

Least squares regression

The problem of linear regression is to find a line that "best fits" the given data. That is we want all the points $\{(x_1,y_1),\ldots,(x_n,y_n)\}$ to satisfy the equation of the line y=mx+c. Since we know that there exists no such line, so we will try to make $y\cong mx+c$, by minimizing some error/distance/cost/loss function between y and mx+c for every point (x_i,y_i) in the dataset. The simplest error function that results in nice answers is squared distance:

$$e(x_i,y_i) = (y_i - (mx_i + c))^2$$

Then we can minimize the total error to find the line:

$$m^*,c^*=rg \min_{m,c}\sum_{i=1}^n e(x_i,y_i)$$

Geometrically, this error minimization corresponds to minimizing the stubs in the following figure:

Vectorization of Least square regression

y = Salt concentration = Variable to predict = Output 2 = Road area = Input variable D= 9 (71,141), 7 (22,42) { Training Dutaset (Zn, yn) 3 model $\hat{y} = f(x) = mx + c = (\omega_1 x + \omega_0)$ $(m_1 c)$ $(m_1 c)$ $(m_1 c)$ $(m_2 c)$ $(m_3 c)$ $(m_4 c)$ $(m_5 c)$ (mLoss function Least square sugression $l(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$ Objective minimize $\sum_{i=1}^{n} l(y_i, \hat{y}_i)$ $m', c'' = ang min \sum_{i=1}^{N} l(y_i, \hat{y_i})$

f(x; (m, c)) = mx + c $= \left[\begin{bmatrix} m, c \end{bmatrix} \begin{bmatrix} x \end{bmatrix} \right]$ WEIR 1x2 $f(x_1; x_2) = x_1 x_2$ (MEIR2XI mtz $l(y_{i}, \hat{y}_{i}) = (y_{i} - \hat{y}_{i})^{2}$ $= (y_{i} - f(x_{i}; m))^{2}$ $= (y_{i} - m_{i} x_{i})^{2}$ = 21.m = 27m parameter's one same for all datapoints Objective Ž l(yi,ŷi) $= \sum_{i=1}^{N} \left(y_i - m^T \chi_i \right)^2$ ei= yi-mtzi = N e? $= \left(\sqrt{\frac{\chi}{2}} e^{\frac{2}{1}}\right)$

$$e:=\begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \begin{bmatrix} y_1 - m^T z_1 \\ y_2 - m^T z_2 \\ \vdots \\ y_n - m^T x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} m^T z_1 \\ m^T z_2 \\ \vdots \\ m^T x_n \end{bmatrix}$$

$$= \underbrace{y_1 - m^T x_1}_{x_1} \underbrace{y_1}_{x_2} + \underbrace{y_2}_{x_1} \underbrace{y_2}_{x_2} + \underbrace{y_2}_{x_2}$$

Objective

minimize
$$|E||^2 = e^{T}e = (y - x m)(y - x m)$$
 (m, c)
 (m)

$$\begin{array}{lll}
\left(A + B\right) &\stackrel{?}{=} & A^{T} + B^{T} \\
\left(a_{11} & a_{12}\right) + \left(b_{11} & b_{12}\right) \\
\left(a_{21} & a_{22}\right) + \left(b_{22} & b_{22}\right)
\end{array}$$

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$$= \left(y^{T} - \frac{m^{T} X^{T}}{1xz} \frac{1}{2xn}\right) \left(y - \frac{1}{2}x\right)$$

$$= \frac{y^{T} y}{y^{T}} - \frac{m^{T} X^{T}}{y^{T}} \left(y - \frac{1}{2}x\right)$$

$$= \frac{y^{T} y}{y^{T}} - \frac{y^{T} X m}{y^{T}} - \frac{m^{T} X^{T} y}{y^{T}} + \frac{m^{T} X^{T} X m}{y^{T}}$$

$$= \frac{y^{T} y}{y^{T}} - \frac{y^{T} X m}{y^{T}} - \frac{m^{T} X^{T} y}{y^{T}} + \frac{m^{T} X^{T} x m}{y^{T}}$$

$$A \in \mathbb{R}^{N}$$

R(m) xy) = yTy - 2yTXm + mTXXm
empirical
risk

Quadrati function = an2+bm+l In 2 var inscalar John = cc d7[3] = an2+by2+ Cn+dy+eny+f $\begin{cases} 2 & y \end{cases} \begin{cases} a_{11} & a_{12} \\ a_{21} & a_{22} \end{cases} \begin{cases} x \\ y \end{cases} = x^{T} A x$ $= \left[\begin{array}{ccc} \chi & \chi \end{array} \right] \left[\begin{array}{ccc} \alpha_{11} \chi & + \alpha_{12} \chi \\ \alpha_{21} \chi & + \alpha_{22} \chi \end{array} \right]$ = a1122 + a12xy + a212xy + a22y2 Quadratic function in vector John is = $x^T A x + b^T x + c$ compare it to the scalar John anz+by²+ cx+ dy = $(x y) \{a e^{y}\} \{y\} + \{c d\} \{y\} + f$ Objective Junction $R(m:xy) = y^{T}y - 2y^{T} \times \frac{m}{m} + m^{T} \times \frac{x^{T}}{m}$ $constant \qquad b^{T} \times m$ mTA M

