Primer on Analysis of Experimental Data and Design of Experiments

Lecture 5. Design of Experiments Scaling of Theory of Equations

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Course Outline

$$\overline{y} = f\,(\overline{x}\,) \qquad \overline{x} = x_1, x_2, \ldots x_n \qquad \overline{y} = y_1, y_2, \ldots y_m$$

Lecture 1: Introduction

Lecture 2: Collecting and plotting $x_1, x_2, \ldots x_n$

Lecture 3: Physical and empirical $f, F, df/dx, \ldots$

Lecture 4: Model selection among $f_1, f_2, \ldots$

Lecture 5: Scaling theory with known f, $f(\overline{x}) = f(\overline{X})$

Lecture 6: Scaling theory with unknown f, $\overline{x} \rightarrow X$

Lecture 7: Design of experiments to determine $\overline{y}_{\max} = f\,(\overline{x}\,)$

Lecture 8: Machine learning … Statistical approach to learn f

Lecture 9: Physics-based machine learning $f = f_{\text{physics}} + \Delta f$

Lecture 10: Principle component analysis for classifying $\{y\}$.

Lecture 11: Conclusions

Outline

1. Introduction
2. Rules of scaling or nondimensionalization
3. Scaling of ordinary differential equations
4. Scaling of partial differential equations
5. Equivalence of equations and solutions
6. Conclusions

Stress-induced cell death

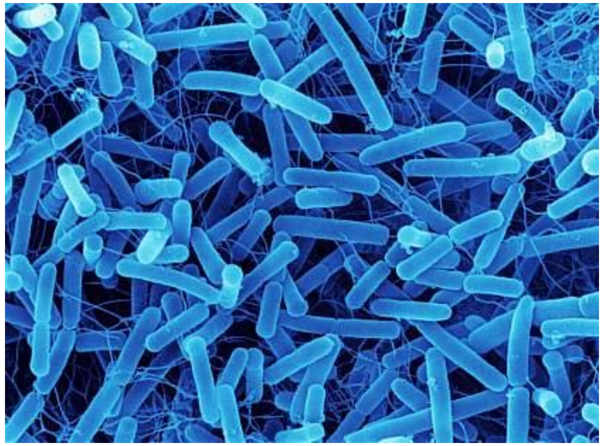
Equation: $\frac{dn}{dt} = -b(T)n$

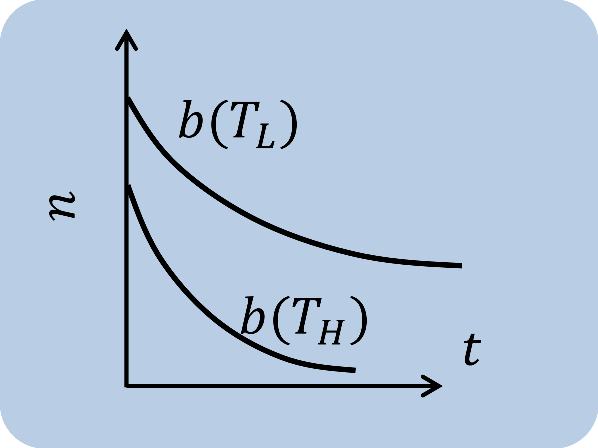
$\Rightarrow \quad n = n_0 \, e^{-b(T)\,t} \equiv f(n_0, b, t)$

5 experiments each for n_0, b, t

... 125 measurements

If with multiple samples, hundreds of measurements required.





Stress-induced cell death

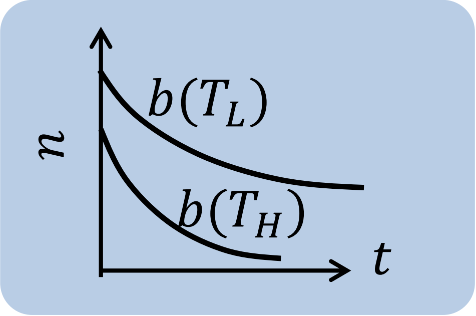
$$n = n_0\, e^{-b(T)\,t} \equiv f(n_0, b, t)$$

Three variables: 125 measurements

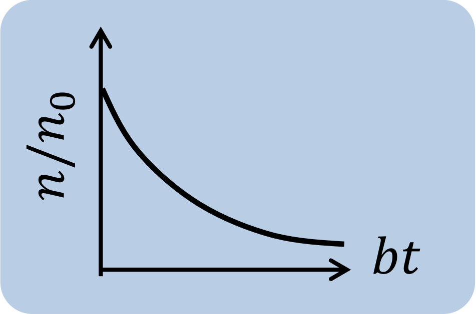
Normalized equation: $\dfrac{n}{n_0} = g(bt) \Rightarrow N = g(\tau)$

Two variables: 25 experiments.

