4. LINEAR LEAST SQUARES

4.1.1 Remember: what we saw during the last lesson

Linear systems $\mathbf{A}\mathrm{x} = \mathrm{b}$ are solved with Gaussian elimination $\Leftrightarrow$ LU factorization.

In general solve using the Matlab command `x=A\b`.
$\mathcal{O}(n^3)$ operations for the LU-factorization, $\mathcal{O}(n^2)$ fwd-/backward substitution.

Triangular solve with fwd-/backward substitution.
$\mathcal{O}(n^2)$ operations required.

Tridiagonal solve using `x=tridia(dia,sup,sub,b)`.
$\mathcal{O}(n)$ operations for the LU-factorization, $\mathcal{O}(n)$ for the fwd-/backward substitution.

Condition number $\mathrm{cond}(\mathbf{A}) = ||\mathbf{A}|| ||\mathbf{A}^{-1}||$ $\rightarrow$ loose $\log_{10}[\mathrm{cond}(\mathbf{A})]$ digits.

4.1.2 Overview: what you will learn today

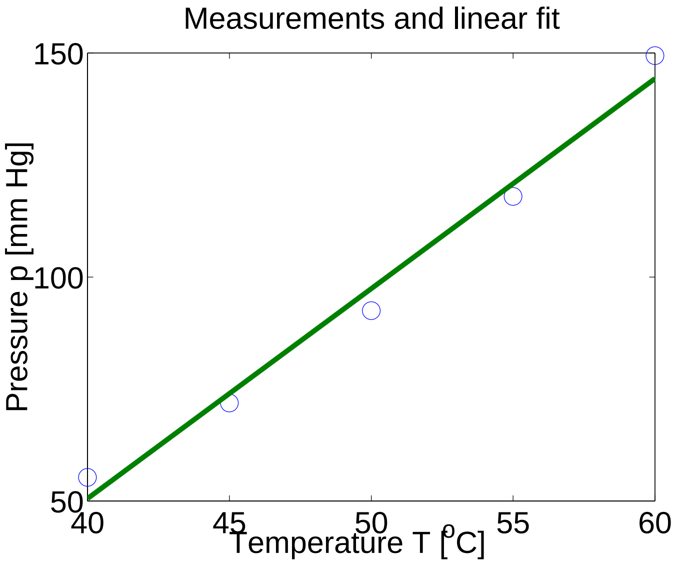
Data fitting to a linear model
Least square solution of an over-determined system

4.2 Data fitting with a linear combination of polynomials (NAM 2.1–2.2, H 3.1)

Example: fitting data from an ideal gas

Measurements:

T^oC	40	45	50	55	60
p mm Hg	55.3	71.9	92.5	118.0	149.4



Model equation: $p(T) = x_1 + x_2 T$

Problem: the system with 5 equations and 2 unknowns is overdetermined = has no exact solution

$$\left\{\begin{array}{rcr} x_1 + 40x_2 & \approx & 55.3 \\ x_1 + 45x_2 & \approx & 71.9 \\ x_1 + 50x_2 & \approx & 92.5 \\ x_1 + 55x_2 & \approx & 118.0 \\ x_1 + 60x_2 & \approx & 149.4 \end{array}\right. \Leftrightarrow \begin{pmatrix} 1 & 40 \\ 1 & 45 \\ 1 & 50 \\ 1 & 55 \\ 1 & 60 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \approx \begin{pmatrix} 55.3 \\ 71.9 \\ 92.5 \\ 118.0 \\ 149.4 \end{pmatrix} \Leftrightarrow$$

$$\Leftrightarrow \mathbf{Ax} \approx \mathbf{b} \quad \Leftrightarrow \quad \mathbf{Ax} - \mathbf{b} \approx \mathbf{0} \quad \Rightarrow \quad \text{minimize } ||\mathbf{Ax} - \mathbf{b}||_2^2 = \sum r_i^2$$

Solution: least square residuals $\sum r_i^2$ when $\mathbf{x}$ satisfies 2 equations for 2 unknowns

$$\mathbf{A}^{\mathbf{T}}\mathbf{Ax} = \mathbf{A}^{\mathbf{T}}\mathbf{b}$$

Apply the recipe

$$\mathbf{A}^{\mathbf{T}}\mathbf{A} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 40 & 45 & 50 & 55 & 60 \end{pmatrix} \begin{pmatrix} 1 & 40 \\ 1 & 45 \\ 1 & 50 \\ 1 & 55 \\ 1 & 60 \end{pmatrix} = \begin{pmatrix} 5 & 250 \\ 250 & 12750 \end{pmatrix}$$

$$\mathbf{A}^{\mathbf{T}}\mathbf{b} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 40 & 45 & 50 & 55 & 60 \end{pmatrix} \begin{pmatrix} 55.3 \\ 71.9 \\ 92.5 \\ 118.0 \\ 149.4 \end{pmatrix} = \begin{pmatrix} 487.1 \\ 25526.5 \end{pmatrix}$$

