathcal{L}}{\partial w_{ij}}$ turevini alacagiz, o sirada $\ln Z(W)$'nin turevi lazim, daha dogrusu $Z(W)$'yi nasil turevi alinir hale getiririz?

$Z(W)$ normalizasyon sabiti olduguna gore, dagilimin geri kalaninin sonsuzlar uzerinden entegrali (ya da toplami) normalizasyon sabitine esittir,

$$Z(W) = \sum_x \exp\left[\frac{1}{2} x^T W x\right]$$

$$\ln Z(W) = \ln\left[\sum_x \exp\big(\frac{1}{2} x^T W x\big)\right]$$

Log bazli turev alinca log icindeki hersey oldugu gibi bolume gider, ve log icindekinin turevi alinirak bolume koyulur. Fakat log icine dikkatli bakarsak bu zaten $Z(W)$'nin tanimidir, boylece denklemi temizleme sansi dogdu, bolume hemen $Z(W)$ deriz, ve turevi log'un icine uygulariz,

$$\frac{\partial}{\partial w_{ij}} \ln Z(W) = \frac{1}{Z(W)}\left[\sum_x \frac{\partial}{\partial w_{ij}} \exp\big(\frac{1}{2} x^T W x\big)\right]$$

$$\frac{\partial}{\partial w_{ij}} \exp\big(\frac{1}{2} x^T W x\big) = \frac{1}{2} \exp\big(\frac{1}{2} x^T W x\big) \frac{\partial}{\partial w_{ij}} x^T W x \tag{2}$$

(2)'in icindeki bolumu acalim,

$$\frac{\partial}{\partial w_{ij}} x^T W x = x_i x_j$$

Simdi (2)'ye geri koyalim,

$$= \frac{1}{2} \exp\big(\frac{1}{2} x^T W x\big) x_i x_j$$

$$\frac{\partial}{\partial w_{ij}} \ln Z(W) = \frac{1}{Z(W)} \bigg[\sum_x \frac{1}{2} \exp\big(\frac{1}{2} x^T W x\big) x_i x_j \bigg]$$

$$= \frac{1}{2} \sum_x \frac{1}{Z(W)} \exp\big(\frac{1}{2} x^T W x\big) x_i x_j$$

$$= \frac{1}{2} \sum_x P(x; W) x_i x_j$$

Ustteki son ifadede bir kisaltma kullanalim,

$$\sum_x P(x; W) x_i x_j = < x_i, x_j >_{P(x;W)}$$

Artik $\ln Z(W)$'nin turevini biliyoruz. O zaman tum log olurlugun turevine (1) donebiliriz,

$$\frac{\partial \mathcal{L}}{\partial w_{ij}} = \sum_{n=1}^{N} \bigg[\frac{\partial}{\partial w_{ij}} \frac{1}{2} x^{(n)^T} W x^{(n)} - \frac{\partial}{\partial w_{ij}} \ln Z(W) \bigg]$$

$$= \sum_{n=1}^{N} \bigg[\frac{1}{2} x_i^{(n)^T} x_j^{(n)} - \frac{\partial}{\partial w_{ij}} \ln Z(W) \bigg]$$

$$= \sum_{n=1}^{N} \bigg[\frac{1}{2} x_i^{(n)^T} x_j^{(n)} - \frac{1}{2} < x_i x_j >_{P(x;W)} \bigg]$$

1/2 sabitlerini atalim,

$$= \sum_{n=1}^{N} \bigg[x_i^{(n)^T} x_j^{(n)} - < x_i x_j >_{P(x;W)} \bigg]$$

Eger

$$< x_i x_j >_{Data} = \frac{1}{N} \sum_{n=1}^{N} x_i^{(n)^T} x_j^{(n)}$$

olarak alirsak, esitligin sag tarafi verisel kovaryansi (empirical covariance) temsil eder. Duzenleyince,

$$N \cdot < x_i x_j >_{Data} = \sum_{n=1}^{N} x_i^{(n)^T} x_j^{(n)}$$

simdi esitligin sag tarafi uc ustteki formule geri koyulabilir,

$$\frac{\partial \mathcal{L}}{\partial w_{ij}} = N \big[< x_i x_j >_{Data} - < x_i x_j >_{P(x;W)} \big]$$

Bu bir gradyan guncelleme formulu olarak gorulebilir, ve N yerine bir guncelleme sabiti alinabilir.

