APA-L4-python

September 6, 2018

1 APA Laboratori 4 - Sistemes lineals (regularitzats)

```
In [1]: # Uncomment to upgrade packages
        # !pip install pandas --upgrade
        # !pip install numpy --upgrade
        # !pip install scipy --upgrade
        # !pip install statsmodels --upgrade
        # !pip install scikit-learn --upgrade
        %load_ext autoreload
```

```
In [2]: import numpy as np
        import matplotlib.pyplot as plt
        import seaborn as sn
        import pandas as pd
        pd.set_option('precision', 3)
        from IPython.core.interactiveshell import InteractiveShell
        InteractiveShell.ast_node_interactivity = "all"
```

```
In [3]: # Extra imports
        from numpy.random import normal
        from numpy.linalg import inv, svd, cond, pinv
        from statsmodels.genmod.generalized_linear_model import GLM
        from pandas import read_csv
        from scipy import stats
        from sklearn.linear_model import RidgeCV, Ridge
        from sklearn.linear_model import LassoCV, Lasso
```

veiem que les matrius AA^T i A^TA són diferents
`1j` es la unitat imaginaria, definim la matriu

```
In [4]: A = np.array([[0,1j],[0,1]])
        A
```

```
Out[4]: array([[0.+0.j, 0.+1.j],
               [0.+0.j, 1.+0.j]])
```

$A \cdot A^T$ és la matriu (-1 i; i 1)

```
In [5]: A@A.T  # el simbol @ es la multiplicació de matrius en numpy

Out[5]: array([[-1.+0.j,  0.+1.j],
               [ 0.+1.j,  1.+0.j]])
```

$A^T \cdot A$ és la matriu tot zeros

```
In [6]: A.T@A

Out[6]: array([[0.+0.j, 0.+0.j],
               [0.+0.j, 0.+0.j]])
```

1.1 EXEMPLE 1

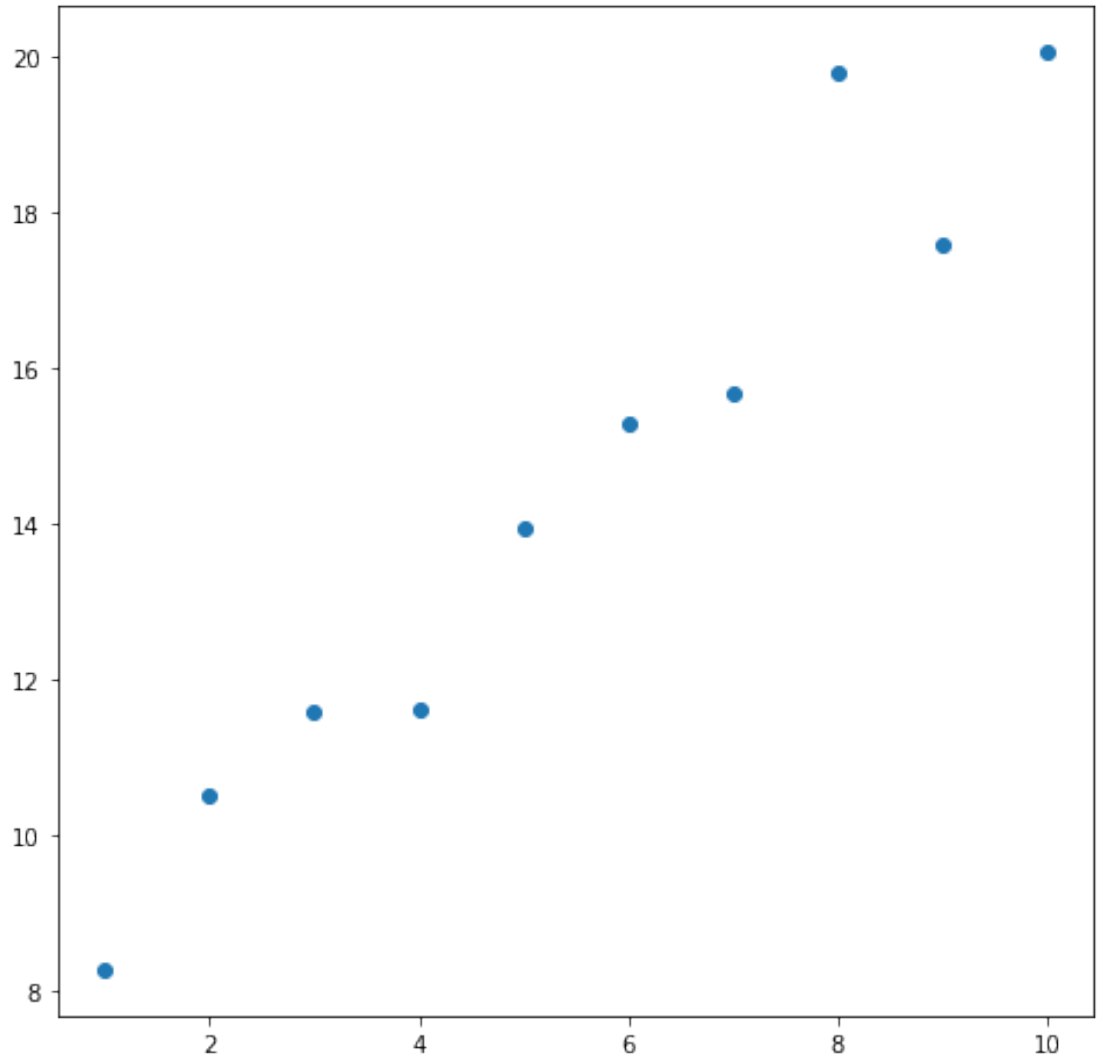
Resolució d'un problema artificial senzill