R(m; x,y) is a quadratic polynomial $\frac{\partial m}{\partial m} R(m; X, y) = 0$ Derivative of a vector-valued functions whit a vector $f(x) \rightarrow f$ $f(x) \rightarrow f$ $\chi \in \mathbb{R}^{n} \rightarrow \mathbb{R}^{m}$ $\chi \in \mathbb{R}^{n} \rightarrow \mathbb{R}^{n}$ $\chi \in \mathbb{R}^{n} \rightarrow \mathbb{R}^$ $\nabla^{f}(x) = \frac{\partial}{\partial x} f(x) - \left[\frac{\partial f(x)}{\partial x_{1}} - - \frac{\partial}{\partial x_{n}} f(x) \right]$

Gradient transpose

$$f(x) = x^{T}Ax + bx + (x + bx)$$

$$\frac{\partial}{\partial x} f(x)$$

$$\frac{\partial}{\partial x} = \begin{bmatrix} 0, 0, \dots & 0 \end{bmatrix}_{1 \times n}$$

$$= \underbrace{0}_{1 \times n}$$

$$\frac{\partial}{\partial x} = \begin{bmatrix} b_{1} & b_{2} & \dots & b_{n} \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \\ \vdots \\ x_{n} \end{bmatrix} = b_{1}x_{1}x \underbrace{b_{2}x_{2}} \\ \frac{\partial}{\partial x_{1}} = \underbrace{b_{1}} \underbrace{b_{2}} \underbrace{b_{2}} \\ \frac{\partial}{\partial x_{1}} = \underbrace{b_{1}} \underbrace{b$$

Remarks) =
$$y^{T}y - 2y^{T}X + m^{T}XX + m^{T}X + m^{T}XX + m^{T}X + m^{T}XX + m^{T}X + m^{T}X$$

Recall that the magnitude of a vector $\|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + \dots + v_n^n}$ has a similar form to the error function. This suggests that we can define an error vector with the signed error for each data point as it's elements

$$\mathbf{e} = egin{bmatrix} y_1 - (mx_1 + c) \ y_2 - (mx_2 + c) \ dots \ y_n - (mx_n + c) \end{bmatrix}$$

Minimizing the total error is same as minimizing the square of error vector magnitude

$$m^*, c^* = rg \min_{m,c} \|\mathbf{e}\|^2$$

While we are at at it let us define $\mathbf{x} = [x_1; \dots; x_n]$ to denote the vector of all x coordinates of the dataset and $\mathbf{y} = [y_1; \dots; y_n]$ to denote y coordinates. Then the error vector is:

$$\mathbf{e} = \mathbf{y} - (\mathbf{x}m + \mathbf{1}_n c)$$

where $\mathbf{1}_n$ is a n-D vector of all ones. Finally, we vectorize parameters of the line $\mathbf{m}=[m;c]$. We will also need to horizontally concatenate \mathbf{x} and $\mathbf{1}_n$. Let's call the result $\mathbf{X}=[\mathbf{x},\mathbf{1}_n]\in\mathbb{R}^{n\times 2}$. Now, the error vector looks like this:

$$e = y - Xm$$

Expanding the error magnitude:

$$\|\mathbf{e}\|^2 = (\mathbf{y} - \mathbf{X}\mathbf{m})^{\top}(\mathbf{y} - \mathbf{X}\mathbf{m})$$

= $\mathbf{y}^{\top}\mathbf{y} + \mathbf{m}^{\top}\mathbf{X}^{\top}\mathbf{X}\mathbf{m} - 2\mathbf{y}^{\top}\mathbf{X}\mathbf{m}$

Homework 3: Problem 4

Expand

$$(\mathbf{y} - \mathbf{X}\mathbf{m})^{\top}(\mathbf{y} - \mathbf{X}\mathbf{m})$$

and show that it is equal to

$$\mathbf{y}^{\mathsf{T}}\mathbf{y} + \mathbf{m}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{m} - 2\mathbf{y}^{\mathsf{T}}\mathbf{X}\mathbf{m}$$

Our minimization problem in vectorized form is:

$$\mathbf{m}^* = \arg \ \min_{\mathbf{m}} \mathbf{y}^{\top} \mathbf{y} + \mathbf{m}^{\top} \mathbf{X}^{\top} \mathbf{X} \mathbf{m} - 2 \mathbf{y}^{\top} \mathbf{X} \mathbf{m}$$

This is a quadratic equation in ${f m}$ that can be minimized by equating the derivate to zero.

