CHEM1033 - Week 7 Lecture - Transcendental equations

Sections 3.1-3.4, 3.6-3.9 of Steiner, "The Chemistry Maths Book", 2nd edition.
Chapters 12 and 16 of Monk and Munro, "Maths for Chemistry", 2nd edition.

1. Number fields

There are many types of numbers in mathematics: integers, rational numbers, real numbers, *etc.* They share some features and provide a good example of formal definitions, as well as notation that is often used in modern physical sciences. In formal mathematics, a *field* is defined as a set $\mathbb{F}$ with two operations, called *addition* ("+") and *multiplication* ("·"), that satisfy the following properties:

1. $\mathbb{F}$ is *closed* under addition and multiplication:

$$\forall a,b \in \mathbb{F}, \quad a+b \in \mathbb{F} \quad \text{and} \quad a \cdot b \in \mathbb{F}$$

   This should be read in the following way: "for any elements a and b belonging to $\mathbb{F}$, their sum and their product also belong to $\mathbb{F}$".

2. Addition and multiplication operations are *associative*:

$$\forall a,b,c \in \mathbb{F} \quad (a+b)+c = a+(b+c) \quad \text{and} \quad (a \cdot b)\cdot c = a \cdot (b \cdot c)$$

3. Addition and multiplication operations are *commutative*:

$$\forall a,b \in \mathbb{F} \quad a+b = b+a \quad \text{and} \quad a \cdot b = b \cdot a$$

4. $\mathbb{F}$ contains a unique *zero element* and a unique *unit element*:

$$\exists 0 \in \mathbb{F}, \quad \forall a \in F \quad a+0=a$$
$$\exists 1 \in \mathbb{F}, \quad \forall a \in F \quad a \cdot 1 = a$$

   The first line should be read in the following way: "there exists an element 0 in $\mathbb{F}$, such that, for any element a belonging to $\mathbb{F}$, $a+0=a$". The second line is: "there exists an element 1 in $\mathbb{F}$, such that, for any element a belonging to $\mathbb{F}$, $a \cdot 1 = a$".

5. Each element in $\mathbb{F}$ has a unique *additive inverse* and a unique *multiplicative inverse*:

$$\forall a \in \mathbb{F} \quad \exists (-a) \in \mathbb{F}, \quad a+(-a)=0$$
$$\forall a \in \mathbb{F} \quad \exists a^{-1} \in \mathbb{F}, \quad a \cdot a^{-1} = 1$$

6. Multiplication is *distributive* over addition:

$$\forall a,b,c \in \mathbb{F} \quad a \cdot (b+c) = a \cdot b + a \cdot c$$

These properties may appear obvious, but elsewhere in mathematics they do not necessarily hold. For example, three-dimensional rotation operators do not, in general, commute (prove this as an exercise). Examples of fields include rational numbers and real numbers. Examples of sets of numbers that are not fields are integers and transcendental numbers (prove this as an exercise).

The following notation for the different fields is commonly used in mathematics: $\mathbb{Z}$ for integers (not a field, but the symbol is there), $\mathbb{Q}$ for rational numbers, $\mathbb{R}$ for real numbers, $\mathbb{C}$ for complex numbers and $\mathbb{H}$ for quaternions. $\mathbb{Z}$ in particular is often used in solutions for trigonometric equations, for example:

$$\cos(x) = 1/\sqrt{2} \quad \Rightarrow \quad x = \pm\pi/4 + 2\pi n, \quad n \in \mathbb{Z}$$

2. Transcendental numbers and functions

A *transcendental number* is defined as a number that is not a root of a polynomial equation with rational coefficients. It is easy to demonstrate that the set of transcendental numbers is not a field – any field must contain a unit element and 1 is not a transcendental number. The most famous transcendental numbers are e and π, but many more exist. All real transcendental numbers are irrational, but not all irrational numbers of are transcendental (for example, $\sqrt{2}$ is not).