Ana dagilim fonksiyonu baz alinarak, yeni veri x uzerinde o x uzerinde biri haric tum ogelerin bilindigi durumda bilinmeyen tek hucre i icin 1 olma olasilik degeri,

$$P(x_i = 1 | x_j, j \neq i) = \frac{1}{1 + e^{-a_i}}$$

ve,

$$a_i = \sum_j w_{ij} x_j$$

Bu kosulsal olasiligin ne kadar temiz oldugu onemli, ustteki gorulen bir sigmoid fonksiyonu. Bu fonksiyonlar hakkinda daha fazla bilgi *Lojistik Regresyon* yazisinda bulunabilir. Ana formul (3)'ten bu noktaya nasil eristik?

x vektoru icinde sadece x_i ogesinin b olmasini x^b olarak alalim. Once kosulsal dagilimda "verili" olan kismi elde etmek lazim. O zaman

$$P(x_j, j \neq i) = P(x^0) + P(x^1)$$

Bu bir marjinalizasyon ifadesi, tum olasi i degerleri uzerinde bir toplam alinca geri kalan j degerlerinin dagilimini elde etmis oluruz.

$$P(x_i = 1 | x_j, j \neq i) = \frac{P(x^1)}{P(x^0) + P(x^1)}$$

cunku $P(A|B) = P(A, B)/P(B)$ bilindigi gibi, ve $P(x^1)$ icinde $x_1 = 1$ setini iceren tum veriler uzerinden.

Esitligin sag tarafinda $P(x^1)$'i bolen olarak gormek daha iyi, ayrica ulasmak istedigimiz $1/1+e^{-a_i}$ ifadesinde $+1$'den kurtulmak iyi olur, boylece sadece e^{-a_i} olan esitligi ispatlariz. Bunun her iki denklemde ters cevirip 1 cikartabiliriz,

$$1/P(x_i = 1|x_j, j \neq i) = \frac{P(x^0) + P(x^1)}{P(x^1)}$$

$$= 1 + \frac{P(x^0)}{P(x^1)}$$

Bir cikartirsak, $\frac{P(x^0)}{P(x^1)}$ kalir. Bu bize ulasmak istedigimiz denklemde e^{-a_i} ibaresini birakir. Artik sadece $\frac{P(x^0)}{P(x^1)}$'in e^{-a_i}'e esit oldugunu gostermek yeterli.

$$\frac{P(x^0)}{P(x^1)} = \exp({x^0}^T W x^0 - {x^1}^T W x^1)$$

Simdi $x^T W x$ gibi bir ifadeyi indisler bazinda acmak icin sunlari yapalim,

$$x^T W x = \sum_{k,j} x_k x_j w_{kj}$$

Ustteki cok iyi bilinen bir acilim. Eger

$$\sum_{k,j} \underbrace{x_k x_j w_{ij}}_{Y_{kj}} = \sum_{k,j} Y_{kj}$$

alirsak birazdan yapacagimiz islemler daha iyi gorulebilir. Mesela $k = i$ olan durumu dis toplamdan disari cekebiliriz

$$= \sum_{k \neq i} \sum_j Y_{kj} + \sum_j Y_{ij}$$

Daha sonra $j = i$ olan durumu ic toplamdan disari cekebiliriz,

$$= \sum_{k \neq i} (\sum_{j \neq i} Y_{kj} + Y_{ki}) + \sum_j Y_{ij}$$

Ic dis toplamlari birlestirelim,

$$= \sum_{k \neq i, j \neq i} Y_{kj} + \sum_{k \neq i} Y_{ki} + \sum_j Y_{ij}$$

$$= \sum_{k \neq i, j \neq i} Y_{kj} + \sum_k Y_{ki} + \sum_j Y_{ij} + Y_{ii}$$

Ustteki ifadeyi $\exp({x^0}^T W x^0 - {x^1}^T W x^1)$ icin kullanirsak,

$$\exp\Big(\sum_k Y^0_{ki} + \sum_j Y^0_{ij} + Y^0_{ii} - \big(\sum_k Y^1_{ki} + \sum_j Y^1_{ij} + Y^1_{ii}\big)\Big)$$

$\sum_{k\neq i, j\neq i} Y_{kj}$ teriminin nereye gittigi merak edilirse, bu ifade i'ye dayanmadigi icin bir eksi bir arti olarak iki defa dahil edilip iptal olacakti.

$$= \exp\Big(0 - \big(\sum_k Y^1_{ki} + \sum_j Y^1_{ij} + Y^1_{ii}\big)\Big)$$

W'nin simetrik matris oldugunu dusunursek, $\sum_k Y^1_{ki}$ ile $\sum_j Y^1_{ij}$ ayni ifadedir,