Original



Non-dimensionalized



Goals of Nondimensionalization

- Simplify differential equations
- Rescale variables to a unitless form
- Get rid of unnecessary parameters
- Reduce the number of experiments needed to test a hypothesis

Rules for nondimentionalization

- Identify the **independent** and **dependent** variables;
- Replace each of them with a quantity **scaled** relative to a characteristic unit of measure to be determined;
- Divide through by the coefficient of the **highest order** polynomial or derivative term;
- Choose judiciously the definition of the characteristic unit for each variable **so that the coefficients** of as many terms as possible become 1;
- Rewrite the system of equations in terms of their **new dimensionless** quantities.

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(1) Constant Coefficient 1st order Equation

1. Equation: $a\frac{dy}{dt} + by = Af(t)$

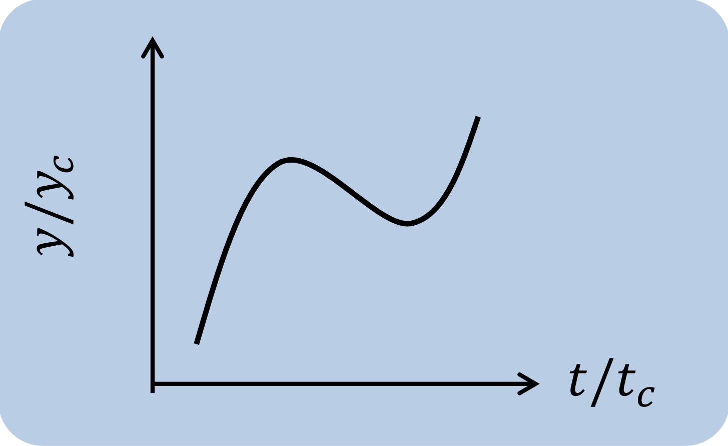
   Define scaled variables: $y = x\, y_c,\ t = \tau\, t_c$

2. Normalized equation: $a\frac{y_c}{t_c}\frac{dx}{d\tau} + by_c x\ = Af(\tau\, t_c)$

$$\frac{dx}{d\tau} + \frac{bt_c}{a}x\ = \frac{At_c}{ay_c}f(\tau\, t_c) = BF(\tau)$$

3. Scale factors: $\frac{bt_c}{a} \equiv 1\ \Rightarrow t_c \equiv \frac{a}{b},\quad B \equiv \frac{At_c}{ay_c} \equiv \frac{A}{by_c}$

4. Final Equation: $\frac{dx}{d\tau} + x\ = BF(\tau)$



Note: What about y_c; Undefined, but scales B.

(1) … Must scale the boundary conditions

Original Equation: $a\frac{dy}{dt} + by = Af(t)$

Final Equation: $\frac{dx}{d\tau} + x \ = BF(\tau)$

Original boundary condition: $y(t = 3) = \ y_0$

Scaled boundary condition:

$y = x\, y_c,\ t = \tau\, t_c$

$$\Rightarrow \ \ xy_c(\tau t_c = 3) = y_0 \Rightarrow x\left(\tau = \frac{3}{t_c}\right) = \frac{y_0}{y_c}$$

(2) Higher order equations

1. Equation: $a\frac{d^2y}{dt^2} + b\frac{dy}{dt} + cy = Af(t)$. With $y = x\, y_c$ and $t = t_c\tau$.

$$\frac{ay_c}{t_c^2}\frac{d^2x}{d\tau^2} + \frac{by_c}{t_c}\frac{dx}{d\tau} + cy_c x = Af(t_c\tau).$$

2. Normalized equation: $\frac{d^2x}{d\tau^2} + \frac{bt_c}{a}\frac{dx}{d\tau} + \frac{ct_c^2}{a}x = \frac{At_c^2}{ay_c}f(t_c\tau) \equiv BF(\tau)$.

3. Two parameters (t_c and y_c), therefore we can two coefficients set to 1.

t_c scaling: Either $\frac{bt_c}{a} = 1 \Rightarrow\ t_c = \frac{a}{b}$ or

$\frac{ct_c^2}{a} = 1 \Rightarrow\ t_c = \sqrt{\frac{a}{c}}$ so that the 1st coefficient is , $b\frac{t_c}{a} = b\sqrt{\frac{a}{c}} = 2\xi$

(2nd normalization is chosen)

y_c scaling: $B = \frac{At_c^2}{ay_c} = 1$, therefore $y_c = A\frac{t_c^2}{a} = \frac{A}{c}$

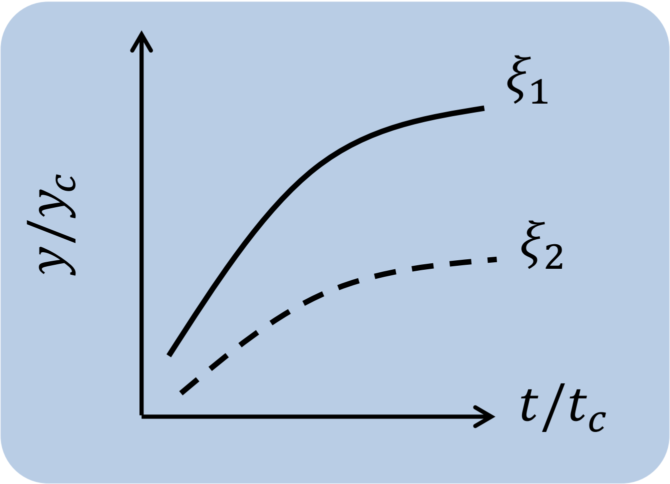
(2) …Higher order equations

1. Equation: $a\frac{d^2y}{dt^2} + b\frac{dy}{dt} + cy = Af(t)$.

Two parameters (t_c and y_c), therefore we can set two coefficients to unity.

$t_c = \sqrt{\frac{a}{c}}$ so that the first coefficient becomes , $b\frac{t_c}{a} = b\sqrt{\frac{a}{c}} = 2\xi$

y_c scaling: $B = \frac{At_c^2}{ay_c} = 1$, therefore $y_c = A\frac{t_c^2}{a} = \frac{A}{c}$



4. Final equation: $\frac{d^2x}{d\tau^2} + 2\xi\frac{dx}{d\tau} + x = \frac{A}{c}f(t_c\tau) \equiv BF(\tau)$.

(3) HW: Coupled Equations

$$\frac{dx}{dt} = \gamma x \left(1 - \frac{\alpha\, x + \beta\, y}{N}\right) \qquad \frac{dy}{dt} = \theta\, y \left(1 - \frac{\alpha\, x \ + \beta\, y}{N}\right)$$

$$x = x_c\, X, \qquad y = y_c\, Y, \qquad t = t_c\, \tau$$

$$\frac{dX}{d\tau} = \frac{t_c}{x_c} x_c \gamma X \ \left(1 - \frac{x_c \alpha X + y_c \beta Y}{N}\right) \qquad \frac{dY}{d\tau} = \frac{t_c}{y_c} y_c \theta Y \ \left(1 - \frac{x_c \alpha X + y_c \beta Y}{N}\right)$$

$$\frac{dX}{d\tau} = t_c \gamma X \ - \frac{t_c \gamma x_c \alpha X + t_c \gamma y_c \beta Y}{N} \qquad \frac{dY}{d\tau} = t_c \theta Y \ - \frac{t_c \gamma x_c \alpha X + t_c \gamma y_c \beta Y}{N}$$

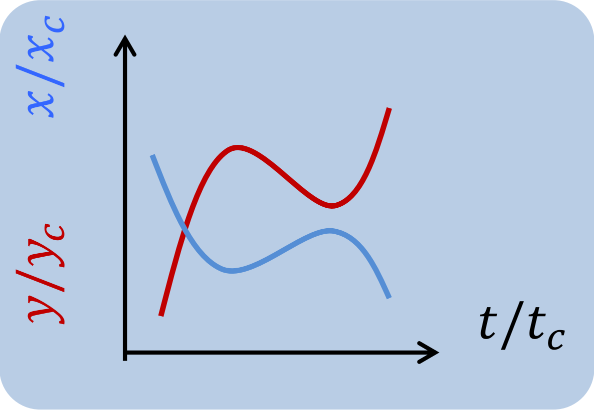
Three variables allows three coefficients to set to 1.

$t_c\,\gamma \ =1 \ \Rightarrow \ \ t_c \ = \gamma^{-1} \qquad t_c \gamma x_c \alpha / N = 1 \ \Rightarrow \ x_c = N\alpha^{-1}, \quad t_c \gamma y_c \beta / N \Rightarrow \ y_c = N\beta^{-1}$

$\frac{dX}{d\tau} = -Y$ and $\frac{dY}{d\tau} = \theta\gamma^{-1} Y - X - Y = (\kappa - 1)Y - X$

$For\ \kappa = 1, \frac{d(X+Y)}{d\tau} = -\,(x + Y) \ \rightarrow (x + Y) \ = \ x_0 \exp(-t/\tau)$

Matrix solution



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Nondimensionalization: example

