12_SVD

March 31, 2016

1 12 Linear Algebra: Singular Value Decomposition

One can always decompose a matrix A

$$\mathsf{A} = \mathsf{U}\,\mathrm{diag}(w_j)\,\mathsf{V}^T \tag{1}$$
$$\mathsf{U}^T\mathsf{U} = \mathsf{U}\mathsf{U}^T = 1 \tag{2}$$
$$\mathsf{V}^T\mathsf{V} = \mathsf{V}\mathsf{V}^T = 1 \tag{3}$$

where the w_j are the singular values.
The inverse (if it exists) can be directly calculated from the SVD:

$$\mathsf{A}^{-1} = \mathsf{V}\mathrm{diag}(1/w_j)\mathsf{U}^T$$

1.1 Solving ill-conditioned coupled linear equations

```
In [ ]: import numpy as np
```

1.1.1 Non-singular matrix

```
In [111]: A = np.array([
                  [1, 2, 3],
                  [3, 2, 1],
                  [-1, -2, -6],
              ])
          b = np.array([0, 1, -1])

In [112]: np.linalg.solve(A, b)

Out[112]: array([ 0.83333333, -0.91666667,  0.33333333])

In [113]: U, w, VT = np.linalg.svd(A)
          print(w)

[ 7.74140616  2.96605874  0.52261473]

In [114]: U.dot(np.diag(w).dot(VT))

Out[114]: array([[ 1.,  2.,  3.],
                 [ 3.,  2.,  1.],
                 [-1., -2., -6.]])

In [115]: np.allclose(A, U.dot(np.diag(w).dot(VT)))

Out[115]: True
```

```
In [116]: inv_w = 1/w
          print(inv_w)
```

```
[ 0.1291755   0.33714774  1.91345545]
```

```
In [117]: A_inv = VT.T.dot(np.diag(inv_w)).dot(U.T)
          print(A_inv)
```

```
[[ -8.33333333e-01   5.00000000e-01  -3.33333333e-01]
 [  1.41666667e+00  -2.50000000e-01   6.66666667e-01]
 [ -3.33333333e-01  -1.11022302e-16  -3.33333333e-01]]
```

```
In [118]: np.allclose(A_inv, np.linalg.inv(A))

Out[118]: True
```

```
In [119]: x = A_inv.dot(b)
          print(x)
          np.allclose(x, np.linalg.solve(A, b))
```

```
[ 0.83333333 -0.91666667  0.33333333]
```

```
Out[119]: True
```

```
In [120]: A.dot(x)

Out[120]: array([ -6.66133815e-16,   1.00000000e+00,  -1.00000000e+00])
```

```
In [121]: np.allclose(A.dot(x), b)

Out[121]: True
```