A *transcendental function* is an analytic function (for our purposes "analytic" means "infinitely differentiable") that does not satisfy any polynomial equation

$$p\left(x, f\left(x\right)\right) = 0$$

where $p\left(x, y\right)$ is a polynomial in x and y with integer coefficients. Transcendental functions cannot be expressed using a finite sequence of addition, multiplication and root extraction operations. The following are common examples of transcendental functions:

$$f\left(x\right) = e^x, \quad f\left(x\right) = \cos\left(x\right), \quad f\left(x\right) = \ln\left(x\right)$$

Equations involving transcendental functions are called *transcendental equations*.

3. Transcendental equations – analytical solutions

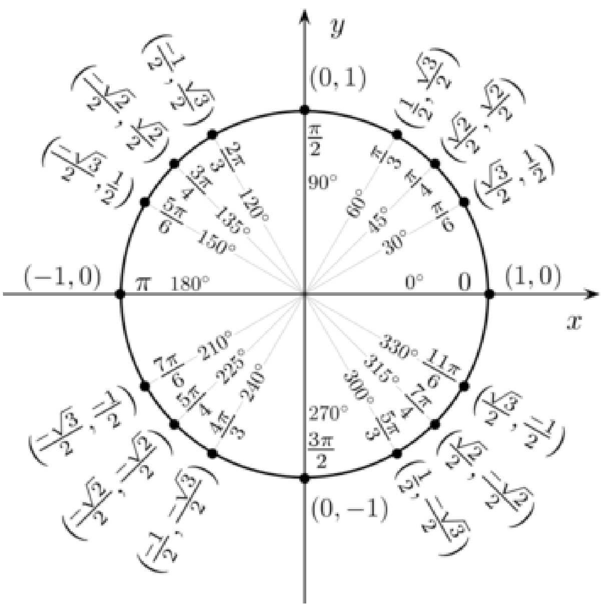
The only type of transcendental equations that are readily soluble are those that may be brought into a non-transcendental form by a variable substitution, for example:

$$\cos^2\left(x\right) - 1 = 0 \quad \Rightarrow \quad \begin{cases} y^2 - 1 = 0 \\ y = \cos\left(x\right) \end{cases} \tag{1}$$

This is a combination of a quadratic equation and an equation in which the variable to be solved for appears only as argument to the transcendental function. Because this equation is trigonometric, it has infinitely many solutions:

$$\begin{cases} y^2 - 1 = 0 \\ y = \cos\left(x\right) \end{cases} \quad \Rightarrow \quad \begin{cases} y = \pm 1 \\ y = \cos\left(x\right) \end{cases} \quad \Rightarrow \quad x = \pi n, \quad n \in \mathbb{Z} \tag{2}$$

To the right is a useful graph that tabulates solutions to common equations involving a single trigonometric function. The X axis corresponds to cosines and the Y axis to sines. Please do not forget about the periodicity and always include n.



Equations involving exponentials and logarithms can usually only be solved analytically if they can be reduced to a form that contains a single transcendental function with all instances of x occurring inside it, for example:

$$\ln\left(2\cos\left(x\right)\right) + \ln\left(\sin\left(x\right)\right) = 0$$

$$\Downarrow$$

$$\ln\left(2\cos\left(x\right)\sin\left(x\right)\right) = 0$$

In this case, the logarithm can be eliminated and the solution process continued:

$$2\cos(x)\sin(x)=1 \quad \Rightarrow \quad \sin(2x)=1 \quad \Rightarrow \quad 2x=\frac{\pi}{2}+2\pi n \quad \Rightarrow \quad x=\frac{\pi}{4}+\pi n, \quad n\in\mathbb{Z}$$

Examples of equations that either have no solutions at all, or have solutions that cannot be expressed in an algebraic form (*i.e.* using additions, multiplications and roots of rational numbers), are:

$$\cos(x)=x, \qquad \frac{E}{kT}\frac{e^{-E/kT}}{1+e^{-E/kT}}=1, \qquad \frac{1}{1+x}=e^{x}$$

Such equations are usually solved numerically.

