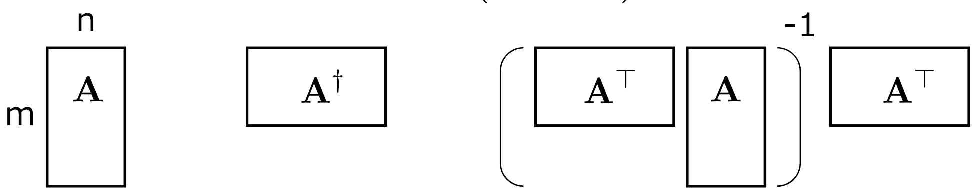
5. Least square method and line fitting

- Pseudoinverse 疑似逆行列
- Overdetermined system of linear equations 線形方程式の過剰決定体系
- Line fitting 線形近似

Pseudoinverse (aka Moore-Penrose pseudoinverse or generalized inverse) 疑似逆行列

- Assuming that a $m\times n$ matrix A is a real matrix and A^TA is invertible, the pseudoinverse $A^\dagger$ for matrix A is defined to be
- 行列Aをm行n列行列とします（正方行列でないものも含む）．A^TAが可逆（正則）で，行列Aの疑似逆行列$A^\dagger$は以下の式で定義される．

$$\mathbf{A}^\dagger \equiv (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top$$



- The following always holds　以下の式が常に成り立つ．：

$$\mathbf{A}^\dagger\mathbf{A} = \mathbf{I}$$

  - This is because　なぜならば，：

$$\mathbf{A}^\dagger\mathbf{A} = ((\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top)\mathbf{A} = (\mathbf{A}^\top\mathbf{A})^{-1}(\mathbf{A}^\top\mathbf{A}) = \mathbf{I}$$

- Note that if $m\neq n$, the following always holds　ただし，もし，mとnが同じ値でない時は，以下の式が常に成り立ちます．：

$$\mathbf{A}\mathbf{A}^\dagger \neq \mathbf{I}$$

Calculating a pseudoinverse　疑似逆行列の計算

- Function pinv gives the pseudoinverse of a given matrix
  pinv関数によってある行列の疑似逆行列は計算される.

```
>> A=randn(5,3)
A =
   -1.000354   0.027611   0.065035
   -3.013282  -0.687265  -0.462170
   -1.345817  -0.410357   1.915242
   -0.480726   0.027323   1.544261
   -0.512782   0.230256  -0.269629
>> pinv(A)
ans =
   -0.3005504  -0.1638335   0.0394693  -0.1490451  -0.3649408
    1.1103074  -0.5201691  -0.5397881   0.7475318   1.6065569
    0.0075412  -0.1606289   0.2720726   0.2571976  -0.0259860
```

- The left multiplication to A yields an identity matrix
  行列Aへの疑似逆行列の左乗算は，単位行列となる.

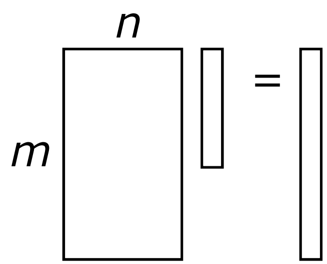
```
>> pinv(A)*A
ans =
    1.0000e+00   2.7756e-16  -1.5266e-16
   -5.5511e-16   1.0000e+00   7.2164e-16
    2.9490e-17   7.9797e-17   1.0000e+00
```

Remark: the right multiplication does not yield an identity
備考：右乗算では単位行列とはならない.

