Primer on Analysis of Experimental Data and Design of Experiments

Lecture 6. Equation-free Scaling Theory for Design of Experiments

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Outline

1. Introduction
2. Buckingham PI Theorem
3. An Illustrative Example
4. Why does the method work
5. Conclusions

Problem definition

Many temperature dependent degradation rate depend on temperature, barrier height, etc.

$$R = f(T, E_B; k_B, \hbar)$$

If I need to perform 10 experiment for T and 10 for E_B, etc. the number of experiments will be 100 – too expensive.

Can the same information be obtained with fewer experiments?

$$\frac{R}{(k_B T/\hbar)} = f_1\left(\frac{E_B}{k_B T}\right)$$

Variables do not matter individually,
They only matter in combination.
Fewer experiments are sufficient.

Buckingham PI Theorem

Assume that a function g depends on parameters $q_1, q_2, \ldots\ q_n$, such that

$$g(q_1, q_2, \ldots, q_n) = 0$$

Here g could a differential equation

$$q_1 \frac{d^2 y}{dx^2} + q_2 \frac{dy}{dx} + q_3 y + q_4 = 0$$

Or, it could be a unknown blackbox, with control parameters q_1, q_2, q_3, etc.

Buckingham PI Theorem

If the function g depends on parameters $q_1, q_2, \ldots\ q_n$, then

$$g(q_1, q_2, \ldots., q_n) = 0$$

The same expression can be expressed in terms of (n-m) independent dimensionless ration, or Π parameters.

$$G(\Pi_1, \Pi_2, \ldots., \Pi_{n-m}) = 0$$

m= minimum number of independent dimension typically given by r, where r is the rank of the matrix

To determine PI …

Determine

$$A = \begin{bmatrix} P & R \\ Q & S \end{bmatrix}$$

P is a $r \times r$ nonsingular matrix

Find the exponent matrix

$$E = (-QP^{-1}, I)$$

Finally,

$$\Pi_i = q_1^{e_{i1}} q_2^{e_{i2}} \ldots\ldots q_N^{e_{iN}}$$

Recall the dimensions of variables

$$\text{Variable} \rightarrow M^{a} \times L^{b} \times t^{c} \times \Theta^{d}$$

$$E_B \rightarrow M^{1} \times L^{2} \times t^{-2} \times \Theta^{0} \quad \left(0.5m\upsilon^{2}\right)$$

$$T \rightarrow M^{0} \times L^{0} \times t^{0} \times \Theta^{1} \quad (\text{kelvin})$$

$$R \rightarrow M^{0} \times L^{0} \times t^{-1} \times \Theta^{0} \quad (\text{sec}^{-1})$$

$$k_B \rightarrow M^{1} \times L^{2} \times t^{-2} \times \Theta^{-1} \quad (\text{energy/kelvin})$$

$$\hbar \rightarrow M^{1} \times L^{2} \times t^{-1} \times \Theta^{0} \quad (\text{energy-sec})$$

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Illustrative Example

$$R = f(T, E_B; k_B, \hbar) \Rightarrow 0 = g(R, T, E_B; k_B, \hbar)$$

$$A = \begin{array}{c} \\ \\ \end{array}\begin{array}{cc} & \begin{array}{cccc} M & L & t & \Theta \end{array} \\ & \left[\begin{array}{cccc} 0 & 0 & 0 & 1 \\ 1 & 2 & -2 & -1 \\ 1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 2 & -2 & 0 \end{array}\right] \end{array} \begin{array}{c} \\ \mathrm{T} \\ \mathrm{k_B} \\ \mathrm{h} \\ \mathrm{R} \\ \mathrm{E_B} \end{array}$$

- Number of unknowns
  $n = 5$
- Rank of the matrix
  $r = 3$ (independent rows)
- Number of parameters (π_1, π_2)
  $n - r = 2$
- Number of repeating variable
  $r = m = 3$

Example: Any nonzero determinant for P

$$A = \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array}\begin{array}{cccc} M & L & t & \Theta \\ \end{array}$$

$$A = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 1 \\ 1 & 2 & -2 & -1 \\ 1 & 2 & -1 & 0 \\ \hline 0 & 0 & -1 & 0 \\ 1 & 2 & -2 & 0 \end{array}\right] \begin{array}{l} T \\ k_B \\ h \\ R \\ E_B \end{array}$$

$$P_1 = \begin{array}{c} \begin{array}{ccc} L & T & \Theta \end{array} \\ \begin{bmatrix} 0 & 0 & -1 \\ 2 & -2 & -1 \\ 2 & -1 & 0 \end{bmatrix} \end{array} \begin{array}{l} T \\ k_B \\ h \end{array}$$

Rank 3 …

$$Q_1 = \begin{array}{c} \begin{array}{ccc} L & T & \Theta \end{array} \\ \begin{bmatrix} 0 & -1 & 0 \\ 2 & -2 & 0 \end{bmatrix} \end{array} \begin{array}{l} R \\ E_B \end{array}$$

$$E = \left[-QP^{-1}, I\right] = \begin{array}{c} \begin{array}{ccccc} T & k_B & h & R & E_B \end{array} \\ \begin{bmatrix} -1 & -1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 0 & 1 \end{bmatrix} \end{array} \Rightarrow \Pi_1 = \frac{\hbar R}{kT}, \Pi_2 = \frac{E_B}{kT}$$

Physical Meaning of the exponent matrix

$$E=\left[-QP^{-1},I\right]=\begin{array}{ccccc} T & k_B & h & R & E_B \\ \end{array}$$

$$E=\left[-QP^{-1},I\right]=\left[\begin{array}{ccc|cc} -1 & -1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 0 & 1 \end{array}\right]\Rightarrow \Pi_1=\frac{\hbar R}{kT},\Pi_2=\frac{E_B}{kT}$$

$$T^a\times k_B{}^b\times h^c\times R=L^0\times t^0\times\Theta^0$$

$\Rightarrow$ 3 equations for a,b,c

$$T^a\times k_B{}^b\times h^c\times E_B=L^0\times t^0\times\Theta^0$$

$\Rightarrow$ 3 equations for a,b,c

Variable $\rightarrow M^a\times L^b\times t^c\times\Theta^d$	
$E_B\rightarrow M^1\times L^2\times t^{-2}\times\Theta^0$	$\left(0.5m\upsilon^2\right)$
$T\rightarrow M^0\times L^0\times t^0\times\Theta^1$	(kelvin)
$R\rightarrow M^0\times L^0\times t^{-1}\times\Theta^0$	$(\sec^{-1})$
$k_B\rightarrow M^1\times L^2\times t^{-2}\times\Theta^{-1}$	(energy/kelvin)
$\hbar\rightarrow M^1\times L^2\times t^{-1}\times\Theta^0$	(energy-sec)

The dimensionless parameters are the Pi parameters

Example continued …

$$E = \left[-QP^{-1}, I\right] = \begin{array}{c} \begin{array}{ccccc} \mathrm{T} & \mathrm{k_B} & \mathrm{h} & \mathrm{R} & \mathrm{E_B} \end{array} \\ \begin{bmatrix} -1 & -1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 0 & 1 \end{bmatrix} \end{array} \Rightarrow \Pi_1 = \frac{\hbar R}{kT}, \Pi_2 = \frac{E_B}{kT}$$

$$G\left(\Pi_1 \equiv \frac{\hbar R}{kT}, \Pi_2 \equiv \frac{E_B}{kT}\right) = 0$$

$$\Rightarrow \frac{\hbar R}{kT} = f\left(\frac{E_B}{kT}\right)$$

If you assumed $\hbar$ to be absent (you did not know about it before Quantum mechanics), then

$$\boxed{\frac{cR}{kT} = f\left(\frac{E_B}{kT}\right)}$$

Example: Any nonzero determinant for P

$$A = \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array}\begin{array}{c} \begin{array}{cccc} M & L & t & \Theta \end{array} \\ \left[\begin{array}{c|ccc} 0 & 0 & 0 & 1 \\ 1 & 2 & -2 & -1 \\ 1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 2 & -2 & 0 \end{array}\right] \end{array} \begin{array}{l} \\ \mathrm{T} \\ \mathrm{k_B} \\ \mathrm{h} \\ \mathrm{R} \\ \mathrm{E_B} \end{array}$$

$$P_2 = \begin{array}{c} \begin{array}{ccc} L & T & \Theta \end{array} \\ \begin{bmatrix} 2 & -2 & -1 \\ 2 & -1 & 0 \\ 0 & -1 & 0 \end{bmatrix} \end{array} \begin{array}{l} \\ T \\ k_B \\ R \end{array}$$

Rank 3 …

$$Q_2 = \begin{bmatrix} 2 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{array}{l} E_B \\ T \end{array}$$

$$E = \left[-QP^{-1}, I\right] = \begin{array}{c} \begin{array}{ccccc} \mathrm{T} & \mathrm{k_B} & \mathrm{h} & \mathrm{R} & \mathrm{E_B} \end{array} \\ \begin{bmatrix} +0 & -1 & -1 & 1 & 0 \\ +1 & -1 & -1 & 0 & 1 \end{bmatrix} \end{array} \Rightarrow \Pi_1 = \frac{E_B}{k_B R}, \Pi_2 = \frac{k_B T}{\hbar R}$$

Example: Any nonzero determinant for P

$$E = \left[-QP^{-1}, I\right] = \begin{array}{c} \begin{array}{ccccc} \mathrm{T} & \mathrm{k_B} & \mathrm{h} & \mathrm{R} & \mathrm{E_B} \end{array} \\ \begin{bmatrix} +0 & -1 & -1 & 1 & 0 \\ +1 & -1 & -1 & 0 & 1 \end{bmatrix} \end{array} \Rightarrow \Pi_1 = \frac{E_B}{k_B R}, \Pi_2 = \frac{k_B T}{\hbar R}$$

$$G\left(\Pi_1 \equiv \frac{E_B}{k_B R}, \Pi_2 \equiv \frac{k_B T}{\hbar R}\right) = 0$$

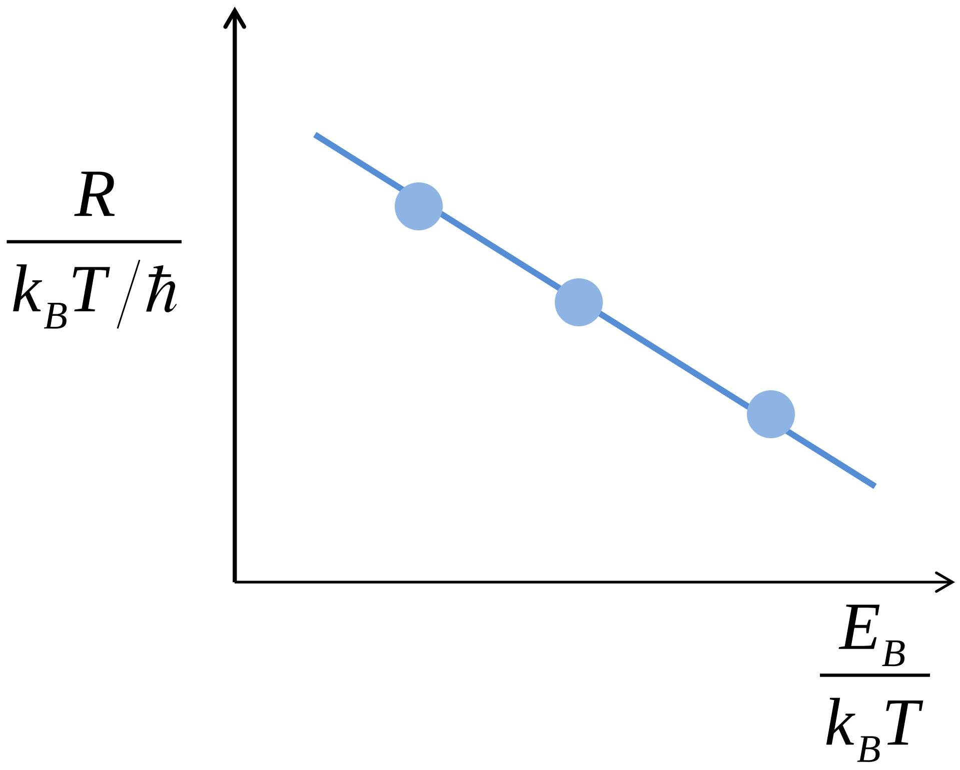
$$\Rightarrow \frac{E_B}{k_B R} = f\left(\frac{k_B T}{\hbar R}\right)$$

$$\Pi_3 \equiv \frac{\Pi_1}{\Pi_2} = \frac{E_B}{k_B T}$$

$$G\left(\Pi_3 \equiv \frac{E_B}{k_B T}, \Pi_2 \equiv \frac{k_B T}{\hbar R}\right) = 0$$

$$\Rightarrow \frac{k_B T}{\hbar R} = f_2\left(\frac{E_B}{k_B T}\right)$$

Plotting with dimensionless variables



Example 2: Newton anticipates Einstein's results

Use Bucking Pi theorem to analyze the remarkable fact that Newton foresaw bending of light by gravity long before Einstein!

Assuming the sun can be treated as a point of mass m and the ray of light passes the mass with a distance of closest approach r, dimensional reasoning helps to predict the defection angle \theta. The problem involves 3 of the 7 fundamental units: mass M, length L, and time T.

a) Write the Buckingham matrix first by thinking about three variables, $\theta, r, and\ m$. We have the following dimensions: angle $[\theta] = L^0\,T^0\,M^0$, $[r] = L^1\,T^0\,M^0$, and $[m] = L^0\,T^0\,M^1$. By putting in Bucking Pi matrix, we find that there is no solution.

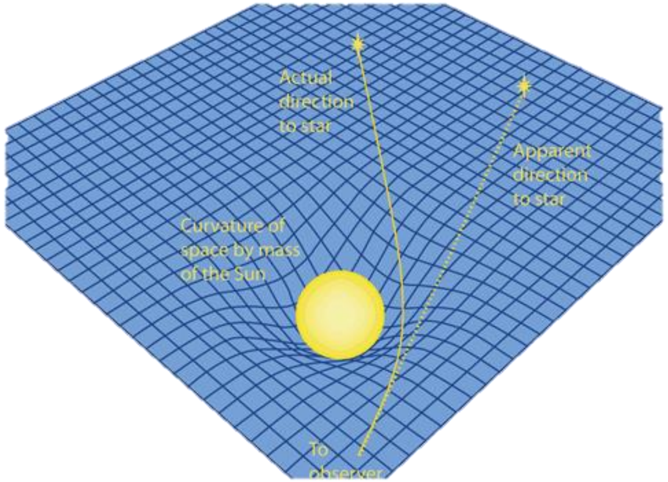
b) Augment the matrix with two other variables, the gravitational constant, $[G] = L^3\,T^{-2}\,M^{-1}$ and velocity of light $[c] = L^1\,T^{-1}\,M^0$. After all, we now light and gravity in the problem. Use the Buckingham pi theorem to show that the scaling factor involved.

c) Show that the final result can be written in the form $\theta = \alpha \frac{G\,m}{c^2 r}$ where α is the dimensionless factor. (Using $r = 6.96 \times 10^8\ m$, $m = 1.99 \times 10^{30}$ kg, and $\alpha = 2$, Newton anticipated the general relativity result within a factor of 2!

Dynamic Similarity , the dimensionless science, A Sept. 2011 (p. 47) physics Today Article by D. Bolster. Also, see R. Kurth, "Dimensional Analysis and Group Theory in Astrophysics" Pergamon Press, Oxford, UK, 1972.

Example 2: Newton anticipates Einstein?!

$$\theta = f(r,m) \Rightarrow 0 = g(\theta, r, m)$$



$$A = \begin{array}{c} \\ \\ \end{array}\begin{array}{ccc} M & L & T \end{array}$$

$$A = \begin{array}{cc} & \begin{array}{ccc} M & L & T \end{array} \\ & \left[\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{array}\right] \begin{array}{c} \theta \\ r \\ m \end{array} \end{array}$$

- The determinant is zero
- Top row is zero
- Two equations and three variables
- No solution
- Incomplete problem specification,
- Must have hidden variable(s)

[a] Here the Buckingha

M	L
0	0
0	1
1	0

The determinant is 0 ar
zero, therefore we have

.... continued

$$\theta = f(G,c,r,m) \Rightarrow 0 = g(\theta,G,c,r,m)$$

$$
\begin{array}{cccccc}
 & M & L & T & \\
\multirow{2}{*}{Q_1} & 0 & 0 & 0 & \theta \\
 & 0 & 1 & 0 & r \\
 & 1 & 0 & 0 & m \\
P_1 & -1 & 3 & -2 & G \\
 & 0 & 1 & -1 & c
\end{array}
$$

- Number of unknowns
  $n = 5$
- Rank of the matrix
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- Number of parameters (π_1, π_2)
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Q should contain the output variables, P the input variables

…. continued

$$\theta = f(G,c,r,m) \Rightarrow 0 = g(\theta,G,c,r,m)$$

$$\begin{array}{c|ccc|c} & M & L & T & \\ \hline \multirow{2}{*}{Q_1} & 0 & 0 & 0 & \theta \\ & 0 & 1 & 0 & r \\ \hline & 1 & 0 & 0 & m \\ P_1 & -1 & 3 & -2 & G \\ & 0 & 1 & -1 & c \end{array}$$

$$E = (-Q_1 P_1^{-1}, I)$$

m	G	c	θ	r
0	0	0	1	0
−1	−1	2	0	1

$$\Pi_1 = \theta^1 m^0 G^0 c^0 r^0$$

$$\Pi_2 = m^{-1} G^{-1} c^2 \theta^0 r$$
$$= c^2 r / Gm$$

$$\theta = f\left(\frac{Gm}{c^2 r}\right) \sim \left(\frac{Gm}{c^2} r\right)$$

$$\Pi_1 = f(\Pi_2)$$

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Example 3: The trick of the magic (Diffusion equation: Standard scaling)

$$D\frac{d^2n}{dx^2} - \frac{n}{\tau} = 0$$

$$n = n_0\, n^* \qquad x = x_0 x^*$$

$$D\frac{n_0 d^2n^*}{x_0^2 dx^{*2}} - \frac{n_0 n^*}{\tau} = 0$$

$$\frac{d^2n^*}{dx^{*2}} - \frac{n_0 x_0^2 n^*}{D\tau} = 0$$

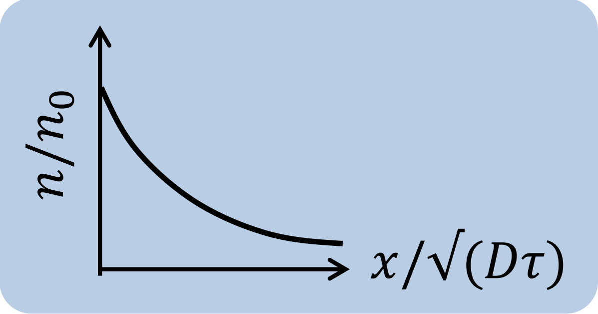
$$\frac{x_0^2}{D\tau} = 1, \qquad \rightarrow \quad x_0 = \sqrt{D\tau}$$

$$\frac{d^2n^*}{dx^{*2}} - n^* = 0$$

$$n^* = Ae^{x^*} + Be^{-x^*}$$

$$\frac{n}{n_0} = Ae^{\frac{x}{\sqrt{D\tau}}} + B\, e^{-\frac{x}{\sqrt{D\tau}}} \equiv f\left(\frac{x}{\sqrt{(D\tau)}}\right)$$

Non-dimensionalized



Example 3: Buckingham Pi approach

$$D\frac{d^2n}{dx^2} - \frac{n}{\tau} = 0$$

	M	L	T	
Q_1	0	-3	0	n
	0	1	0	x
P_1	0	2	-1	D
	0	0	1	τ

$Q_1 =$

L	T	
-3	0	n
1	0	x

$P_1 =$

L	T	
2	-1	D
0	1	τ

$$E = (-Q_1\, P_1^{-1}, I)$$

D	τ	n	x
-1.5	-1.5	1	0
-0.5	-0.5	0	1

Variables … n=4
Rank … r=2
Scaled dimension … (4-2)=2

$$\Pi_1 = n^1 D^{-1.5}\tau^{-1.5} \equiv \frac{n}{n_0}$$

$$\Pi_2 = x^1 D^{-0.5}\tau^{-0.5} \equiv \frac{x}{\sqrt{D\tau}}$$

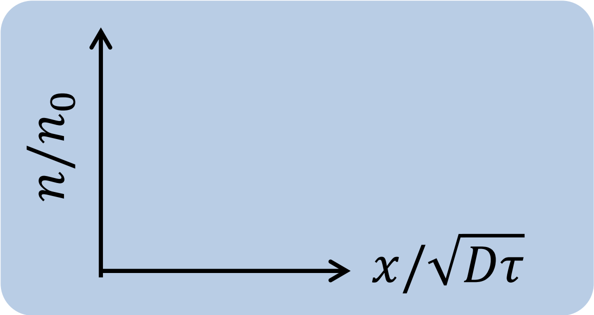
$$\Pi_1 = f(\Pi_2) \equiv \frac{n}{n_0} = f\left(\frac{x}{\sqrt{D\tau}}\right)$$

D implies a second order term

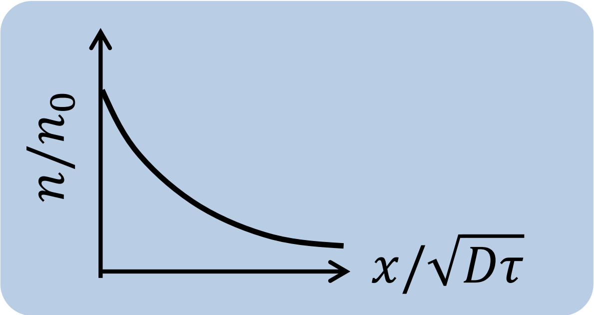
Example 3: continued …

$$\Pi_1 = f(\Pi_2) \equiv \frac{n}{n_0} = f\left(\frac{x}{\sqrt{D\tau}}\right)$$

D implies a second order term!



Scaling theory defines the axes



Experiments gets the function

Deep essence of machine learning … you do not need to know the equation

Discussion

1. Widely used in fluid mechanics (Rayleigh, Reynold, Pandtl numbers), percolation theory, reliability problems, etc. Newton predicted bending of light by gravitational field simply by dimensional analysis. He was off by a factor of 2 compared to Einstein.

   HW. $F = f(D, V, \rho, \mu)$, show that $\frac{F}{\rho V^2 D^2} = f(\frac{\mu}{\rho V D})$.

   We did not solve for Navier-Stokes equation.
   Similitude explains why Wind-tunnels work. And why Wright brothers succeeded why others failed.

2. If you add extra variables, which are unimportant – they will other disappear or appear as normalized variable that will be shown to be irrelevant experimentally.

3. Related to the principle component analysis in a interesting way (e.g. 'Recommended for you' by Amazon and Netflix)

Significant Dimensionless Group

Viscous force: $\tau A = \mu \frac{du}{dy} A \propto \mu \frac{V}{L} L^2 = \mu V L$

Pressure force: $(\Delta p)A \propto (\Delta p)L^2$

Compressibility force: $E_v A \propto E_v L^2$

Gravity force: $mg \propto g\rho L^3$

Surface tension force: σL

$$Re = \frac{\rho \bar{V} D}{\mu} = \frac{\bar{V} D}{\nu}$$

$$Eu = \frac{\Delta p}{\frac{1}{2}\rho V^2}$$

$$M = \frac{V}{c} = \frac{V}{\sqrt{\frac{dp}{d\rho}}} = \frac{V}{\sqrt{\frac{E_v}{\rho}}}$$

$$Ca = \frac{p - p_v}{\frac{1}{2}\rho V^2}$$

$$Fr = \frac{V}{\sqrt{gL}}$$

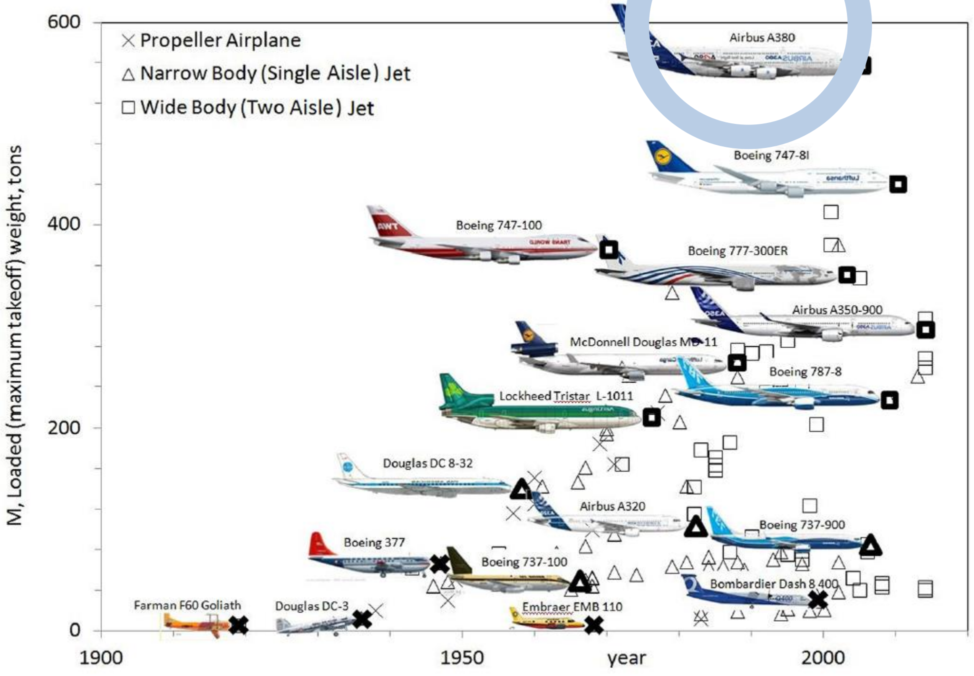
$$M^2 = \frac{\rho V^2 L^2}{E_v L^2}$$

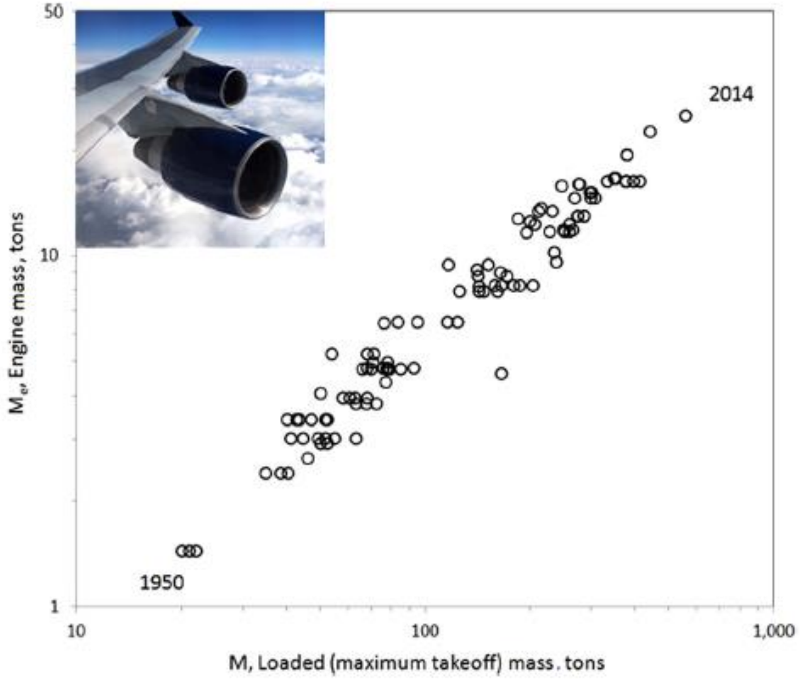
$$We = \frac{\rho V^2 L}{\sigma}$$

$$Fr^2 = \frac{V^2}{gL} = \frac{\rho V^2 L^2}{\rho g L^3}$$

The evolution of airplanes

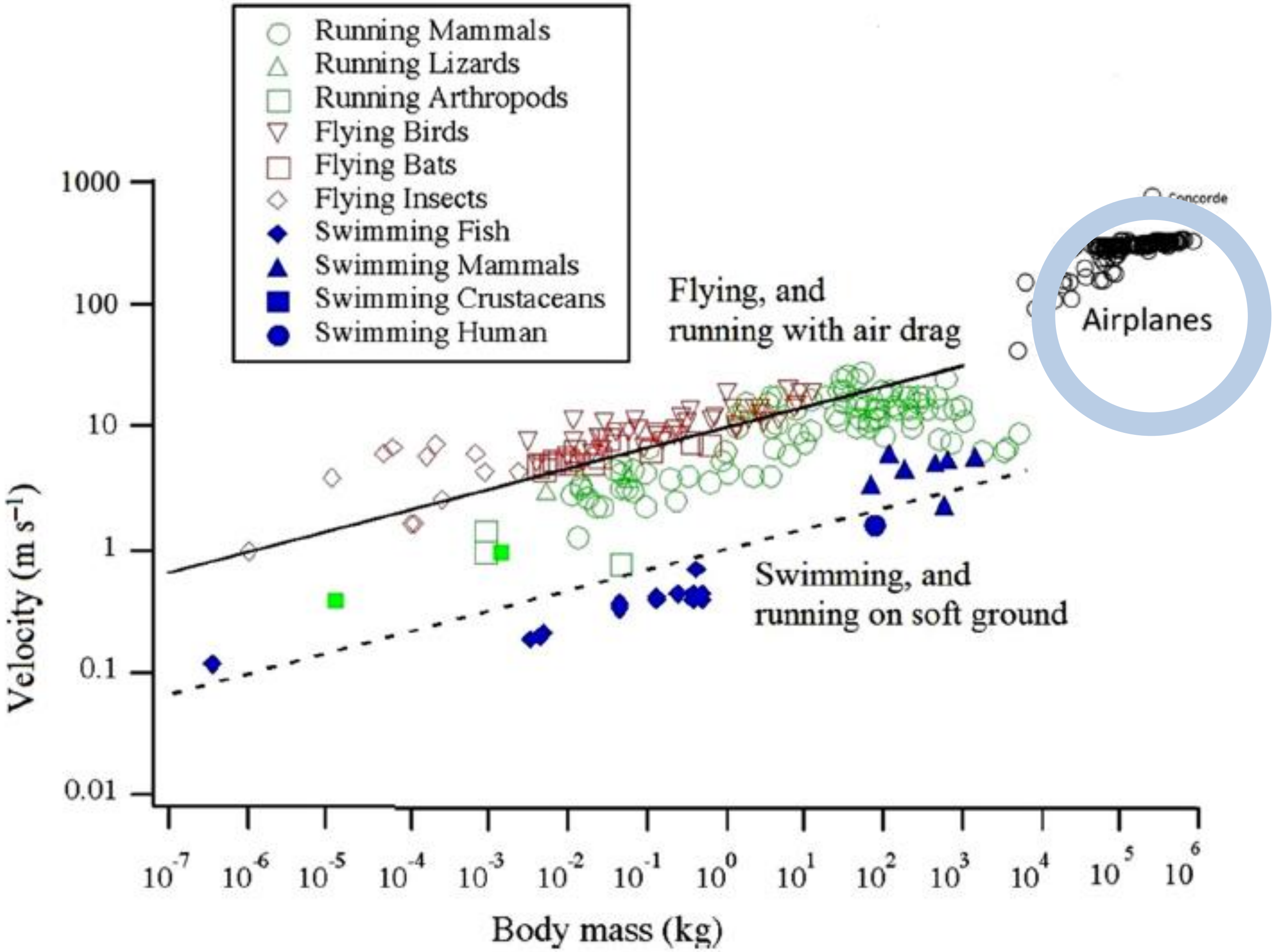
A. Bejan et al. JAP, 116, 044901, 2014

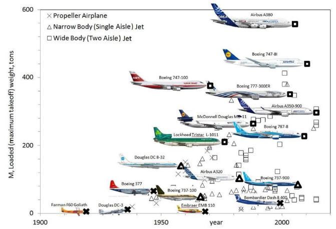




Engine lifts 10x its mass: $M_e = 0.13\, M^{0.83}$

Scaling theory of things that move





Conclusions

1. Fundamentally, the laws of physics must be non-dimensional, because otherwise laws will depend where you are in the universe.
2. Scaling of variables is a very important way of reducing the number of variables in an experiment. However, scaling requires that we have some idea about the key variables.

3. There are many applications of the scaling theory, especially in fluid mechanics, phase transition, percolation theory, etc. The problem is complex, similar to that of reliability, and therefore scaling provides enormous simplification.

4. Some of the problems may not be fully specified in terms of explicitly stated variables. The Fisher/Taguchi method help design those experiments.

References

Dimensional Analysis:
Most books on Fluid mechanics has a chapter on "Dimensional Analysis". See for example,http://en.wikibooks.org/wiki/Fluid_Mechanics/Dimensional_Analysis

One of the best articles on this topic is by D. Bolster, R. Hershberger, and R. J. Donnelly, Physics Today, p. 42, 2011. http://astro.berkeley.edu/~eliot/Astro202/dimensional_PhysicsToday.pdf

The reliability example I used is from a bookchapter on "Some Unifying Concepts in Reliability Physics, Mathematical Models, and Statistics" by R. E. Thomas,

Another excellent book is Introduction to Fluid mechanics, 5th Edition written by R.W. Fox and A.T. McDonald, John Wiley and Sons, Inc.

Review Questions

1. How does one choose the variables in for Buckingham Pi analysis?
2. Convince yourself that Rayleigh, Reynold, Womersley, Prandtl numbers are dimensionless.
3. Use the example of wind-tunnel and Dennard scaling to argue that scaling reduces the number of experiments while simultaneously reducing the physical size of the experimental setup.
4. The scaling theory may give fundamentally wrong results, if the choice of the variables is not guided by physical insights of the problem. Explain.
5. What are the advantages and disadvantages of nature units?
6. What is the difference among geometric similarity, kinetic similarity and dynamic similarity?