4. Transcendental equations – numerical solutions

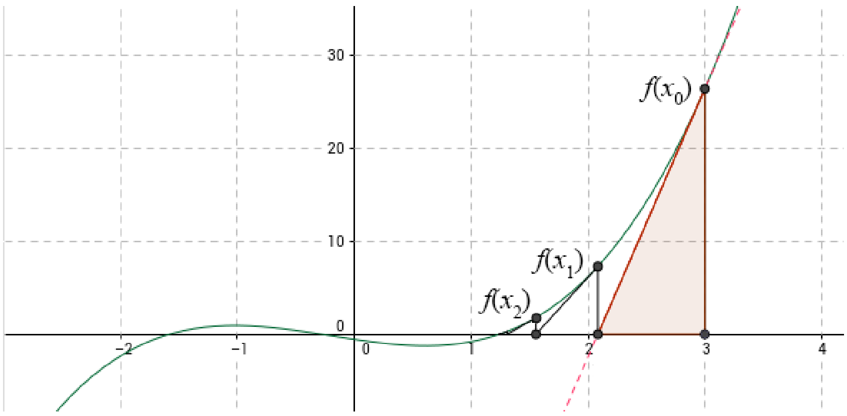
A large number of methods exist for numerical root finding. One method that is simple enough to be used in manual calculations and efficient enough to produce a solution in reasonable time is *Newton-Raphson method*. Isaac Newton observed in 1669 (and Joseph Raphson did, independently, in 1690) that the equation for the tangent line to a function $f(x)$ at a particular point x_n

$$y=f'(x_n)(x-x_n)+f(x_n) \tag{3}$$

may be used as a basis for an iterative algorithm that moves closer and closer to the root:

$$f'(x_n)(x_{n+1}-x_n)+f(x_n)=0 \quad \Rightarrow \quad x_{n+1}=x_n-\frac{f(x_n)}{f'(x_n)} \tag{4}$$

At each step, the algorithm replaces the difficult problem of finding the root of the original function with the simple problem of finding the root of its tangent line.



It may be demonstrated that the point x_n moves closer and closer to the nearest root of $f(x)$ when n is increased. Note that Newton-Raphson algorithm requires an *initial guess* x_0, that it converges to the *nearest* root to that initial guess and that it may fail to converge if the initial guess is not well chosen.

As an example, consider the root finding problem for $\exp(x)-5x=0$. The corresponding Newton-Raphson iteration equation is:

$$x_{n+1}=x_n-\frac{\exp(x_n)-5x_n}{\exp(x_n)-5}$$

If we begin our iterations at $x_0=3$, we obtain the following sequence of numbers: $x_1=2.6629$, $x_2=2.5533$, $x_3=2.5427$, $x_4=2.5426$ and the five significant digits quoted stop changing at the point when $n=4$, meaning that our root is found. As an exercise, find the other root by starting at $x_0=-1$.

Week 8 workshop exercises

In Problems 1–12, find exact solutions

1. $2 \sin x + 1 = 0, 0 \le x < 2\pi$

2. $2 \cos x + 1 = 0, 0 \le x < 2\pi$

3. $2 \sin x + 1 = 0$, all real x

4. $2 \cos x + 1 = 0$, all real x

5. $\tan x + \sqrt{3} = 0, 0 \le x < \pi$

6. $\sqrt{3} \tan x + 1 = 0, 0 \le x < \pi$

7. $\tan x + \sqrt{3} = 0$, all real x

8. $\sqrt{3} \tan x + 1 = 0$, all real x

9. $2 \cos \theta - \sqrt{3} = 0, 0° \le \theta < 360°$

10. $\sqrt{2} \sin \theta - 1 = 0, 0° \le \theta < 360°$

11. $2 \cos \theta - \sqrt{3} = 0$, all θ

12. $\sqrt{2} \sin \theta - 1 = 0$, all θ

Solve problems 19–22 to four decimal places

19. $1 - x = 2 \sin x$, all real x

20. $2x - \cos x = 0$, all real x

21. $\tan (x/2) = 8 - x, 0 \le x < \pi$

22. $\tan 2x = 1 + 3x, 0 \le x < \pi/4$

In Problems 23–34, find exact solutions

23. $2 \sin^2 \theta + \sin 2\theta = 0$, all θ

24. $\cos^2 \theta = \frac{1}{2} \sin 2\theta$, all θ

25. $\tan x = -2 \sin x, 0 \le x < 2\pi$

26. $\cos x = \cot x, 0 \le x < 2\pi$

27. $\sec (x/2) + 2 = 0, 0 \le x < 2\pi$

28. $\tan (x/2) - 1 = 0, 0 \le x < 2\pi$

29. $2 \cos^2 \theta + 3 \sin \theta = 0, 0° \le \theta < 360°$

30. $\sin^2 \theta + 2 \cos \theta = -2, 0° \le \theta < 360°$

31. $\cos 2\theta + \cos \theta = 0, 0° \le \theta < 360°$

32. $\cos 2\theta + \sin^2 \theta = 0, 0° \le \theta < 360°$

33. $2 \sin^2 (x/2) - 3 \sin (x/2) + 1 = 0, 0 \le x \le 2\pi$

34. $4 \cos^2 2x - 4 \cos 2x + 1 = 0, 0 \le x \le 2\pi$

Solve Problems 43–52 to four decimal places

43. $2 \sin x = \cos 2x, 0 \le x < 2\pi$

44. $\cos 2x + 10 \cos x = 5, 0 \le x < 2\pi$

45. $2 \sin^2 x = 1 - 2 \sin x$, all real x

46. $\cos^2 x = 3 - 5 \cos x$, all real x

Enhanced difficulty problems for the brave

1. Prove the identities:

   (a) $\tan\alpha + \cot\alpha = \sec\alpha\csc\alpha$

   (b) $\cot^2\alpha = \cos^2\alpha + \left(\cot\alpha\cos\alpha\right)^2$

   (c) $\dfrac{1}{\sec^2 x} = \sin^2 x\cos^2 x + \cos^4 x$

   (d) $\cot\beta\sec\beta = \csc\beta$

   (e) $\sec^2\alpha + \csc^2\alpha = \dfrac{1}{\sin^2\alpha\cos^2\alpha}$

2. Simplify:

   (a) $\dfrac{1+\tan^2 x}{1+\cot^2 x}$

   (b) $\dfrac{\sec^2 y - \cos^2 y}{\tan^2 y}$

   (c) $\dfrac{\csc^2\alpha - \sin^2\alpha}{\csc^2\alpha\left(2-\cos^2\alpha\right)}$

3. Prove the identities:

   (a) $\sin\beta\cos\left(\alpha-\beta\right) + \cos\beta\sin\left(\alpha-\beta\right) = \sin\alpha$

   (b) $\cot\left(\alpha+\beta\right) = \dfrac{\cot\alpha\cot\beta - 1}{\cot\alpha + \cot\beta}$

4. Simplify:

   (a) $\dfrac{\sin 2x}{1+\cos 2x}$

   (b) $\dfrac{\sin 2\alpha}{1-\cos^2\alpha}\dfrac{\sin 2\alpha}{\cos\alpha}$

   (c) $\dfrac{\sin 3\alpha - \sin 5\alpha}{\cos 3\alpha + \cos 5\alpha}$

5. Express as a monomial:

$$\sin\left(x-y\right) + \sin\left(y-z\right) + \sin\left(z-x\right)$$

6. Prove that

$$\left(1+\frac{a}{\sin x}\right)\left(1+\frac{b}{\cos x}\right) \ge \left(1+\sqrt{2ab}\right)^2$$

   for all real numbers a,b,x with $a,b \ge 0$ and $0 < x < \pi/2$.

7. Prove that

$$\left(4\cos^2 9° - 3\right)\left(4\cos^2 27° - 3\right) = \tan 9°$$

8. Simplify:

$$\sqrt{\sin^4 x + 4\cos^2 x} - \sqrt{\cos^4 x + 4\sin^2 x}$$