1.1.2 Singular matrix

```
In [376]: C = np.array([
                [ 0.87119148,  0.9330127,  -0.9330127],
                [ 1.1160254,   0.04736717, -0.04736717],
                [ 1.1160254,   0.04736717, -0.04736717],
              ])
          b1 = np.array([ 2.3674474,  -0.24813392, -0.24813392])
          b2 = np.array([0, 1, 1])
```

```
In [310]: np.linalg.solve(C, b1)
```

```
        ---------------------------------------------------------------------------

        LinAlgError                               Traceback (most recent call last)

        <ipython-input-310-d689ff5cc60e> in <module>()
    ----> 1 np.linalg.solve(C, b)


        /opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/numpy/li
        382     signature = 'DD->D' if isComplexType(t) else 'dd->d'
        383     extobj = get_linalg_error_extobj(_raise_linalgerror_singular)
    --> 384     r = gufunc(a, b, signature=signature, extobj=extobj)
        385
```

```
    386     return wrap(r.astype(result_t, copy=False))


    /opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/numpy/li
     88
     89 def _raise_linalgerror_singular(err, flag):
---> 90     raise LinAlgError("Singular matrix")
     91
     92 def _raise_linalgerror_nonposdef(err, flag):


    LinAlgError: Singular matrix
```

```
In [377]: U, w, VT = np.linalg.svd(C)
          print(w)
```

```
[  1.99999999e+00   1.00000000e+00   2.46519033e-32]
```

```
In [378]: U.dot(np.diag(w).dot(VT))
```

```
Out[378]: array([[ 0.87119148,  0.9330127 , -0.9330127 ],
                 [ 1.1160254 ,  0.04736717, -0.04736717],
                 [ 1.1160254 ,  0.04736717, -0.04736717]])
```

```
In [379]: np.allclose(C, U.dot(np.diag(w).dot(VT)))
```

```
Out[379]: True
```

```
In [380]: singular_values = np.abs(w) < 1e-12
          print(singular_values)
```

```
[False False  True]
```

```
In [381]: inv_w = 1/w
          inv_w[singular_values] = 0
          print(inv_w)
```

```
[ 0.5  1.   0. ]
```

```
In [382]: C_inv = VT.T.dot(np.diag(inv_w)).dot(U.T)
          print(C_inv)
```

```
[[-0.04736717  0.46650635  0.46650635]
 [ 0.5580127  -0.21779787 -0.21779787]
 [-0.5580127   0.21779787  0.21779787]]
```

```
In [383]: x1 = C_inv.dot(b1)
          print(x1)
```

```
[-0.34365138  1.4291518  -1.4291518 ]
```

```
In [384]: C.dot(x1)
```

```
Out[384]: array([ 2.3674474 , -0.24813392, -0.24813392])
```

```
In [385]: C.dot(x1) - b1
```

```
Out[385]: array([ -4.44089210e-16,   4.99600361e-16,   4.99600361e-16])
```

- The columns $U_{:,i}$ of U (i.e. `U.T[i]` or `U[:, i]`) corresponding to non-zero w_i, i.e. $\{i : w_i \neq 0\}$, form the basis for the range of the matrix A.
- The columns $V_{:,i}$ of V (i.e. `V.T[i]` or `V[:, i]`) corresponding to zero w_i, i.e. $\{i : w_i = 0\}$, form the basis for the null space of the matrix A.

Note that `x1` can be written as a linear combination of `U.T[0]` and `U.T[1]`:

```
In [408]: x1

Out[408]: array([-0.34365138,  1.4291518 , -1.4291518 ])

In [402]: U.T

Out[402]: array([[ -7.07106782e-01,  -4.99999999e-01,  -4.99999999e-01],
                 [  7.07106780e-01,  -5.00000001e-01,  -5.00000001e-01],
                 [ -2.47010760e-16,  -7.07106781e-01,   7.07106781e-01]])

In [410]: VT

Out[410]: array([[-0.8660254 , -0.35355339,  0.35355339],
                 [-0.5       ,  0.61237244, -0.61237244],
                 [-0.        , -0.70710678, -0.70710678]])

In [411]: U.T[0].dot(x1), U.T[1].dot(x1)

Out[411]: (0.24299822382783731, -0.24299822305983199)

In [412]: VT[2].dot(x1)

Out[412]: 2.2204460492503131e-16

In [413]: U.T[0].dot(x1) * U.T[0] + U.T[1].dot(x1) * U.T[1] + 2 * VT[2]

Out[413]: array([-0.34365138, -1.41421356, -1.41421356])
```

The solution vector x_2 is in the null space:

```
In [349]: x2 = C_inv.dot(b2)
          print(x2)
          print(C.dot(x2))
          print(C.dot(x2) - b2)

[ 0.9330127  -0.43559574  0.43559574]
[ -3.33066907e-16   1.00000000e+00   1.00000000e+00]
[ -3.33066907e-16  -3.33066907e-16  -3.33066907e-16]

In [352]: C.dot(10*x2)

Out[352]: array([ -3.55271368e-15,   1.00000000e+01,   1.00000000e+01])

In [350]: C.dot(VT[2])

Out[350]: array([  0.00000000e+00,  -6.93889390e-18,  -6.93889390e-18])

In [351]: VT[2]

Out[351]: array([-0.        , -0.70710678, -0.70710678])

In [138]: null_basis = VT[singular_values]

In [140]: C.dot(null_basis.T)

Out[140]: array([[  0.00000000e+00],
                 [  4.44089210e-16],
                 [  0.00000000e+00]])
```