Definició del sistema lineal a resoldre

$t = f(x) + \epsilon$

on $f(x) = (1 + 1/9)(x - 1) + 10$ i $\epsilon \sim N(0, 1)$

```
In [7]: N=10
        X=np.array([[1]*N,range(1,11)]).T
        X

Out[7]: array([[ 1,  1],
               [ 1,  2],
               [ 1,  3],
               [ 1,  4],
               [ 1,  5],
               [ 1,  6],
               [ 1,  7],
               [ 1,  8],
               [ 1,  9],
               [ 1, 10]])

In [8]: t= np.linspace(9,20,num=N)+normal(size=N)
        t

Out[8]: array([ 8.27098422, 10.52270153, 11.57451043, 11.61698802, 13.93946336,
               15.27490323, 15.66396609, 19.78918239, 17.59525074, 20.07005656])

In [9]: fig, ax = plt.subplots(figsize=(8,8))
        ax.plot(X[:,1], t, 'o');
```



1.1.1 Solució de problemes de mínims quadrats de l'estil

$\min_w ||t - Xw||^2$

1) Resolució mitjançant la pseudo-inversa

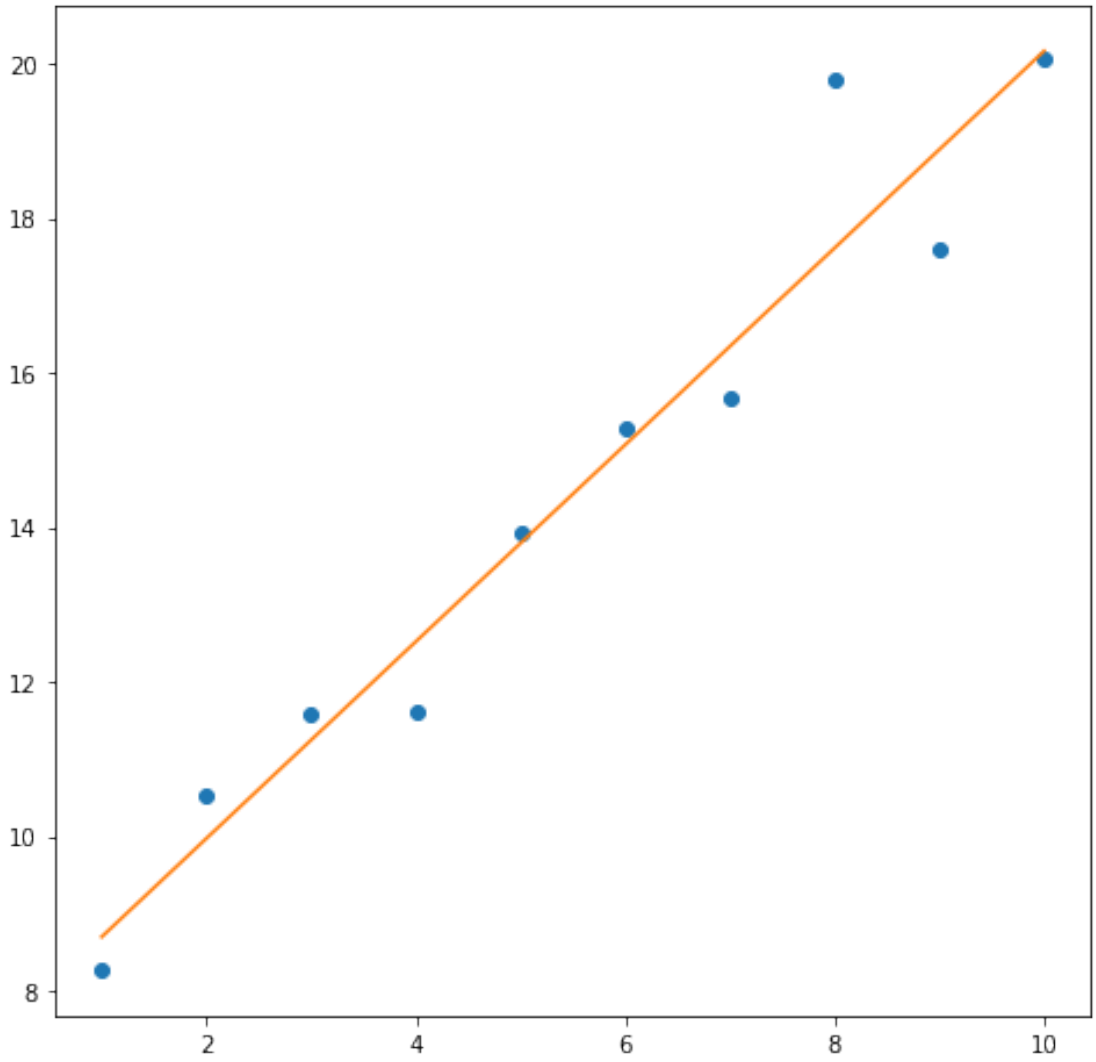
$X^T \cdot X$

```
In [10]: C = X.T @ X
         C
```

```
Out[10]: array([[ 10,  55],
                [ 55, 385]])
```

$(X^T \cdot X)^{-1} \cdot X^T$

```
In [11]: X_pseudo = inv(C) @ X.T
         X_pseudo

Out[11]: array([[ 0.4       ,  0.33333333,  0.26666667,  0.2       ,  0.13333333,
                   0.06666667,  0.        , -0.06666667, -0.13333333, -0.2       ],
                 [-0.05454545, -0.04242424, -0.03030303, -0.01818182, -0.00606061,
                   0.00606061,  0.01818182,  0.03030303,  0.04242424,  0.05454545]])

In [12]: X_pseudo @ X # és pseudo-inversa esquerra d'X

Out[12]: array([[1.00000000e+00, 8.88178420e-16],
                 [1.38777878e-17, 1.00000000e+00]])

In [13]: w = X_pseudo @ t
         w

Out[13]: array([7.42349301, 1.27423775])

In [14]: fig, ax = plt.subplots(figsize=(8,8))
         ax.plot(X[:,1], t, 'o');
         ax.plot(X[:,1], w[0] + X[:,1] * w[1], '-');
```



2) Resolució mitjançant la SVD

```
In [15]: u, d, v = svd(X, full_matrices=False)
         u,d,v

Out[15]: (array([[ 0.0571102 ,  0.58497262],
                 [ 0.10704739,  0.48685286],
                 [ 0.15698459,  0.38873309],
                 [ 0.20692178,  0.29061332],
                 [ 0.25685898,  0.19249355],
                 [ 0.30679617,  0.09437379],
                 [ 0.35673337, -0.00374598],
                 [ 0.40667056, -0.10186575],
                 [ 0.45660776, -0.19998551],
```

```
       [ 0.50654495, -0.29810528]]),
array([19.82171108,  1.44905821]),
array([[ 0.14218125,  0.98984064],
       [ 0.98984064, -0.14218125]]))
```

Les dues columnes d'X són linealment independents, i per tant els dos valors singulars són diferents de 0; en altres paraules, $rang(X) = 2 = min(10, 2)$, per tant X és "full rank"

ara comprovem que $X = UDV^T$

```
In [16]: D = np.diag(d)

         u @ D @ v.T

Out[16]: array([[ 1.,  1.],
                [ 1.,  2.],
                [ 1.,  3.],
                [ 1.,  4.],
                [ 1.,  5.],
                [ 1.,  6.],
                [ 1.,  7.],
                [ 1.,  8.],
                [ 1.,  9.],
                [ 1., 10.]])
```

Ara ho apliquem a la solució del problema de mínims quadrats

$\min_w ||t - Xw||^2$

```
In [17]: D = np.diag(1/d)
         w = v @ D @ u.T @ t
         w

Out[17]: array([7.42349301, 1.27423775])
```

noteu que obtenim la mateixa solució

La rutina `glm()` implementa regressió lineal per mínims quadrats si li demanem mitjançant el paràmetre `family = gaussian`

```
In [18]: mostra = pd.DataFrame({'x1':X[:,0], 'x2':X[:,1],'t':t})
         mostra

Out[18]:    x1  x2       t
         0   1   1   8.271
         1   1   2  10.523
         2   1   3  11.575
         3   1   4  11.617
         4   1   5  13.939
         5   1   6  15.275
         6   1   7  15.664
         7   1   8  19.789
         8   1   9  17.595
         9   1  10  20.070
```

Noteu que glm sempre afegeix un terme *intercept* o *offset* (un regressor constant 1) per defecte, així que tenim dues opcions:

1) desactivar-lo (el "-1" a la fòrmula següent) i usar la nostra pròpia columna de 1's

```
In [19]: model1 = GLM.from_formula('t ~ x2 + x1 -1', mostra)
         result = model1.fit()
```

2) usar la que glm ja posa (recomanat) i desactivar la nostra pròpia columna de 1's

```
In [20]: model2 = GLM.from_formula('t ~ x2', mostra)
         result = model2.fit()
```

Els coefficients (el vector w)

```
In [21]: result.params

Out[21]: Intercept    7.423
         x2           1.274
         dtype: float64
```

** Per què la SVD?**

a. En formar la matriu $X^T X$ es pot perdre informació

```
In [22]: eps = 1e-3
         X_eps = np.array([[1,1],[eps,0],[0,eps]])
         X_eps

Out[22]: array([[1.   , 1.   ],
                [0.001, 0.   ],
                [0.   , 0.001]])

In [23]: C_eps = X_eps.T @ X_eps
         C_eps

Out[23]: array([[1.000001, 1.      ],
                [1.      , 1.000001]])

In [24]: inv(C_eps)# comencem a tenir problemes ...

Out[24]: array([[ 500000.25003573, -499999.75003598],
                [-499999.75003598,  500000.25003573]])

In [25]: eps = 1e-10
         X_eps = np.array([[1,1],[eps,0],[0,eps]])
         X_eps

Out[25]: array([[1.e+00, 1.e+00],
                [1.e-10, 0.e+00],
                [0.e+00, 1.e-10]])
```

```
In [26]: C_eps = X_eps.T @ X_eps
         C_eps

Out[26]: array([[1., 1.],
                [1., 1.]])

In [27]: inv(C_eps)# dóna error (la matriu 2x2 "tot uns" és singular)


         ---------------------------------------------------------------------------

         LinAlgError                               Traceback (most recent call last)

         <ipython-input-27-3e489997295d> in <module>()
     ----> 1 inv(C_eps)# dóna error (la matriu 2x2 "tot uns" és singular)


         /usr/local/lib64/python3.6/site-packages/numpy/linalg/linalg.py in inv(a)
         530     signature = 'D->D' if isComplexType(t) else 'd->d'
         531     extobj = get_linalg_error_extobj(_raise_linalgerror_singular)
     --> 532     ainv = _umath_linalg.inv(a, signature=signature, extobj=extobj)
         533     return wrap(ainv.astype(result_t, copy=False))
         534


         /usr/local/lib64/python3.6/site-packages/numpy/linalg/linalg.py in _raise_linalgerror_si
          87
          88 def _raise_linalgerror_singular(err, flag):
     ---> 89     raise LinAlgError("Singular matrix")
          90
          91 def _raise_linalgerror_nonposdef(err, flag):


         LinAlgError: Singular matrix
```

(el determinant és 1ů1 - 1ů1 = 0)

però no ho hauria de ser ... aquesta no és la nostra matriu ... el problema és que l'operacio X^T X fa perdre molta precissió numèrica (hem perdut epsilon)

b. El número de condició d'una matriu

El número de condició d'una matriu és el producte entre la norma de la matriu i la norma de la seva inversa Dóna una indicació de l'exactitud dels resultats de la inversió d'una matriu Valors prop d'1 indiquen una matriu ben condicionada

El número de condició de la matriu $X^T X$ és el quadrat del de la matriu X

Incidentalment, el número de condició corresponent a usar la norma-2 equival al quocient entre el valor singular més gran i el més petit (no nul) de la matriu