The best fit with the coefficients (x_1, x_2) satisfies the linear system

$$\mathbf{A}^{\mathbf{T}}\mathbf{A}\mathbf{x} = \begin{pmatrix} 5 & 250 \\ 250 & 12750 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 487.1 \\ 25526.5 \end{pmatrix} = \mathbf{A}^{\mathbf{T}}\mathbf{b}$$

The solution $\mathbf{x} = (-136.9; 4.686)^T$ yields a model $p(T) = -136.9 + 4.686T$

In Matlab simply use the solver `x=A\b` on a rectangular system matrix

```
>> T=(40:5:60)'; b=[55.3 71.9 92.5 118 149.4]';
>> A=[ones(5,1) T]; coeff=A\b, bfit=A*coeff;
>> resid=b-bfit, sumsq=resid'*resid, k=cond(A'*A), plot(T,b,'o',T,bfit)
coeff = -136.8800    4.6860
resid =    4.7400   -2.0900   -4.9200   -2.8500    5.1200
sumsq =   85.3790
k     =    1.3015E+05
```

The polynomial fit $p(T) = -136.9 + 4.686T$ approximates the experimental data with residues $r_i \in [-5.5; 5.5]$ and for a mean square error of $\sum r_i^2 \simeq 85.4$.

Centering The bad condition of the 2×2 matrix $\mathrm{cond}(\mathbf{A}) \simeq 1.3 \times 10^5$ can be improved by centering the argument of the polynomial basis functions around the mean:

Centered model: $p(T) = x_1 + x_2(T - \bar{T})$, $\quad \bar{T} = \frac{1}{m}\sum_{i=1}^{m} t_i$

$$\mathbf{A}^{\mathrm{T}} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -10 & -5 & 0 & 5 & 10 \end{pmatrix} \Rightarrow \begin{pmatrix} 5 & 0 \\ 0 & 250 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 487.1 \\ 1171.5 \end{pmatrix}$$

In Matlab

```
>> T=(40:5:60)'; b=[55.3 71.9 92.5 118 149.4]'; Tm=mean(T);
>> A=[ones(5,1) T-Tm]; coeff=A\b, bfit=A*coeff
>> resid=b-bfit, sumsq=resid'*resid, k=cond(A'*A), plot(T,b,'o',T,bfit)
coeff =   97.4200    4.6860
resid =    4.7400   -2.0900   -4.9200   -2.8500    5.1200
sumsq =   85.3790
k     =   50
```

4.3 Normal equations (NAM 2.3, H 3.2)

Minimize residuals $Q(\mathbf{x}) = \sum r_i^2 = ||\mathbf{Ax} - \mathbf{b}||_2^2 \Rightarrow$ derivatives equal to zero $\nabla r = 0$

$$\begin{aligned}\nabla Q(\mathbf{x}) &= \nabla\left[(\mathbf{Ax}-\mathbf{b})^T(\mathbf{Ax}-\mathbf{b})\right] = \nabla\left[\mathbf{x}^{\mathbf{T}}\mathbf{A}^{\mathbf{T}}\mathbf{Ax} - \mathbf{x}^{\mathbf{T}}\mathbf{A}^{\mathbf{T}}\mathbf{b} - \mathbf{b}^{\mathbf{T}}\mathbf{Ax} + \mathbf{b}^{\mathbf{T}}\mathbf{b}\right] \\ &= \mathbf{A}^{\mathbf{T}}\mathbf{Ax} + \mathbf{x}^{\mathbf{T}}\mathbf{A}^{\mathbf{T}}\mathbf{A} - 2\mathbf{A}^{\mathbf{T}}\mathbf{b} = 2(\mathbf{A}^{\mathbf{T}}\mathbf{Ax} - \mathbf{A}^{\mathbf{T}}\mathbf{b}) = 0\end{aligned}$$

i.e. $\sum r_i^2$ has a minimum where x satisfies the normal equations $\mathbf{A}^{\mathbf{T}}\mathbf{Ax} = \mathbf{A}^{\mathbf{T}}\mathbf{b}$.