$$= \exp\Big(-\big(2\sum_j Y^1_{ij} + Y^1_{ii}\big)\Big)$$

W sifir caprazli bir matristir, o zaman $Y^1_{ii} = 0$,

$$= \exp\Big(2\sum_j Y^1_{ij}\Big) = \exp(-2a_i)$$

Orijinal dagilim denkleminde $1/2$ ifadesi vardi, onu basta islemlere dahil etmemistik, edilseydi sonuc $\exp(-a_i)$ olacakti.

```python
import numpy as np

class Boltzmann:

    def __init__(self,n_iter=100,eta=0.1,sample_size=100,init_sample_size=10):
        self.n_iter = n_iter
        self.eta = eta
        self.sample_size = sample_size
        self.init_sample_size = init_sample_size

    def sigmoid(self, u):
        return 1./(1.+np.exp(-u));

    def draw(self, Sin,T):
        """
        draw - perform single Gibbs sweep to draw a sample from distribution
        """
        N=Sin.shape[0]
        S=Sin.copy()
        rand = np.random.rand(N,1)
        for i in xrange(N):
            h=np.dot(T[i,:],S)
            S[i]=rand[i]<self.sigmoid(h);
        return S

    def sample(self, T):
        N=T.shape[0]
        s=np.random.rand(N)<self.sigmoid(0)
```

```
        for k in xrange(self.init_sample_size):
            s=self.draw(s,T)
        S=np.zeros((N,self.sample_size))
        S[:,0]=s
        for i in xrange(1,self.sample_size):
            S[:,i]=self.draw(S[:,i-1],T)
        return S.T

    def normc(self, X):
        """
        Return the normalization constant
        """
        def f(x): return np.exp(0.5 * np.dot(np.dot(x,self.W), x))
        S = 2*self.sample(self.W)-1
        res = dict((tuple(s),f(s)) for s in S)
        return np.sum(res.values())

    def fit(self, X):
        W=np.zeros((X.shape[1],X.shape[1]))
        W_data=np.dot(X.T,X)/X.shape[1];
        for i in range(self.n_iter):
            if i % 10 == 0: print 'Iteration', i
            S = self.sample(W)
            S = (S*2)-1
            W_guess=np.dot(S.T,S)/S.shape[1];
            W += self.eta * (W_data - W_guess)
            np.fill_diagonal(W, 0)
        self.W = W
        self.C = self.normc(X)

    def predict_proba(self, X):
        return np.diag(np.exp(0.5 * np.dot(np.dot(X, self.W), X.T))) / self.C
```

```
import boltz
A = np.array([\
[0.,1.,1.,1],
[1.,0.,0,0],
[1.,1.,1.,0],
[0, 1.,1.,1.],
[1, 0, 1.,0]
])
A[A==0]=-1

np.random.seed(0)
clf = boltz.Boltzmann(n_iter=30,eta=0.05,sample_size=100,init_sample_size=50)
clf.fit(A)
print 'W'
print clf.W
print 'normalizasyon sabiti', clf.C

test = np.array([\
[0.,1.,1.,1],
```

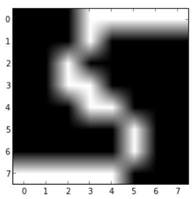
```
[1.,1.,0,0],
[0.,1.,1.,1]
])
print clf.predict_proba(test)
```

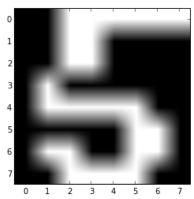
```
Iteration 0
Iteration 10
Iteration 20
W
[[ 0.     0.05  -0.075 -0.375]
 [ 0.05   0.     0.05   0.45 ]
 [-0.075  0.05   0.     0.325]
 [-0.375  0.45   0.325  0.   ]]
normalizasyon sabiti 20.1580365398
[ 0.11319955  0.05215146  0.11319955]
```

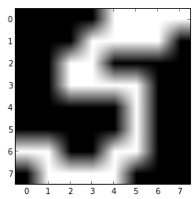
```
Y = np.loadtxt('../../stat/stat_mixbern/binarydigits.txt')
label = np.ravel(np.loadtxt('../../stat/stat_mixbern/bindigitlabels.txt'))
Y5 = Y[label==5]
plt.imshow(Y5[0,:].reshape((8,8),order='C'), cmap=plt.cm.gray)
plt.savefig('boltzmann_01.png')

plt.imshow(Y5[1,:].reshape((8,8),order='C'), cmap=plt.cm.gray)
plt.savefig('boltzmann_02.png')

plt.imshow(Y5[2,:].reshape((8,8),order='C'), cmap=plt.cm.gray)
plt.savefig('boltzmann_03.png')
```







```
!python testbm.py
```

```
Iteration 0
Iteration 10
Iteration 20
Iteration 0
Iteration 10
Iteration 20
Iteration 0
Iteration 10
Iteration 20
0.975
KNN 0.975
```

Information Theory, Inference and Learning Algorithms, D. MacKay

http://nbviewer.ipython.org/gist/aflaxman/7d946762ee99daf739f1

http://math.stackexchange.com/questions/1095491/from-pxw-frac1zw-exp-bigl-frac12-xt-w-x-bigr-to-sigmoid/