La rutina `cond()` calcula el número de condició

```
In [28]: cond(X)
         cond(X.T @ X)

Out[28]: 13.679030222900371

Out[28]: 187.1158678390236
```

veiem-ho amb un exemple:

```
In [29]: X= np.array([[1]*N, np.linspace(101,110,num=10)]).T
         X

Out[29]: array([[  1., 101.],
                [  1., 102.],
                [  1., 103.],
                [  1., 104.],
                [  1., 105.],
                [  1., 106.],
                [  1., 107.],
                [  1., 108.],
                [  1., 109.],
                [  1., 110.]])

In [30]: cond(X)
         cond(X.T @ X)

Out[30]: 3878.275839190437

Out[30]: 15041023.484257316
```

Una solució molt senzilla és centrar la segona columna:

```
In [31]: X= np.array([[1]*N, np.linspace(101,110,num=10)]).T
         X[:,1] = X[:,1] - np.mean(X[:,1])
         X

Out[31]: array([[ 1. , -4.5],
                [ 1. , -3.5],
                [ 1. , -2.5],
                [ 1. , -1.5],
                [ 1. , -0.5],
                [ 1. ,  0.5],
                [ 1. ,  1.5],
                [ 1. ,  2.5],
                [ 1. ,  3.5],
                [ 1. ,  4.5]])

In [32]: cond(X)
         cond(X.T @ X)
```

```
Out[32]: 2.8722813232690134

Out[32]: 8.25
```

Hi ha una relació senzilla entre els dos sistems lineals; en altres paraules, podem "post-processar els coeficients de sortida perquè corresponguin a la matriu inicial

Nota: hi ha una rutina que calcula directament la pseudo-inversa (ho fa via la SVD):

```
In [33]: pinv(X)

Out[33]: array([[ 0.1       ,  0.1       ,  0.1       ,  0.1       ,  0.1       ,
                  0.1       ,  0.1       ,  0.1       ,  0.1       ,  0.1       ],
                [-0.05454545, -0.04242424, -0.03030303, -0.01818182, -0.00606061,
                  0.00606061,  0.01818182,  0.03030303,  0.04242424,  0.05454545]])
```

1.2 EXEMPLE 2

Anem a analitzar dades de greix corporal mitjançant regressió normal i ridge (regularitzada)

```
In [34]: bodyfat_data = read_csv("bodyfatdata.txt",
                                 delim_whitespace=True,
                                 names=['triceps', 'thigh', 'midarm', 'bodyfat'])
         bodyfat_data.describe()
         N=bodyfat_data.shape[0]

Out[34]:        triceps   thigh  midarm  bodyfat
         count   20.000  20.000  20.000   20.000
         mean    25.305  51.170  27.620   20.195
         std      5.023   5.235   3.647    5.106
         min     14.600  42.200  21.300   11.700
         25%     21.500  47.775  24.750   17.050
         50%     25.550  52.000  27.900   21.200
         75%     29.900  54.625  30.025   24.275
         max     31.400  58.600  37.000   27.200
```

let us start with standard linear regression

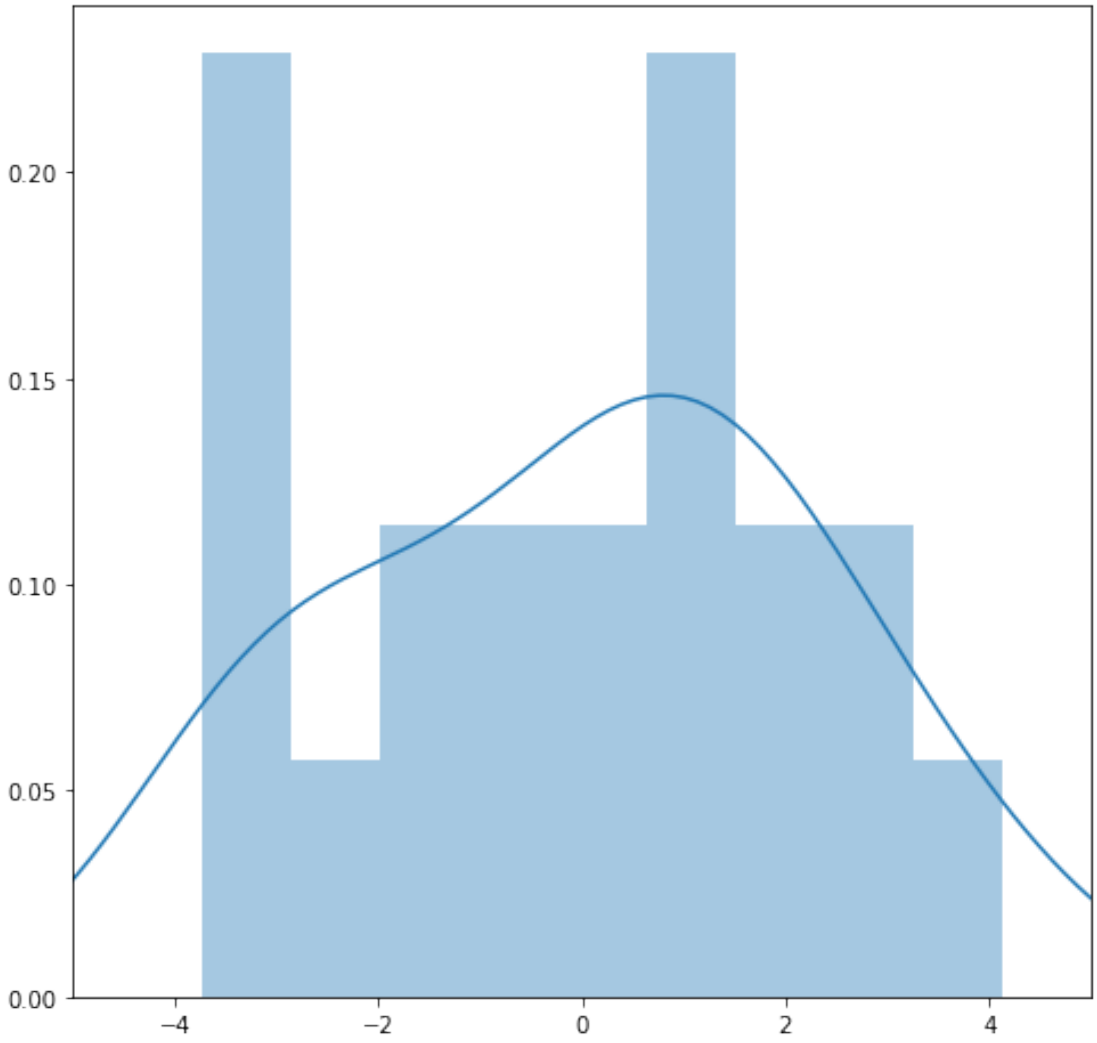
```
In [35]: model = GLM.from_formula('bodyfat ~ triceps + thigh + midarm', bodyfat_data)
         result = model.fit()
         result.summary()

Out[35]: <class 'statsmodels.iolib.summary.Summary'>
         """
                          Generalized Linear Model Regression Results
         ==============================================================================
         Dep. Variable:                bodyfat   No. Observations:                   20
         Model:                            GLM   Df Residuals:                       16
         Model Family:                Gaussian   Df Model:                           3
```

```
Link Function:                identity   Scale:                          6.1503
Method:                           IRLS   Log-Likelihood:                -44.312
Date:                Thu, 06 Sep 2018   Deviance:                       98.405
Time:                        14:33:55   Pearson chi2:                     98.4
No. Iterations:                     3   Covariance Type:             nonrobust
==============================================================================
                 coef    std err          z      P>|z|      [0.025      0.975]
------------------------------------------------------------------------------
Intercept    117.0847     99.782      1.173      0.241     -78.485     312.655
triceps        4.3341      3.016      1.437      0.151      -1.576      10.244
thigh         -2.8568      2.582     -1.106      0.269      -7.918       2.204
midarm        -2.1861      1.595     -1.370      0.171      -5.313       0.941
==============================================================================
"""
```

How to read this output:
$x = (1, triceps, thigh, midarm)^T$
$w = (117.085, 4.334, -2.857, -2.186)^T$
the model is $y(x;w) = w^T x = 117.085 + 4.334 * triceps - 2.857 * thigh - 2.186 * midarm$
The residuals are the differences $(t_n - y(x_n;w)), n = 1, \ldots N$
let's inspect `model$residuals`

In [36]:
```
fig, ax = plt.subplots(figsize=(8,8))
ax.set_xlim([-5,5])
sn.distplot(result.resid_response,bins=9);
```

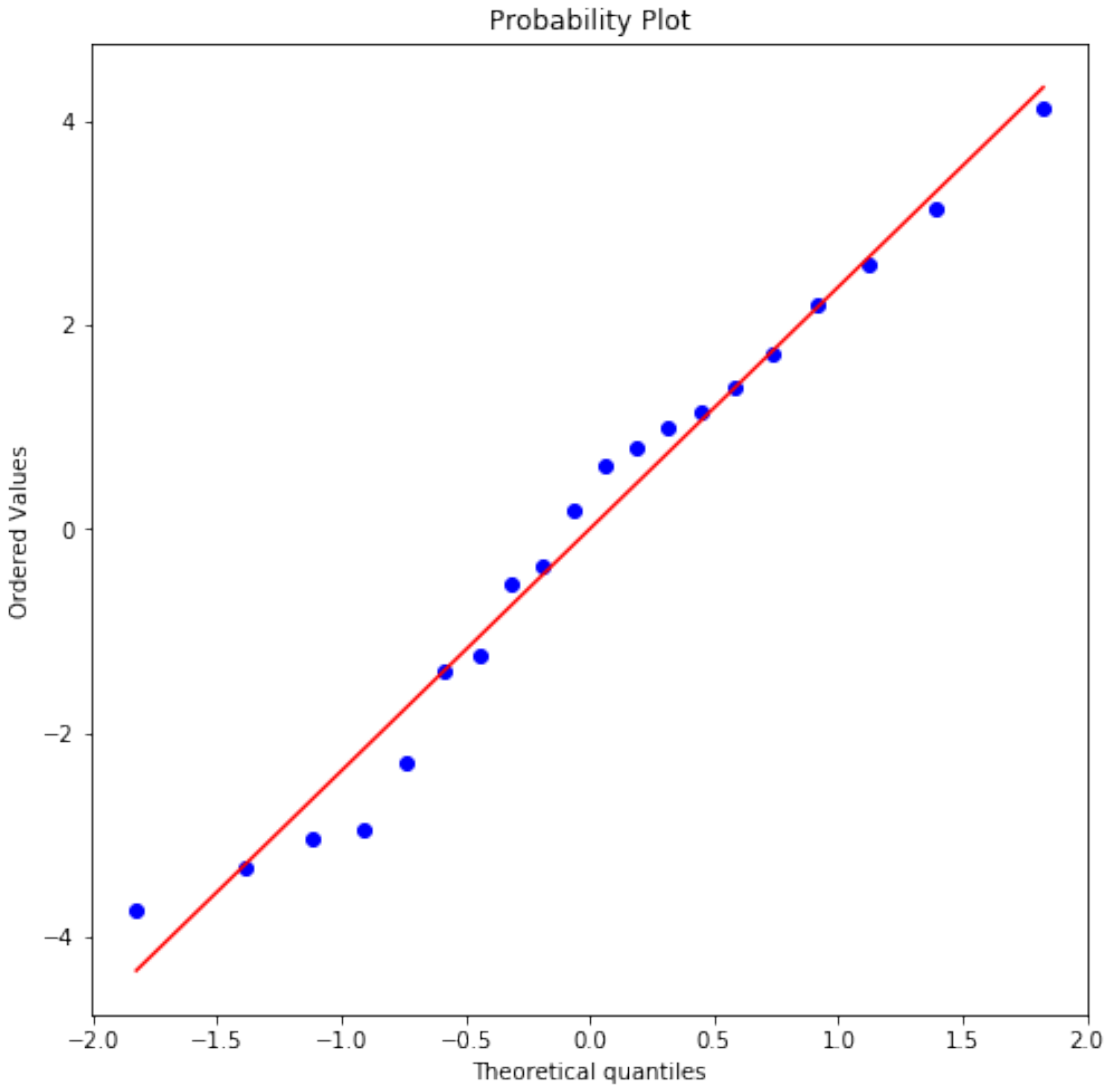
```
/usr/lib64/python3.6/site-packages/scipy/stats/stats.py:1706: FutureWarning: Using a non-tuple s
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
```



Do the residuals look Gaussian? this is direct indication of model validity (since it was our departing assumption)

Let's do a more informative plot (a QQ-plot), which plots actual quantiles against theoretical quantiles of a comparison distribution (Gaussian in this case)

```
In [37]: fig, ax = plt.subplots(figsize=(8,8))
         stats.probplot(result.resid_response, plot=plt);
```



The solid line corresponds to the theoretical quantiles therefore in this case the residuals are not even close (the tails are heavier, the central part is flatter)

This is how we can compute the mean square error

```
In [38]: prediction = result.predict(bodyfat_data.loc[:,'triceps':'midarm'])
         mean_square_error = np.sum((bodyfat_data.bodyfat - prediction)**2)/N
         mean_square_error
```

```
Out[38]: 4.92024440837829
```

Is this number large or small? it depends on the magnitude of the targets! a very good practice is to normalise it, by dividing by the variance of the target:

```
In [39]: norm_mse = np.sum((bodyfat_data.bodyfat - prediction)**2) /  \
                            ((N-1)*np.var(bodyfat_data.bodyfat))
         norm_mse
```

```
Out[39]: 0.2090962622501365
```

If we divide the mean square error by the variance of the targets t, we get the proportion of the variability of the target that is NOT explained by the model

A model with 'norm.mse' equal to 1 is as good as the best constant model (namely, the model that always outputs the average of the target)

models with 'norm.mse' above 0.5 are so so, beyond 0.7 they begin to be quite bad

models with 'norm.mse' below 0.2 are quite good

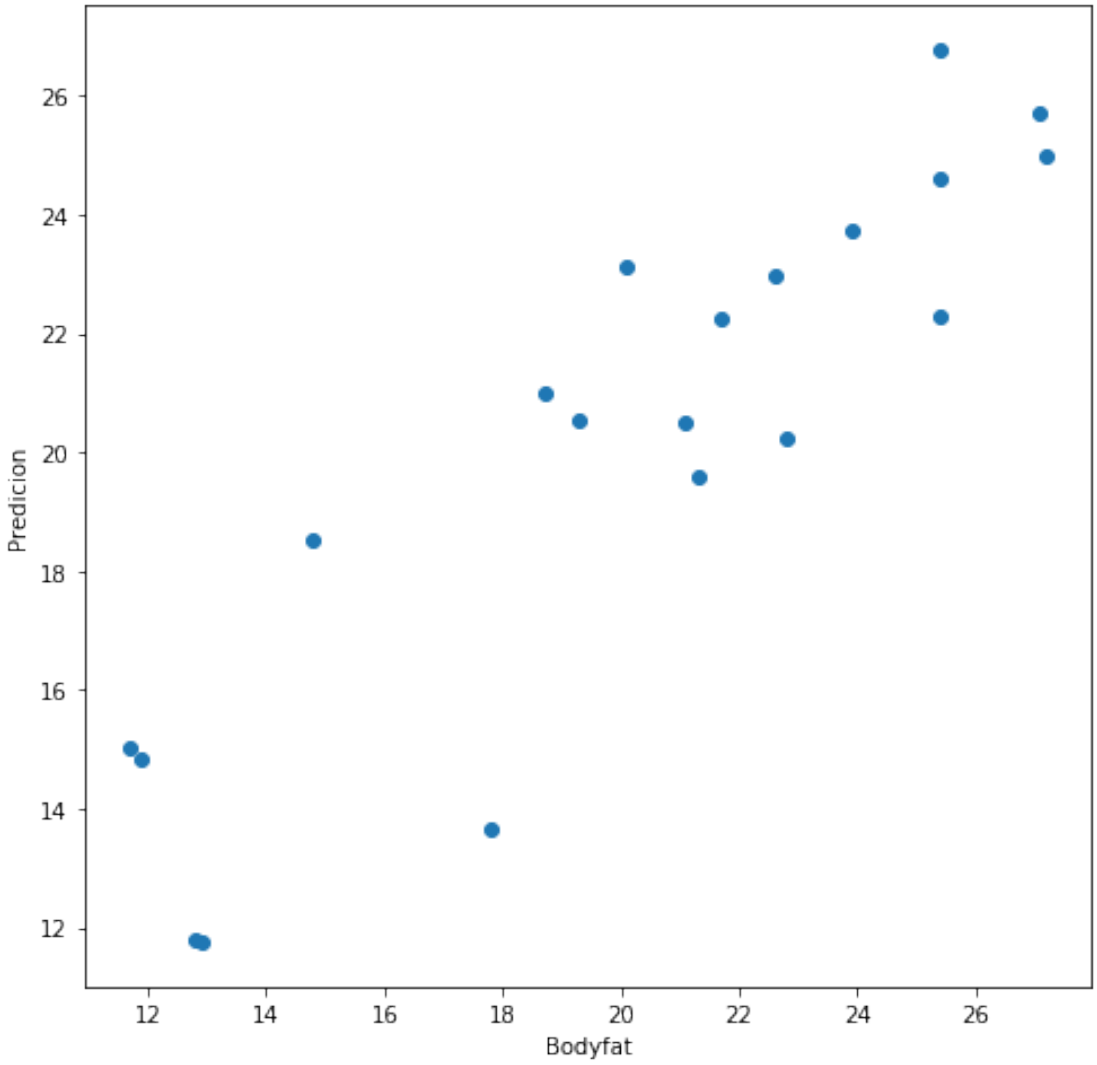
The Multiple R-squared (usually used by statisticians) is obtained by subtracting this quantity form one; that is, the proportion of the target variability that is explained by the model; in this case it reaches ~80%

```
In [40]: R_squared = (1 - norm_mse)*100
         R_squared

Out[40]: 79.09037377498636
```

The "adjusted R-squared" is the same thing, but adjusted for the complexity of the model, i.e. the number of parameters (three in our case)

Now let us try to see how are the real predictions by plotting the real predictions against the targets:

```
In [41]: fig, ax = plt.subplots(figsize=(8,8))
         plt.plot(bodyfat_data.bodyfat,prediction,'o')
         ax.set_xlabel('Bodyfat')
         ax.set_ylabel('Predicion');
```



It is difficult to see if the model is a good predictor; what we need is a numerical assessment of predictive ability. We compute the exact LOOCV as seen in class:

$LOOCV = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i-\hat{y}_i}{1-h_i}\right)^2$

where $H = X(X^TX)^{-1}X^T$ and $h_i = diag(H)_i$

```
In [42]: H= np.diag(model.exog@inv(model.exog.T@model.exog)@model.exog.T)

         LOOCV = np.sum( (result.resid_response/(1-H))**2) / N
         LOOCV
```

```
Out[42]: 8.036828037162582
```

and the corresponding predictive R-square

```
In [43]: R2_LOOCV = (1 - LOOCV*N/((N-1)*np.var(bodyfat_data.bodyfat)))*100
         R2_LOOCV
```

```
Out[43]: 65.8457880658071
```

we can see that prediction quality is not as good as it seemed (since CV error is worse than training error)

this last number is the one I recommend to do model selection!!!

Let us continue now with *regularized linear regression* (aka ridge regression) this time we need to use scikit-learn RidgeCV

We must first choose a value for lambda (the regularization constant) there are several criteria to do this, the most used of which is the GCV so we optimize the GCV for several values of lambda in a sequence

notice we start with a wide logarithmic search

```
In [44]: lambdas = 10**np.arange(-6,2,0.1)
         ridge = RidgeCV(alphas=lambdas,normalize=True)
         ridge.fit(bodyfat_data.loc[:,'triceps':'midarm'],
                   bodyfat_data.bodyfat)
         print('LAMBDA=',ridge.alpha_);

LAMBDA= 0.0019952623149688256
```

best value (according to GCV) is 0.01995262

we perform a finer search

```
In [45]: lambdas = np.arange(0.0001,1,0.0001)
         ridge = RidgeCV(alphas=lambdas,
                         normalize=True,
                         store_cv_values=True)
         ridge.fit(bodyfat_data.loc[:,'triceps':'midarm'],
                   bodyfat_data.bodyfat)
         print('LAMBDA=',ridge.alpha_);

LAMBDA= 0.0019000000000000002
```

Definitely the best value is 0.019, so we refit the model with this precise value:

```
In [46]: bodyfat_ridge_reg = Ridge(alpha=0.0019,
                                   normalize=True).fit(bodyfat_data.loc[:,'triceps':'midarm'],
                                                       bodyfat_data.bodyfat)
         pd.DataFrame([bodyfat_ridge_reg.intercept_,
                       bodyfat_ridge_reg.coef_[0],
                       bodyfat_ridge_reg.coef_[1],
                       bodyfat_ridge_reg.coef_[2]],
                      index=['Intercept','triceps','thigh','midarm'])
```

```
Out[46]:                0
         Intercept  23.587
         triceps     1.504
         thigh      -0.435
         midarm     -0.695
```

Now let us compare these results with those obtained by standard regression (without regularization)

Hand calculation of coefficients, since we know the theory:

```
In [47]: X= np.concatenate((np.ones((bodyfat_data.shape[0],1)),
                            bodyfat_data.loc[:,'triceps':'midarm']),
                           axis=1).T
         w = pinv(X) @ bodyfat_data.bodyfat
         pd.DataFrame(w, index=['Intercept','triceps','thigh','midarm'])
```

```
Out[47]:                 0
         Intercept  117.085
         triceps      4.334
         thigh       -2.857
         midarm      -2.186
```

they should coincide with the results of GLM

```
In [48]: result.params
```

```
Out[48]: Intercept    117.085
         triceps        4.334
         thigh         -2.857
         midarm        -2.186
         dtype: float64
```

Notice that the regularized weights are smaller (in absolute value), one by one

Now we calculate the corresponding prediction errors First by standard regression (without regularization, we already did this)

```
In [49]: R2_LOOCV
```

```
Out[49]: 65.8457880658071
```

Now those with ridge regression (with regularization):

```
In [50]: resid = bodyfat_ridge_reg.\
                   predict(bodyfat_data.loc[:,'triceps':'midarm'])-bodyfat_data.bodyfat
         LOOCV_ridge = np.sum( (resid/(1-H))**2) / N
         LOOCV_ridge
         R2_LOOCV_ridge = (1 - LOOCV_ridge*N/((N-1)*np.var(bodyfat_data.bodyfat)))*100
         R2_LOOCV_ridge
```

```
Out[50]: 8.422173377848805
```

```
Out[50]: 64.2081809933659
```

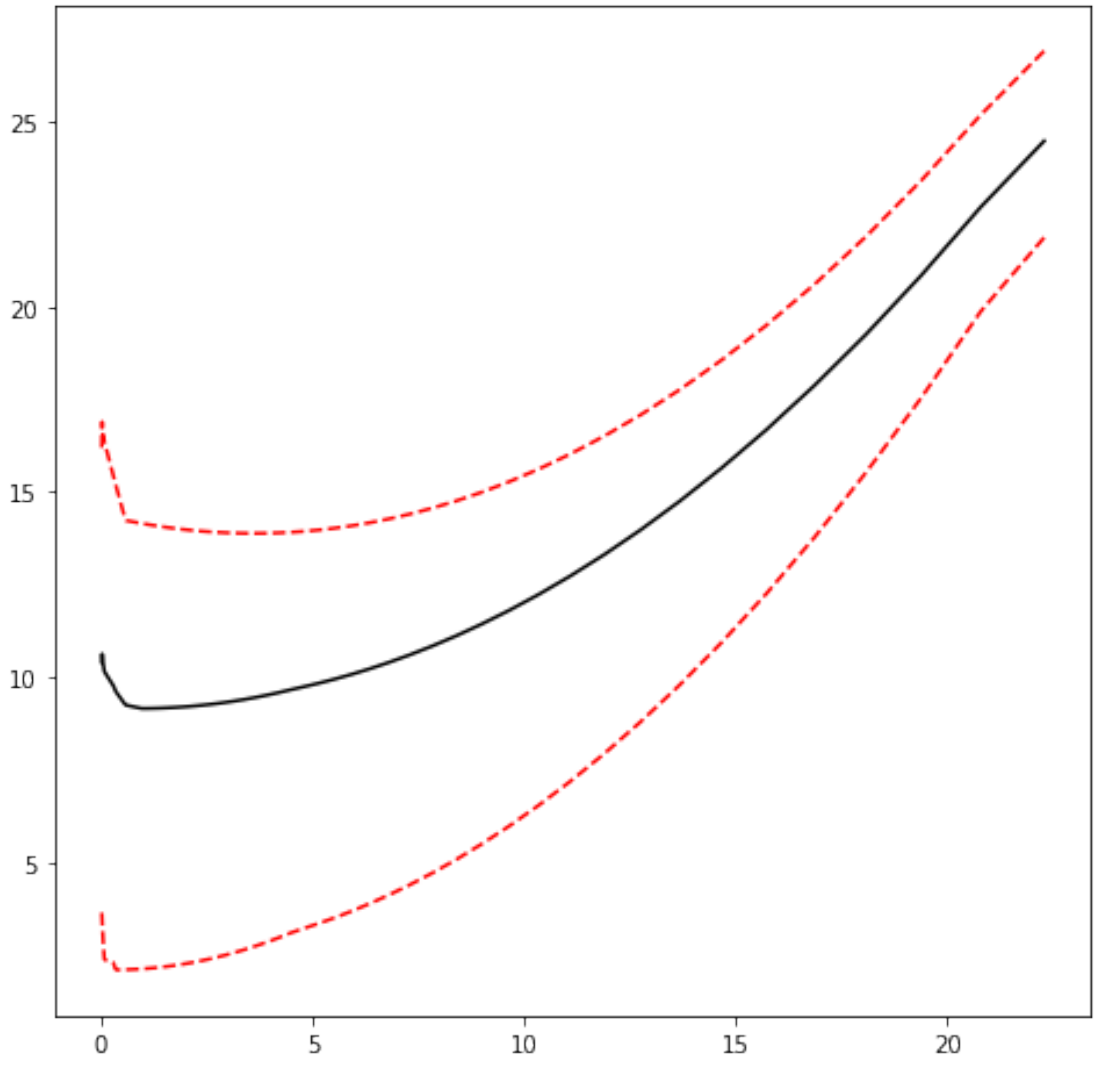
The prediction errors are quite close and the model is way simpler: we would probably prefer the regularized one

---

Now we use the LASSO: here the coefficients are penalized by the L1 norm. The optimal value for lambda is again chosen by cross-validation

```
In [51]: lasso =LassoCV(max_iter=5000)
         lasso.fit(bodyfat_data.loc[:,'triceps':'midarm'],bodyfat_data.bodyfat)
         print('LAMBDA=',lasso.alpha_)
         fig, ax = plt.subplots(figsize=(8,8))
         plt.plot(lasso.alphas_,lasso.mse_path_.mean(axis=1),'k-')
         plt.plot(lasso.alphas_,lasso.mse_path_.max(axis=1),'r--')
         plt.plot(lasso.alphas_,lasso.mse_path_.min(axis=1),'r--');
```

```
LAMBDA= 1.0349280998473913
```



Predictions can be made based on the fitted object; for instance, this would be the TR error with the *optimal* lambda as chosen by LOOCV

```
In [52]: bodyfat_lasso_reg =Lasso(alpha=1.0349, max_iter=5000)
         bodyfat_lasso_reg.fit(bodyfat_data.loc[:,'triceps':'midarm'],
                               bodyfat_data.bodyfat)
         print('Intercept:', bodyfat_lasso_reg.intercept_)
         print('triceps:', bodyfat_lasso_reg.coef_[0])
         print('thigh:', bodyfat_lasso_reg.coef_[1])
         print('midarm:', bodyfat_lasso_reg.coef_[2]);
```

```
Intercept: -17.803172901893376
triceps: 0.18928783908462435
thigh: 0.6489787792428563
midarm: 0.0
```

```
In [53]:  pd.DataFrame(bodyfat_lasso_reg.predict(bodyfat_data.loc[:,'triceps':'midarm']))
```

Out[53]:

	0
0	13.859
1	19.191
2	21.690
3	23.077
4	13.199
5	22.023
6	26.106
7	21.290
8	18.764
9	21.744
10	24.816
11	24.748
12	15.914
13	14.611
14	12.672
15	23.085
16	23.329
17	25.943
18	17.774
19	20.065

And this would be corresponding LOOCV and the corresponding predictive R-square

```
In [54]: resid = bodyfat_lasso_reg.\
                   predict(bodyfat_data.loc[:,'triceps':'midarm'])-bodyfat_data.bodyfat
         LOOCV_lasso = np.sum( (resid/(1-H))**2) / N
         LOOCV_lasso
```

```
R2_LOOCV_lasso = (1 - LOOCV_lasso*N/((N-1)*np.var(bodyfat_data.bodyfat)))*100
R2_LOOCV_lasso
```

```
Out[54]: 9.023634611567775
```

```
Out[54]: 61.652143418386096
```