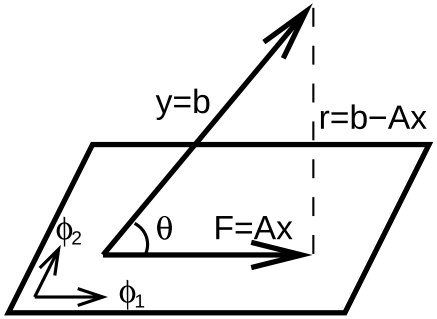
Geometrically this can be understood with two basis functions (or vectors) ϕ_1, ϕ_2

Measurements: $F(t_i) \approx y_i, \quad i = 1, 2, ..., m$

Model equation: $\mathbf{F}(\mathbf{t}) = x_1\phi_1(\mathbf{t}) + x_2\phi_2(\mathbf{t}) = \mathbf{Ax}$

Least squares: $\mathbf{F} \approx \mathbf{y}$, i.e. minimize $||\mathbf{y} - \mathbf{F}||_2^2$

$$\mathbf{F} = x_1\begin{pmatrix}\phi_1(t_1)\\ \phi_1(t_2)\\ \vdots \\ \phi_1(t_m)\end{pmatrix} + x_2\begin{pmatrix}\phi_2(t_1)\\ \phi_2(t_2)\\ \vdots \\ \phi_2(t_m)\end{pmatrix} = \begin{pmatrix}\phi_1(t_1) & \phi_2(t_1)\\ \phi_1(t_2) & \phi_2(t_2)\\ \vdots & \vdots \\ \phi_1(t_m) & \phi_2(t_m)\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix}$$



The minimum length of $r(\mathbf{x}) = ||\mathbf{y} - \mathbf{F}||_2^2$ is obtained when the residual vector $\mathbf{y} - \mathbf{F}$ is perpendicular to the plane defined by two basis vectors (ϕ_1, ϕ_2):

$$\begin{cases}\phi_1 \cdot (\mathbf{F} - \mathbf{y}) = 0 \\ \phi_2 \cdot (\mathbf{F} - \mathbf{y}) = 0\end{cases} \quad \Rightarrow \quad \mathbf{A}^{\mathbf{T}}(\mathbf{F} - \mathbf{y}) = \begin{pmatrix}0\\ 0\end{pmatrix} \quad \Rightarrow \quad \mathbf{A}^{\mathbf{T}}(\mathbf{Ax} - \mathbf{b}) = \mathbf{0}$$

4.4 Analysis of the residuals (NAM 2.5, H 3.2)

Measurements

T	40	45	50	55	60	65	70	75	80	85	90	95	100
p	55	72	93	118	149	188	234	289	355	434	526	634	760

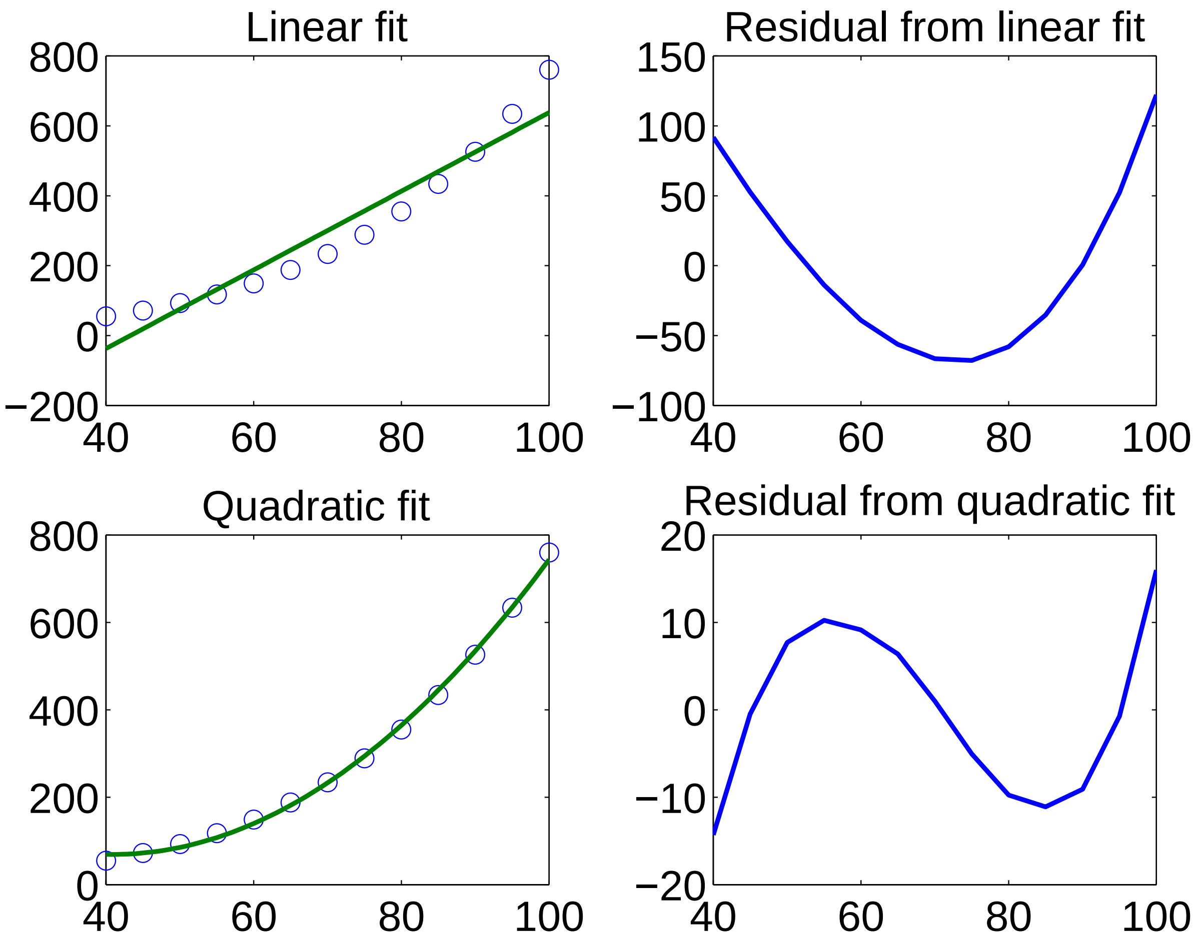
First guess with a linear model $p(T) = c_0 + c_1(T - \bar{T})$

Improvement with a quadratic model $p(T) = c_0 + c_1(T - \bar{T}) + c_2(T - \bar{T})^2$

In Matlab

```
>> % --- First order
>> T=(40:5:100)’; p=[55 72 93 118 149 188 234 289 355 434 526 634 760]’;
>> A=[ones(size(T)) (T-mean(T))]; c=A\p; r=p-A*c; r1sq=r’*r, k1=cond(A’*A)
r1sq = 4.7660e+04
k1   = 350
>> X=(40:100)’; A1=[ones(size(X)) (X-mean(X))]; F1=A1*c;
>> subplot(2,2,1);plot(T,p,’o’,X,F1); title(’Linear fit’)
>> subplot(2,2,2);plot(T,r); title(’Residual from linear fit’)
>>
>> % --- Second order
>> A=[A (T-mean(T)).^2]; c=A\p; r=p-A*c; r2sq=r’*r, k2=cond(A’*A)
r2sq = 1.0778e+03
k2 = 4.9716e+05
>> A2=[A1 (X-mean(X)).^2]; F2=A2*c;
>> subplot(2,2,3);plot(T,p,’o’,X,F2); title(’Quadratic fit’)
>> subplot(2,2,4);plot(T,r); title(’Residual from quadratic fit’)
```

Linear and quadratic fit with the corresponding residuals



Increasing the fitting polynomial from 1st to 2nd order reduces the mean square error $\sum r_i^2$ from 48000 down to 1100; an even lower value could be achieved with a cubic fit to remove the cubic component that is clearly visible in the residual. But watch out for the system condition number!

4.5 Simulation of uncertainties / statistical confidence interval (NAM 2.6–2.7)

Two properties are desirable when fitting, but are often in contradiction:

- **robustness**: the fitting coefficients should be insensitive to data perturbations,
- **accuracy**: the mean square error should be small.

This is particularly important when the measurements have an uncertainty; for example, assume an uncertainty of ±0.5 mm Hg in the measured pressures.

In Matlab this can be simulated with random perturbations of the data

```
>> % --- First order
>> T=(40:5:100)'; p=[55 72 93 118 149 188 234 289 355 434 526 634 760]';
>> A=[ones(size(T)) (T-mean(T))]; c=A\p; c1d=[]; c2d=[];
>> for i=1:100                                      % generate 100 samples
>>   pp=p+0.5*(2*rand(size(T))-1); cp=A\pp;         % random perturbation
>>   c1d=[c1d cp(1)-c(1)]; c2d=[c2d cp(2)-c(2)];    % accumulate deviations
>> end
>> c1err=[c(1) max(abs(c1d))], c2err=[c(2) max(abs(c2d))]  % result
c1err =  300.5385    0.21
c2err =   11.2451    0.01
>> % --- Second order
>> A=[A (T-mean(T)).^2]; c=A\p; r=p-A*c; c1d=[]; c2d=[]; c3d=[];
>> for i=1:100                                      % generate 100 samples
>>   pp=p+0.5*(2*rand(size(T))-1); cp=A\pp;         % random perturbation
>>   c1d=[c1d cp(1)-c(1)]; c2d=[c2d cp(2)-c(2)]; c3d=[c3d cp(3)-c(3)];
>> end
>> c1err=[c(1) max(abs(c1d))],c2err=[c(2) max(abs(c2d))],c3err=[c(3) max(abs(c3d))]
c1err =  233.0070    0.3000
c2err =   11.2451    0.0120
c3err =    0.1929    0.0009
```

The fitted value for $\bar{T} = 70$ is less accurate using a linear $p(\bar{T}) = 300.5 \pm 0.2$ than a quadratic polynomial $p(\bar{T}) = 233.0 \pm 0.3$, but the uncertainty is larger in the latter.

Statistically the least square solution is also the most significant.

Define $\mathbf{c}^*$ as the (unknown) coefficients obtained from perfect (exact) measurements $\mathbf{Ac}^*$; experimental uncertainties perturb the exact value with $\mathbf{y} = \mathbf{Ac}^* + \mathbf{d}$. Inserting in the normal equations

$$\mathbf{A}^{\mathrm{T}}\mathbf{Ac} = \mathbf{A}^{\mathrm{T}}\mathbf{y} \quad \Rightarrow$$

$$\mathbf{c} = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{y} = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}(\mathbf{Ac}^* + \mathbf{d}) = \mathbf{c}^* + (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{d}$$

shows that a larger variance in the measurement errors $d_i,\ i = 1, \ldots m$ increases the uncertainty of the fitting coefficients $c_j,\ j = 1, \ldots n$, but doesn't affect their value. Using the diagonal of the matrix $\mathbf{W} = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}$ to define the variance

$$\sigma^2(c_i) \approx w_{ii}\mathbf{r}^{\mathrm{T}}\mathbf{r}/(m-n)$$

there is a 95% confidence of having normally distributed errors in the interval $\pm 2\sigma$.

4.6 Fitting with a linear superposition of non-linear basis functions (NAM 2.3, H 3.2)

Linear fitting is performed using a **linear combination** of suitable basis functions:

$$
\begin{aligned}
F(t) &= c_0\phi_0(t) + c_1\phi_1(t) + c_2\phi_2(t) + \ldots + c_n\phi_n(t) && \text{(in general)} \\
F(t) &= c_0 + c_1(t-\bar{t}) + c_2(t-\bar{t})^2 + \ldots + c_n(t-\bar{t})^n && \text{(polynomial)} \\
F(t) &= c_0 + c_1\sin(\pi t) + c_2\cos(\pi t) + \ldots + c_{2n}\cos(n\pi t) && \text{(periodic)} \\
F(t) &= c_1/t + c_2\exp(-2t) + c_3 && \text{(blended)}
\end{aligned}
$$

Non-linear fitting cannot, in general, be performed in this manner – later in this course

Except when the model can be re-written as a linear superposition:

Example Radioactive decay.

Measurements:

t sec	0	500	1000	1500	2000	2500	3000
x $counts$	0.1	0.0892	0.0776	0.0705	0.0603	0.0542	0.0471

Model equation: $x(t) = x_0 \exp(-kt)$

Take logarithm: $y = \ln x = \ln x_0 - kt = c_1 + c_2 t$

In the transformed problem, the logarithm of the measured values $y = \ln x$ is fitted to a linear combination of polynomials.

In Matlab

```
>> t=(0:500:3000)'; x=[0.1 0.0892 0.0776 0.0705 0.0603 0.0542 0.0471]';
>> y=log(x); A=[ones(size(t)) t]; c=A\y; yfit=A*c; r=y-yfit;
>> m=size(A,1); n=size(A,2); s2=r'*r/(m-n), W=inv(A'*A); sigma2c=diag(W)*s2;
>> stdev=sqrt(sigma2c);
>> x0int=[exp(c(1)-2*stdev(1)) exp(c(1)) exp(c(1)+2*stdev(1))]
>> kint=[-c(2)-2*stdev(2) -c(2) -c(2)+2*stdev(2)]
x0int = 0.0989       0.1006       0.1023
kint  = 0.0002600    0.0002505    0.0002411
```

The least square fit of the coefficient finally yields $x_0 = 0.101 \pm 0.002$ and a decay constant $k = 0.00025 \pm 0.00001$ with a confidence of 95%.