1.2 SVD for fewer equations than unknowns

M equations for N unknowns with $M < N$:

- no unique solutions (underdetermined)
- $N - M$ dimensional family of solutions
- SVD: at least $N-M$ zero or negligible w_j: columns of V corresponding to singular w_j span the solution space when added to a particular solution.

1.3 SVD for more equations than unknowns

M equations for N unknowns with $M > N$:

- no exact solutions in general (overdetermined)
- but: SVD can provide best solution in the least-square sense

$$\mathbf{x} = \mathsf{V}\,\mathrm{diag}(1/w_j)\,\mathsf{U}^T\,\mathbf{b}$$

where

- $\mathbf{x}$ is a N-dimensional vector of the unknowns,
- V is a $N \times M$ matrix
- the w_j form a square $M \times M$ matrix,
- U is a $N \times M$ matrix (and U^T is a $M \times N$ matrix), and
- $\mathbf{b}$ is the M-dimensional vector of the given values

It provides the $\mathbf{x}$ that minimizes the residual

$$\mathbf{r} := |\mathsf{A}\mathbf{x} - \mathbf{b}|.$$

1.3.1 Linear least-squares fitting

This is the liner least-squares fitting problem: Given data points (x_i, y_i), fit to a linear model $y(x)$, which can be any linear combination of functions of x.

For example:

$$y(x) = a_1 + a_2 x + a_3 x^2 + \cdots + a_M x^{M-1}$$

or in general

$$y(x) = \sum_{k=1}^{M} a_k X_k(x)$$

The goal is to determine the coefficients a_k.

Define the **merit function**

$$\chi^2 = \sum_{i=1}^{N} \left[\frac{y_i - \sum_{k=1}^{M} a_k X_k(x_i)}{\sigma_i} \right]^2$$

(sum of squared deviations, weighted with standard deviations σ_i on the y_i).

Best parameters a_k are the ones that minimize χ^2.

Design matrix A ($N \times M$, $N \geq M$), vector of measurements $\mathbf{b}$ (N-dim) and parameter vector $\mathbf{a}$ (M-dim):

$$A_{ij} = \frac{X_j(x_i)}{\sigma_i} \tag{4}$$

$$b_i = \frac{y_i}{\sigma_i} \tag{5}$$

$$\mathbf{a} = (a_1, a_2, \ldots, a_M) \tag{6}$$

Minimum occurs when the derivative vanishes:

$$0 = \frac{\partial \chi^2}{\partial a_k} = \sum_{i=1}^{N} {\sigma_i}^{-2} \left[y_i - \sum_{k=1}^{M} a_k X_k(x_i) \right] X_k(x_i), \quad 1 \leq k \leq M$$

(M coupled equations)

$$\sum_{j=1}^{M} \alpha_{kj} a_j = \beta_k \tag{7}$$

$$\alpha \mathbf{a} = \beta \tag{8}$$

with the $M \times M$ matrix

$$\alpha_{kj} = \sum_{i=1}^{N} \frac{X_j(x_i) X_k(x_i)}{\sigma_i^2} \tag{9}$$

$$\alpha = \mathsf{A}^T \mathsf{A} \tag{10}$$

and the vector of length M

$$\beta_k = \sum_{i=1}^{N} \frac{y_i X_k(x_i)}{\sigma_i^2} \tag{11}$$

$$\beta = \mathsf{A}^T \mathbf{b} \tag{12}$$

The inverse of α is related to the uncertainties in the parameters:

$$\mathsf{C} := \alpha^{-1}$$

in particular

$$\sigma(a_i) = C_i i$$

(and the C_{ij} are the co-variances).