- Minority carrier diffusion equation: $\frac{dn}{dt} = D\frac{d^2n}{dx^2} - \frac{n}{\tau} + G_L$
  - 3 parameters: D, τ, and G_L
  - 3 variables: n, x, and t
- Goal: convert n, x, and t to dimensionless $\tilde{n}, \tilde{x}, \tilde{t}$ in terms of D, τ, and G_L
- Technique:
  - Set $\tilde{n} = \frac{n-n_r}{n_0}$, $\tilde{x} = \frac{x-x_r}{x_0}$, $\tilde{t} = \frac{t-t_r}{t_0}$

    (n_r, x_r, t_r: reference values; n_0, x_0, t_0: scaling factors)

  - Assume: n, x, t starts at n=0 x=0 and t =0 , so $\mathrm{n_r} = 0$, $x_r = 0$, $t_r = 0$
  - $\tilde{n} = \frac{n}{n_0}$, $\tilde{x} = \frac{x}{x_0}$, $\tilde{t} = \frac{t}{t_0}$
  - Insert $n = \tilde{n}n_0$, $x = \tilde{x}x_0$, $t = \tilde{t}t_0$ into the original PDE

Nondimensionalization: example

- Rewrite: $\frac{dn}{dt} = D\frac{d}{dx}\left(\frac{dn}{dx}\right) - \frac{n}{\tau} + G_L$, insert $n = \tilde{n}n_0, x = \tilde{x}x_0, t = \tilde{t}t_0$

$$=> \frac{d\tilde{n}n_0}{d\tilde{t}t_0} = D\frac{d}{d\tilde{x}x_0}\left(\frac{d\tilde{n}n_0}{d\tilde{x}x_0}\right) - \frac{\tilde{n}n_0}{\tau} + G_L$$

Divide by this factor on both sides

$$=> \boxed{\frac{n_0}{t_0}}\frac{d\tilde{n}}{d\tilde{t}} = D\frac{n_0}{x_0^2}\frac{d}{d\tilde{x}}\left(\frac{d\tilde{n}}{d\tilde{x}}\right) - \frac{n_0}{\tau}\tilde{n} + G_L$$

$$=> \frac{d\tilde{n}}{d\tilde{t}} = \boxed{D\frac{t_0}{x_0^2}}\frac{d}{d\tilde{x}}\left(\frac{d\tilde{n}}{d\tilde{x}}\right) - \boxed{\frac{t_0}{\tau}}\tilde{n} + \boxed{\frac{t_0}{n_0}G_L}$$

New coefficients

- Choose $t_0 = \tau, x_0 = \sqrt{D\tau}, n_0 = \tau G_L$ so that PDE become as simple as possible:

$$=> \frac{d\tilde{n}}{d\tilde{t}} = \frac{d^2\tilde{n}}{d\tilde{x}^2} - \tilde{n} + 1$$

  - 3 unitless variables and 0 parameter

- Q: Where are the original 3 parameters D, τ, and G_L?

  A: They are combined into scaling factors $x_0, t_0, and\ n_0$

Conclusions

1. Scaling of equations is a powerful concept.
2. Scaling of the equations involves very specific rules; the equations and the boundary conditions must be scaled simultaneously.
3. The power of scaling involves reducing the number of experiments or simulations needed to investigate a hypothesis.
4. The scaling makes numerical solution simpler by making the variables of similar magnitude.
5. The scaling also allows one to look up solutions from in differential equations handbook or websites.
6. Scaling allows one to compare equations from very different fields and solve the problem in one field by borrowing solution from a different field.

References

Book on dimensional analysis including python code: https://hplgit.github.io/scaling-book/doc/pub/book/pdf/scaling-book-4screen-sol.pdf

Nondimensionalized models produce physically universal and numerically robust results. The topic is easily learned from the following articles.
ODE: https://en.wikipedia.org/wiki/Nondimensionalization
PDE: https://link.springer.com/article/10.1007/s11071-015-2233-8

Examples: https://user.engineering.uiowa.edu/~fluids/Posting/Schedule/Example/Dimensional%20Analysis_11-03-2014.pdf

Coupled Equation: https://math.stackexchange.com/questions/845891/nondimensionalization-of-coupled-ode

References: R. W. Robinett, "Dimensional Analysis at the Other Language of Physics," American Journal of Physics, 83(4), 353, 2015.

Review Questions

1. A non-dimensionalized equation is also called a scaled equation. Explain.
2. If there are two variables (one independent, the other dependent), how many scaled coefficients can be set to 1?
3. When scaling the differential equation, do you also need to scale the boundary conditions as well?
4. Why is it important to plot the experimental and simulation results in terms of scaled variables?
5. Why is it helpful to non-dimensionalize an equation before looking up the solution in a handbook?