Two rules of vector derivatives

There are two conventions in vector derivatives:

- 1. Gradient convention
- 2. Jacobian convention

Gradient convention

Under gradient convention the derivative of scalar-valued vector function function $f(\mathbf{x}): \mathbb{R}^n \to \mathbb{R}$ is defined as vertical stacking of element-wise derivatives

$$rac{\partial}{\partial \mathbf{x}} f(\mathbf{x}) = egin{bmatrix} rac{\partial f(\mathbf{x})}{\partial x_1} \ dots \ rac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix} \in \mathbb{R}^n$$

Jacobian convention

Under gradient convention the derivative of scalar-valued vector function function $f(\mathbf{x}): \mathbb{R}^n \to \mathbb{R}$ is defined as horizontal stacking of element-wise derivatives

$$rac{\partial}{\partial \mathbf{x}} f(\mathbf{x}) = \left[rac{\partial f(\mathbf{x})}{\partial x_1} \quad \dots \quad rac{\partial f(\mathbf{x})}{\partial x_n}
ight] \in \mathbb{R}^{1 imes n}$$

For a vector-value vector function $\mathbf{f}(\mathbf{x}): \mathbb{R}^n \to \mathbb{R}^m$, Jacobian of $\mathbf{f}(\mathbf{x})$ is the vertical concatentation of gradients transposed, resulting in $m \times n$ matrix

$$\mathbf{J}_{\mathbf{x}}(\mathbf{f}(\mathbf{x})) = rac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{x}) = egin{bmatrix} rac{\partial f_1(\mathbf{x})}{\partial \mathbf{x}} \ \dots \ rac{\partial f_m(\mathbf{x})}{\partial \mathbf{x}} \end{bmatrix}$$

We will use Jacobian convention in this course, because it works nicely with chain rule.

Derivative of a linear function

All scalar-valued linear functions of $\mathbf x$ can be written in the form $f(\mathbf x) = \mathbf b \mathbf f \mathbf c^{\top} \mathbf x$.

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{c}^{\top} \mathbf{x} = \mathbf{c}^{\top} \tag{10}$$

Derivative of a quadratic function

All scalar-valued homogeneous quadratic functions of \mathbf{x} can be written in the form $f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{A} \mathbf{x}$.

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{x}^{\top} \mathbf{A} \mathbf{x} = \mathbf{x}^{\top} (\mathbf{A} + \mathbf{A}^{\top}) \tag{11}$$

Homework 3: Problem 5

Proof of above two derivatives is left as an exercises.

Back to Least square regression

$$\mathbf{0}^{\top} = \frac{\partial}{\partial \mathbf{m}} (\mathbf{y}^{\top} \mathbf{y} + \mathbf{m}^{\top} \mathbf{X}^{\top} \mathbf{X} \mathbf{m} - 2 \mathbf{y}^{\top} \mathbf{X} \mathbf{m})$$
(12)

$$= 2\mathbf{m}^{*\top} \mathbf{X}^{\top} \mathbf{X} - 2\mathbf{y}^{\top} \mathbf{X} \tag{13}$$

This gives us the solution

$$\mathbf{m}^* = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$$

The symbol \mathbf{V}^{-1} is called inverse of matrix \mathbf{V} .

The term $(\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}$ is also called the pseudo-inverse of a matrix \mathbf{X} , denoted as \mathbf{X}^{\dagger} .

```
In [26]: n = salt_concentration_data.shape[0]
bfx = salt_concentration_data[:, 2:3]
bfy = salt_concentration_data[:, 1]
bfX = np.hstack((bfx, np.ones((bfx.shape[0], 1))))
bfX
```

```
Out[26]: array([[0.19, 1.
                [0.15, 1.],
                [0.57, 1. ],
                [0.4 , 1. ],
                [0.7, 1.],
                [0.67, 1.
                          ],
                [0.63, 1.],
                [0.47, 1.],
                [0.75, 1.],
                [0.6, 1.],
                [0.78, 1. ],
                [0.81, 1. ],
                [0.78, 1. ],
                [0.69, 1.],
                [1.3 , 1. ],
                [1.05, 1.],
                [1.52, 1. ],
                [1.06, 1. ],
                [1.74, 1.],
                [1.62, 1. ]])
In [27]: bfm = np.linalg.inv(bfX.T @ bfX) @ bfX.T @ bfy
         print(bfm)
         bfm, * = np.linalg.lstsq(bfX, bfy, rcond=None)
         print(bfm)
        [17.5466671
                      2.67654631]
        [17.5466671
                     2.67654631]
In [28]: m = bfm.flatten()[0]
         c = bfm.flatten()[1]
         # Plot the points
         fig, ax = plt.subplots()
         ax.scatter(salt_concentration_data[:, 2], salt_concentration_data[:, 1])
         ax.set xlabel(r"Roadway area $\%$")
         ax.set ylabel(r"Salt concentration (mg/L)")
         x = salt concentration data[:, 2]
         y = m * x + c
         # Plot the points
         ax.plot(x, y, 'r-') # the line
```

Out[28]: [<matplotlib.lines.Line2D at 0x7fd3ed57a4a0>]