Solution of the linear least-squares fitting problem with SVD We need to solve the overdetermined system of M coupled equations

$$\sum_{j=1}^{M} \alpha_{kj} a_j = \beta_k \tag{13}$$

$$\alpha \mathbf{a} = \beta \tag{14}$$

SVD finds $\mathbf{a}$ that minimizes

$$\chi^2 = |\mathsf{A}\mathbf{a} - \mathbf{b}|$$

The errors are

$$\sigma^2(a_j) = \sum_{i=1}^{M} \left(\frac{V_{ji}}{w_i} \right)^2$$

Example Synthetic data

$$y(x) = 3\sin x - 2\sin 3x + \sin 4x$$

with noise r added (uniform in range $-5 < r < 5$).

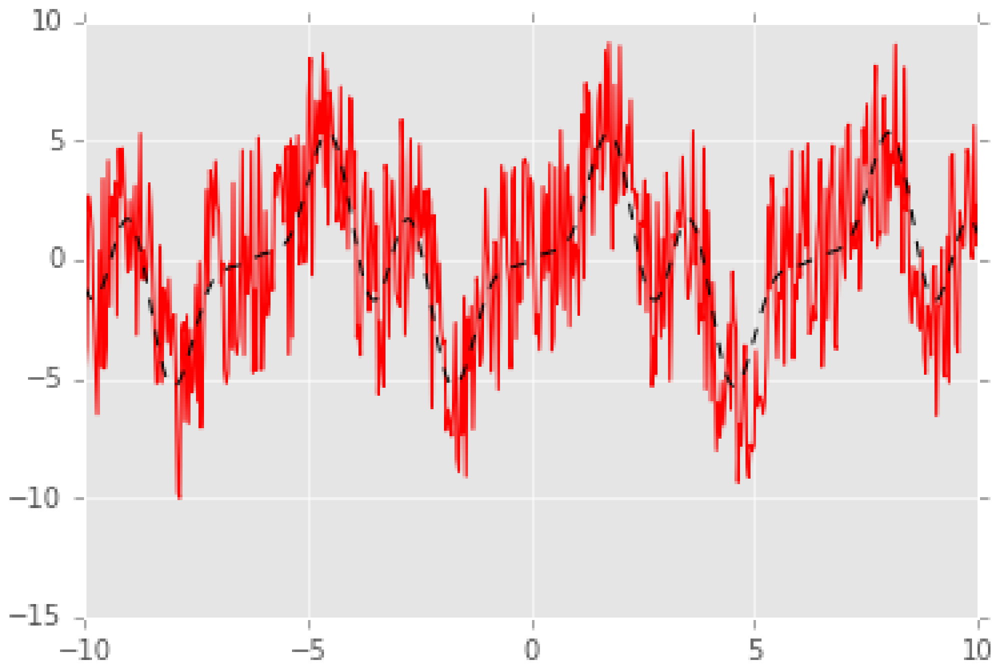
In [2]:
```
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
matplotlib.style.use('ggplot')

import numpy as np
```

In [3]:
```
def signal(x, noise=0):
    r = np.random.uniform(-noise, noise, len(x))
    return 3*np.sin(x) - 2*np.sin(3*x) + np.sin(4*x) + r
```

In [6]:
```
X = np.linspace(-10, 10, 500)
Y = signal(X, noise=5)
```

In [7]:
```
plt.plot(X, Y, 'r-', X, signal(X, noise=0), 'k--')
```

Out[7]:
```
[<matplotlib.lines.Line2D at 0x10765da90>,
 <matplotlib.lines.Line2D at 0x10765dc50>]
```