Overdetermined system of linear equations
線形方程式の過剰決定体系

- Consider a system of linear equations with a more number of equations than unknowns　未知数よりも多くの方程式を持つ線形方程式の系を考える
  - A: m x n matrix（m>n）

$$\mathbf{Ax} = \mathbf{b}$$



m>n → Called overdetermined　過剰決定系

m<n → Called underdetermined　劣決定系

  - In general, an overdetermined system does not have a solution
    一般に，過剰決定系には解がない

- We calculate a “solution” as follows　以下の式から”解”を計算します:

$$\mathbf{x} = \mathbf{A}^{\dagger}\mathbf{b}$$

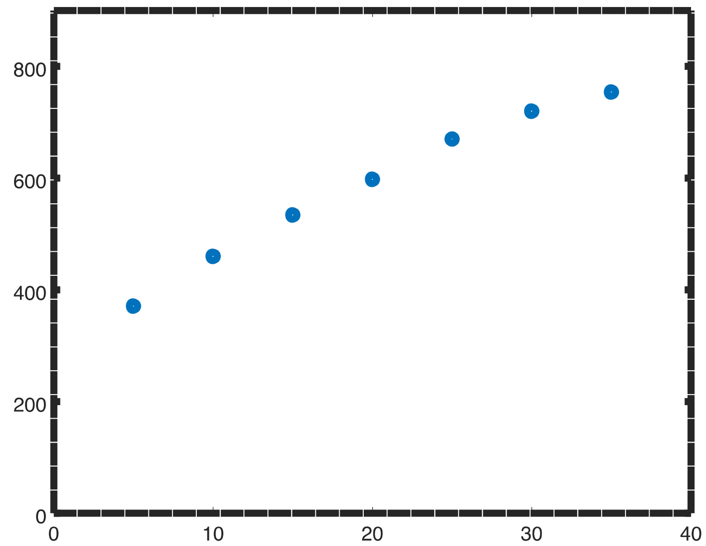
  - It can be shown that this solution x minimizes $\|\mathbf{Ax} - \mathbf{b}\|^2$
    この解xは右式を最小化する $\|\mathbf{Ax} - \mathbf{b}\|^2$
  - This solution is thus called the least square solution
    したがって，この解は最小自乗解（最小二乗解）と呼ばれます

Line fitting: an example
線形近似：例

- Salary and years of service of employees in Japan
  日本における年収と勤続年数

Years of service	<5	<10	<15	<20	<25	<30	<35
Salary (mil. JPY)	370.8	459.4	533.8	597.7	669.7	719.7	753.8

```
>> years=5:5:35
years =
     5    10    15    20    25    30    35
>> income=[371,460,534,598,670,720,754];
>> plot(years,income,"o")
>> axis([0,40,0,900])
>> set(gca,"fontsize",14)
```



Line fitting: least square method (1/2)
線形近似：最小二乗法（1/2）

- Fit a line $y=ax+b$ to a set of points $\{(x_1,y_1), \cdots, (x_N,y_N)\}$ so that the difference in y axis will be small for each (x_i,y_i)
  それぞれの(x_i,y_i)に対してy軸の差が小さくなるように，点集合$\{(x_1,y_1), \cdots, (x_N,y_N)\}$に線$y=ax+b$をフィッティングします．

$$\varepsilon_i \equiv \|y_i - \hat{y}_i\| = \|y_i - (ax_i + b)\|$$

- To do so, find (a,b) that minimizes the sum of the differences for all the points
  これを行うには，すべての点の差の合計を最小にする（a,b）を見つけます

$$\sum_{i=1}^{N} \varepsilon_i^2 = \sum_{i=1}^{N} \|y_i - (ax_i + b)\|^2$$

The right hand side can be rewritten as　右辺は以下のように書き直せます．：

$$\sum_i \|y_i - (ax_i + b)\|^2 = \left\| \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} ax_1 + b \\ ax_2 + b \\ \vdots \\ ax_N + b \end{bmatrix} \right\|^2 = \left\| \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_N & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \right\|^2$$

$$ax_i + b = \begin{bmatrix} x_i & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

Line fitting: least square method (2/2)
線形近似：最小二乗法（2/2）

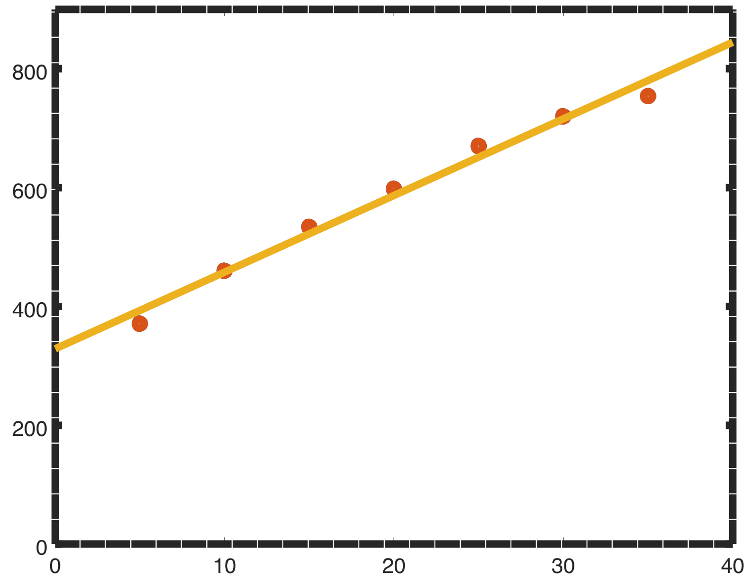
- Thus, the problem reduces to solution of a linear equation Xp=y
  したがって，この問題は，線形方程式Xp = yの解に帰着する.

$$\|\mathbf{X}\mathbf{p}-\mathbf{y}\|^2 \to \min \qquad \mathbf{X} \equiv \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_N & 1 \end{bmatrix}, \quad \mathbf{p} \equiv \begin{bmatrix} a \\ b \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

- Its solution (i.e., least square solution) is given using pseudoinverse X†as
  その解（すなわち、最小自乗解）は，疑似逆行列X†を用いて次のように与えられる．：$\hat{\mathbf{p}} \equiv \mathbf{X}^{\dagger}\mathbf{y}$

```
>> X=ones(7,2);
>> X(:,1)=years';
>> y=income';
>> p=pinv(X)*y;
>> hold on
>> xx=0:1:40;
>> plot(xx,p(1)*xx+p(2))
```

この命令以降のプロット命令を同一のグラフ上に上書きする



Exercises 5.1

- The table to the right shows the number of Nobel laureates per capita (i.e., divided by population) and chocolate consumption per capita for different countries
- It has been discovered that there is a strong link between these two cultural traits (Nobel laureates and chocolate consumption)
  - Franz H. Messerli, Chocolate Consumption, Cognitive Function, and Nobel Laureates, the New England Journal of Medicine, 367, 1562-1564, 2012
- Fit a line to the data and plot the results
  - You can download a file ('Nobel_vs_choco.txt') from the course page

	Nobel laureates per capita	Chocolate consumption per capita (kg/y/head)
Sweden	31.855	6.6
Switzerland	31.544	10.8
Denmark	25.255	8.6
Austria	24.332	7.9
Norway	23.368	9.8
UK	18.875	10.3
Ireland	12.706	8.8
Germany	12.668	11.4
USA	10.706	5.1
Hungary	9.038	3.5
France	8.99	7.4
Belgium	8.622	6.8
Finland	7.6	7
Australia	5.451	6
Italy	3.265	3.3
Poland	3.124	4.5
Lithuania	2.836	6.1
Greece	1.857	4.5
Portugal	1.855	4.5
Spain	1.701	3.3
Japan	1.492	2.2
Bulgaria	1.421	2.2
Brazil	0.05	2.5

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3743834/

Exercises 5.1

- 右の表は、各国の1人当りのノーベル賞受賞者数（人口で割ったもの）と1人当たりのチョコレート消費量を示しています.
- これらの2つの文化的特性（ノーベル賞受賞者とチョコレート消費）の間には強い関連性があることが発見されている.
  - Franz H. Messerli, Chocolate Consumption, Cognitive Function, and Nobel Laureates, the New England Journal of Medicine, 367, 1562-1564, 2012
- データに線形近似し、結果をプロットせよ
  - コースページからデータファイル（ 'Nobel_vs_choco.txt'）をダウンロードできます

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