In [8]:
```
def fitfunc(x, a):
    return a[0]*np.cos(x) + a[1]*np.sin(x) + \
           a[2]*np.cos(2*x) + a[3]*np.sin(2*x) + \
           a[4]*np.cos(3*x) + a[5]*np.sin(3*x) + \
           a[6]*np.cos(4*x) + a[7]*np.sin(4*x)
```

```
def basisfuncs(x):
    return np.array([np.cos(x), np.sin(x),
                     np.cos(2*x), np.sin(2*x),
                     np.cos(3*x), np.sin(3*x),
                     np.cos(4*x), np.sin(4*x)])
```

```
In [9]: M = 8
        sigma = 1.
        alpha = np.zeros((M, M))
        beta = np.zeros(M)
        for x in X:
            Xk = basisfuncs(x)
            for k in range(M):
                for j in range(M):
                    alpha[k, j] += Xk[k]*Xk[j]
        for x, y in zip(X, Y):
            beta += y * basisfuncs(x)/sigma
```

```
In [10]: U, w, VT = np.linalg.svd(alpha)
         V = VT.T
```

In this case, the singular values do not immediately show if any basis functions are superfluous (this would be the case for values close to 0).

```
In [11]: w
```

```
Out[11]: array([ 296.92809624,  282.94804954,  243.7895787 ,  235.7300808 ,
                 235.15938555,  235.14838812,  235.14821093,  235.14821013])
```

... nevertheless, remember to routinely mask any singular values or close to singular values:

```
In [12]: w_inv = 1/w
         w_inv[np.abs(w) < 1e-12] = 0
         alpha_inv = V.dot(np.diag(w_inv)).dot(U.T)
```

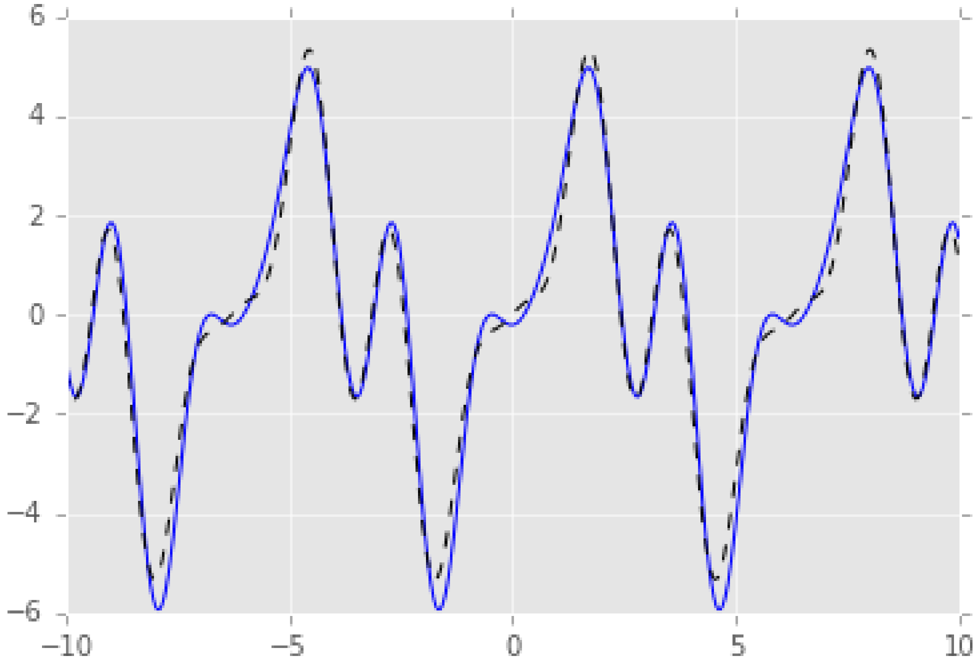
Compare the fitted values to the original parameters $a_j = 0, +3, 0, 0, 0, -2, 0, +1$.

```
In [15]: a_values = alpha_inv.dot(beta)
         print(a_values)
```

```
[-0.01571487  3.15536126  0.14649695  0.27795436  0.04792114 -2.17431709
 -0.38617743  0.72017528]
```

```
In [14]: plt.plot(X, fitfunc(X, a_values), 'b-')
         plt.plot(X, signal(X, noise=0), 'k--')
```

```
Out[14]: [<matplotlib.lines.Line2D at 0x1075cbba8>]
```



In [ ]: