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Lecture 08: From Data to Functions

Sergei V. Kalinin

This and That

1. Hackathon impressions?
2. Please submit homeworks, midterms, finals, and hackathons to gmail
3. GitHub opportunity!

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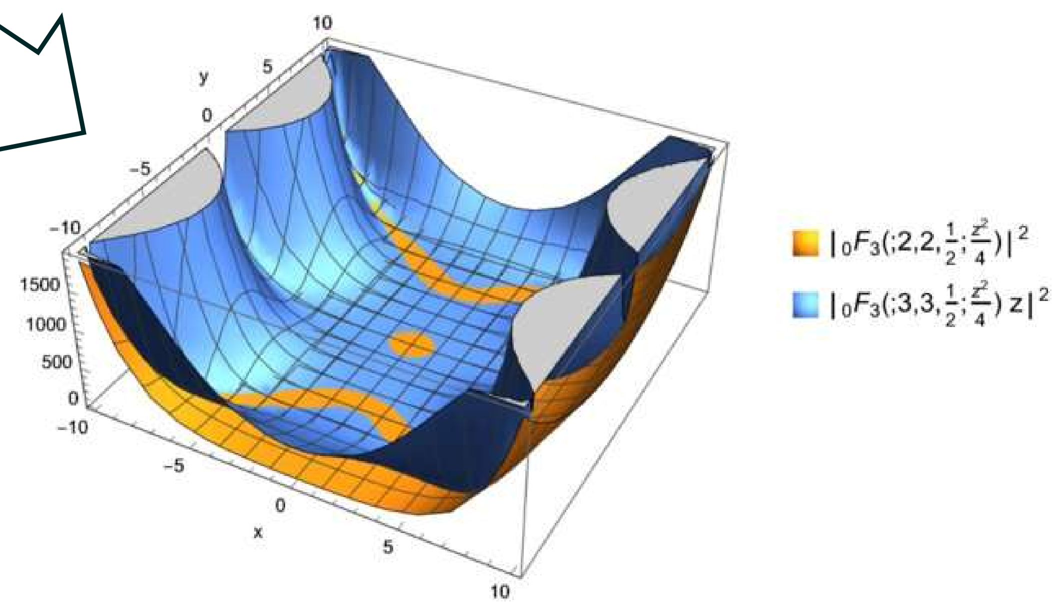
$Y = a\,x + b$



https://www.researchgate.net/publication/364521547_3D_Quantum_Gravity_from_Holomorphic_Blocks/

Astronomy

1. Correlative Observations (Egyptians, Celts, Chinese, Indians)

Nature of Observations: Ancients made astute observations of the stars, planets, and celestial events. Their primary motivation was practical, such as calendar development for agriculture and religious ceremonies.

Impact: These observations laid the groundwork for systematic astronomical study. However, they were largely correlative, noting patterns and cycles without a theoretical framework to explain them.

https://ras.ac.uk/events-and-meetings/friends-ras/friends-ras-only-lecture-astronomy-ancient-egypt

https://www.pexels.com/photo/stonehenge-england-1448136/

Astronomy

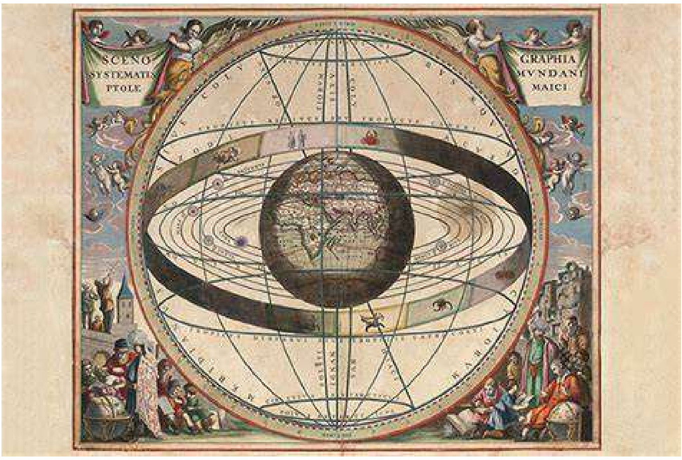
2. Geocentric Models (Ptolemy)

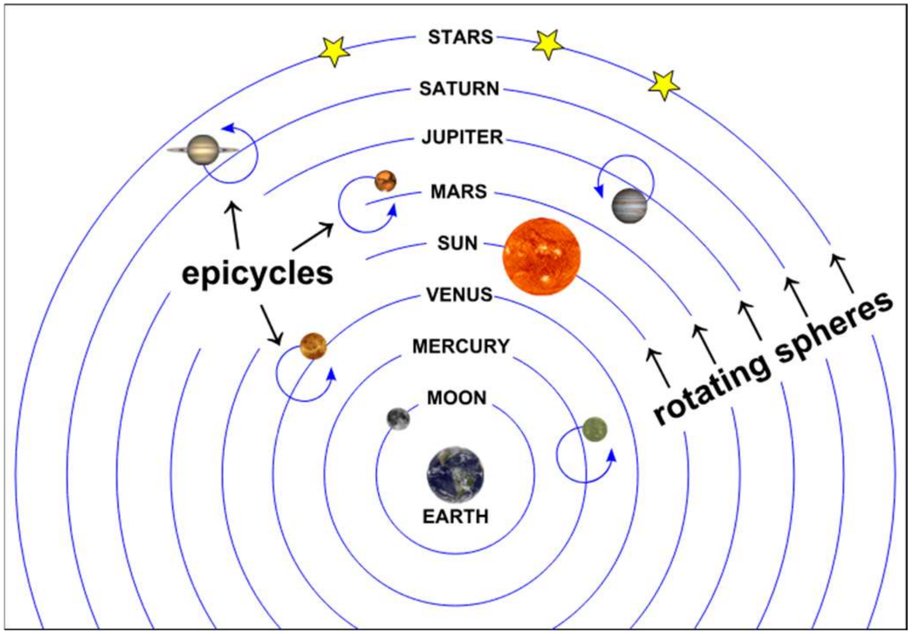
Development of Models: Claudius Ptolemy, among others, developed the geocentric model, placing Earth at the universe's center. This was an attempt to not just correlate but also explain the movements of celestial bodies.

Significance: This model, despite its inaccuracies, represented a shift towards trying to understand why celestial bodies moved as they did, not just how.

https://en.24smi.org/celebrity/104407-ptolemy.html

http://www.faithfulscience.com/science-and-faith/brief-history-of-faithful-science.html



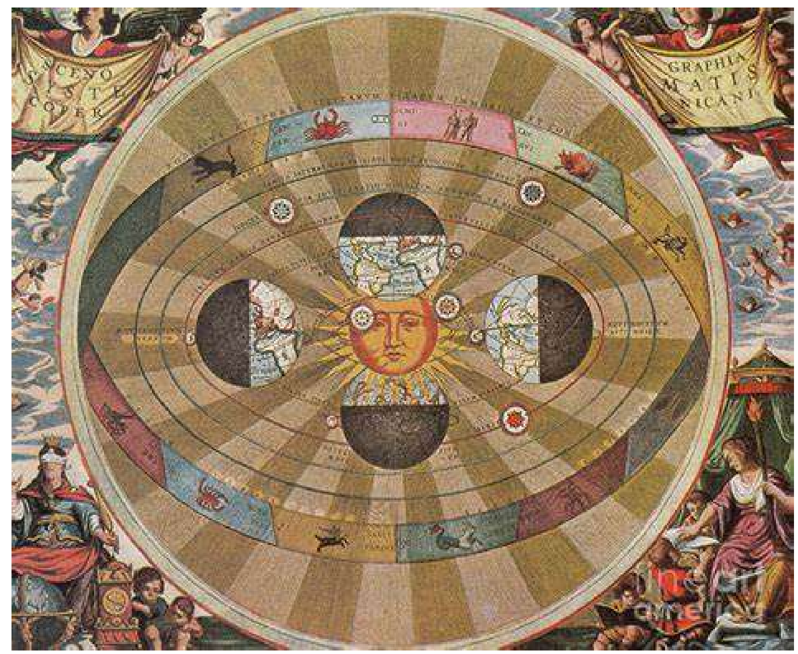


Astronomy

3. Heliocentric Shift (Copernicus)

Revision of Models: Nicolaus Copernicus proposed a heliocentric model, placing the Sun at the center of the universe. This challenged the long-standing geocentric view.

Consequence: This shift was crucial as it reoriented the perspective of the universe and laid the foundation for a more accurate understanding of celestial mechanics.



https://www.pinterest.com/pin/744923594607711152/

https://fineartamerica.com/featured/copernican-world-system-17th-century-science-source.html

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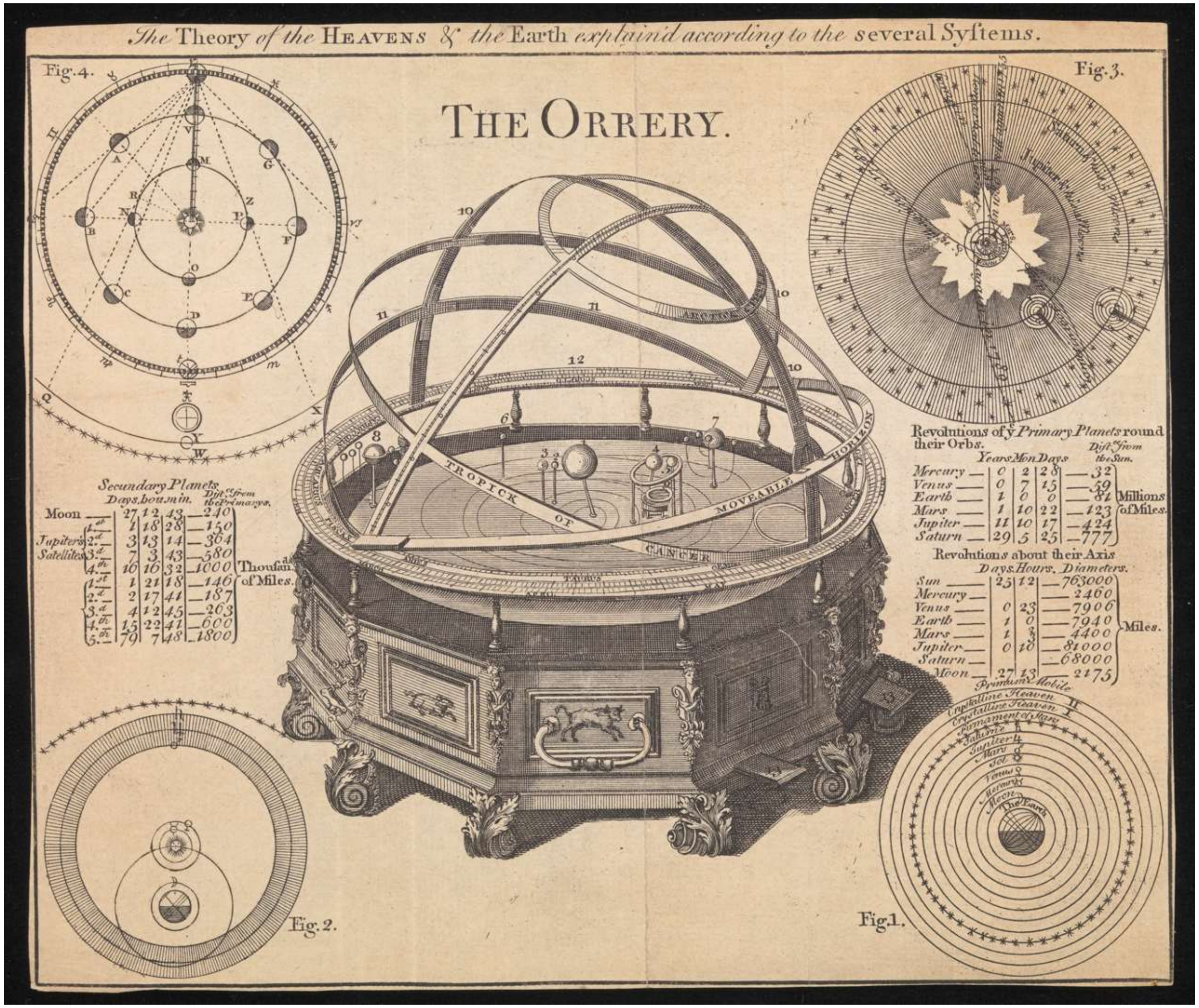

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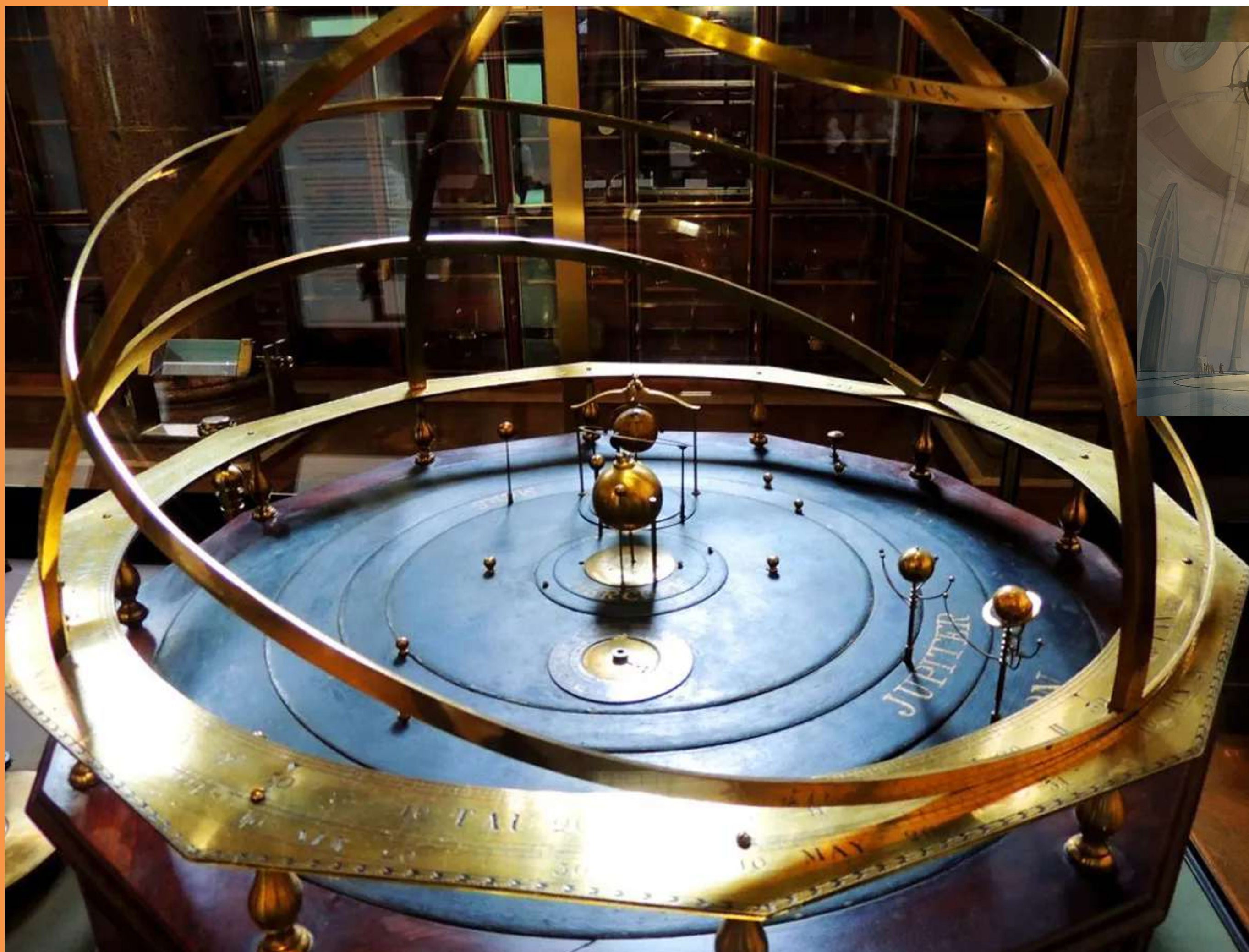
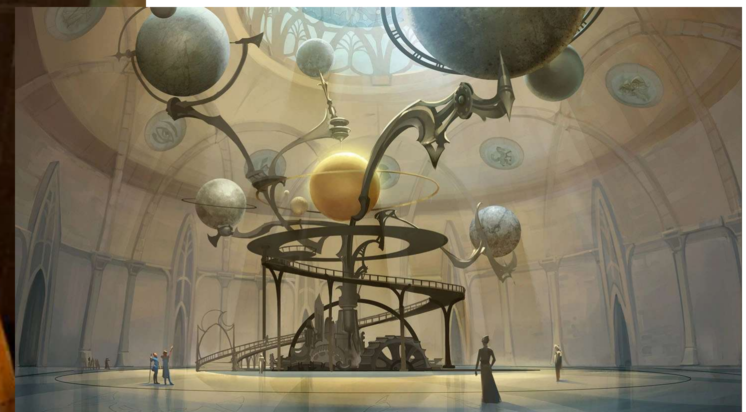




Astronomy

4. Empirical Observations (Tycho Brahe, Galileo)

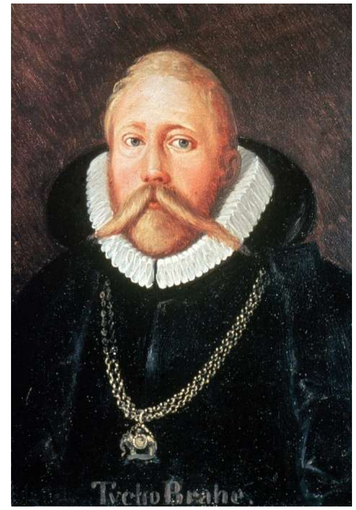
Enhanced Observations: Tycho Brahe's precise measurements of planetary positions and Galileo's telescopic observations provided empirical data that questioned existing models.

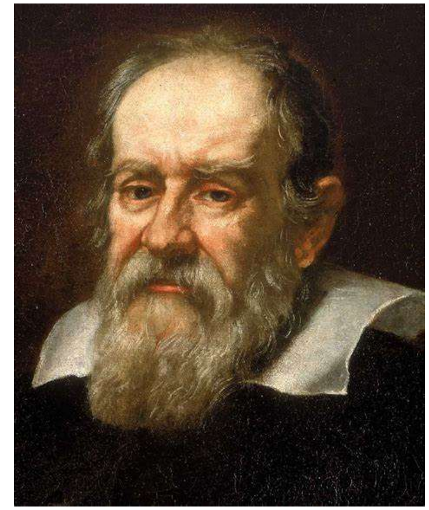
Role in Scientific Method: These observations underscored the importance of empirical evidence in validating or refuting scientific models.

https://www.britannica.com/biography/Tycho-Brahe-Danish-astronomer

https://it.wikipedia.org/wiki/Galileo_Galilei

https://www.messagetoeagle.com/galilei-galileo-demonstrates-his-first-telescope-august-25-1609/





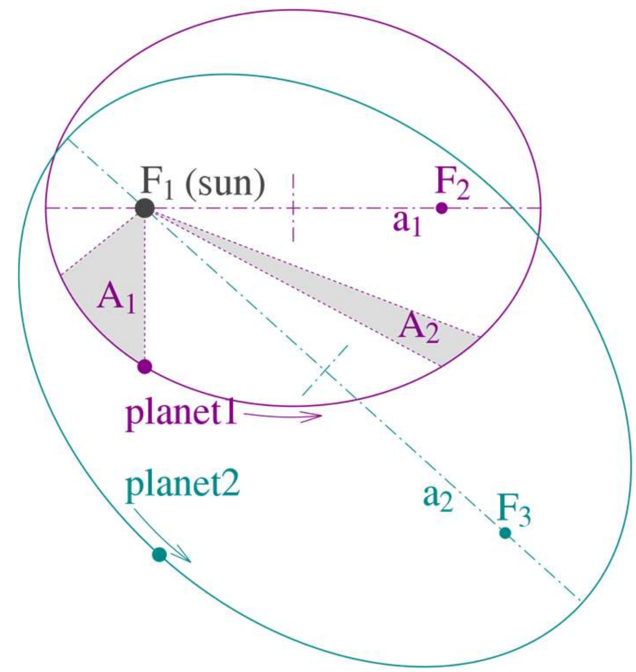
Astronomy

5. Laws of Planetary Motion
(Kepler)

From Data to Laws: Johannes Kepler used Brahe's data to develop three laws of planetary motion, mathematically describing the orbits of planets around the Sun.

Transition to Laws: Kepler's laws were significant as they represented a move from descriptive models to predictive and mathematical laws.

https://en.wikipedia.org/wiki/Kepler's_laws_of_planetary_motion



1. The orbit of a planet is an ellipse with the Sun at one of the two foci.
2. A line segment joining a planet and the Sun sweeps out equal areas during equal intervals of time.
3. The square of a planet's orbital period is proportional to the cube of the length of the semi-major axis of its orbit.

Astronomy

6. Synthesis and Universal Laws
(Newton)

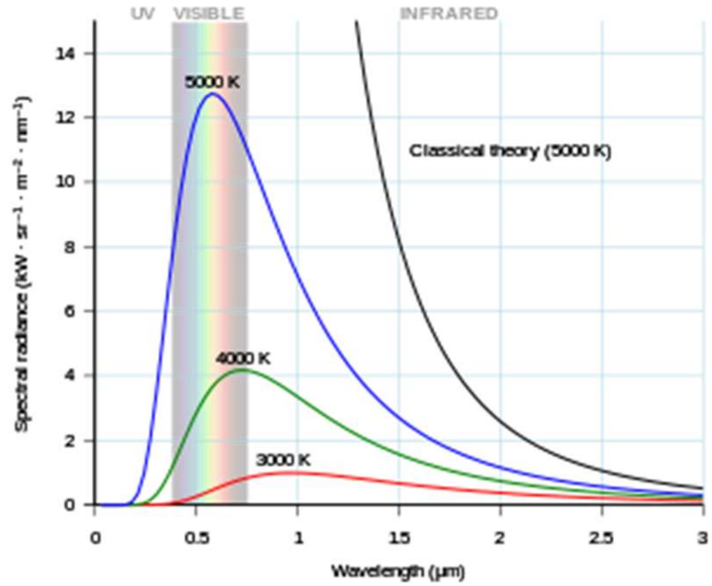
Universal Gravitation: Isaac Newton synthesized previous findings and introduced the law of universal gravitation, explaining the force that governs celestial motion.

Formulation of Mechanics: Newton's laws of motion established the foundational principles of classical mechanics, explaining not just celestial but also terrestrial motion.

$$F = d(mv)/dt$$

1. A body remains at rest, or in motion at a constant speed in a straight line, unless acted upon by a force.
2. The net force on a body is equal to the body's acceleration multiplied by its mass or, equivalently, the rate at which the body's momentum changes with time.
3. If two bodies exert forces on each other, these forces have the same magnitude but opposite directions.

Quantum physics



1. Planck's Quantum Hypothesis (1900)
Problem: The Ultraviolet Catastrophe in blackbody radiation, where classical physics predicted infinite energy at short wavelengths
Accomplishment: Introduced quantization of energy, solving the Ultraviolet Catastrophe by allowing only discrete energy levels.

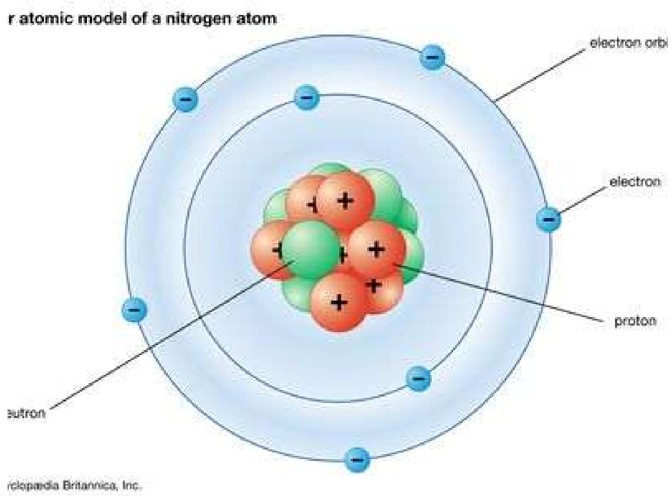
2. Planck's Radiation Law (1901)
Problem: Inaccuracies in the classical prediction of electromagnetic radiation emitted by black bodies.
Creation: The Planck Law accurately described the intensity and distribution of blackbody radiation across different wavelengths.

3. The Photoelectric Effect (Einstein) (1905)
Problem : Classical physics couldn't explain why light of certain frequencies could eject electrons from materials.
Discovery: Demonstrated that light is made of quanta (photons), explaining the frequency threshold for the photoelectric effect.

Quantum physics

4. Bohr's Model of the Atom (1913)
•**Problem**: Classical models failed to explain atomic stability and discrete spectral lines.
•**Model Development**: Bohr's quantized orbits explained why atoms are stable and why their emission spectra are discrete.

https://www.britannica.com/science/Bohr-model

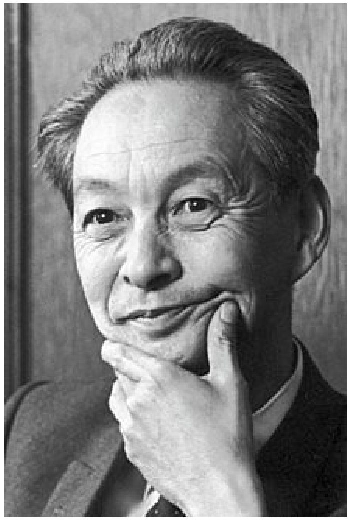


5. De Broglie's Wave-Particle Duality (1924)
•**Problem**: The classical particle theory of matter was insufficient to explain phenomena at atomic and subatomic levels.
•**Hypothesis**: Proposed wave-particle duality, suggesting that particles like electrons exhibit both wave and particle characteristics.

6. Schrödinger's Wave Mechanics (1926)
•**Problem**: Needed a comprehensive mathematical framework to describe quantum phenomena.
•**Development**: Schrödinger's equation provided a way to calculate the wave function of quantum systems, describing their behavior over time.

Quantum physics

7. Uncertainty Principle (Heisenberg) (1927)
Problem: The classical assumption of precise measurability of physical properties.
Principle Formulation: Introduced the uncertainty principle, establishing a fundamental limit to the precision of certain pairs of physical properties.



8. The Copenhagen Interpretation (Late 1920s)
Problem: The need for a coherent interpretation of the probabilistic nature of quantum mechanics.
Interpretation: Provided a framework for understanding quantum mechanics, focusing on probabilistic measurements and observer effects.

9. Quantum Field Theory Development (1940s-1950s)
Problem: Unifying quantum mechanics with the theory of relativity.
Theory Formation: Quantum field theory reconciled quantum mechanics with special relativity, crucial for understanding particle physics and forces.

Tomonaga, Feynman, Schwinger, source: Wikipedia

General relativity

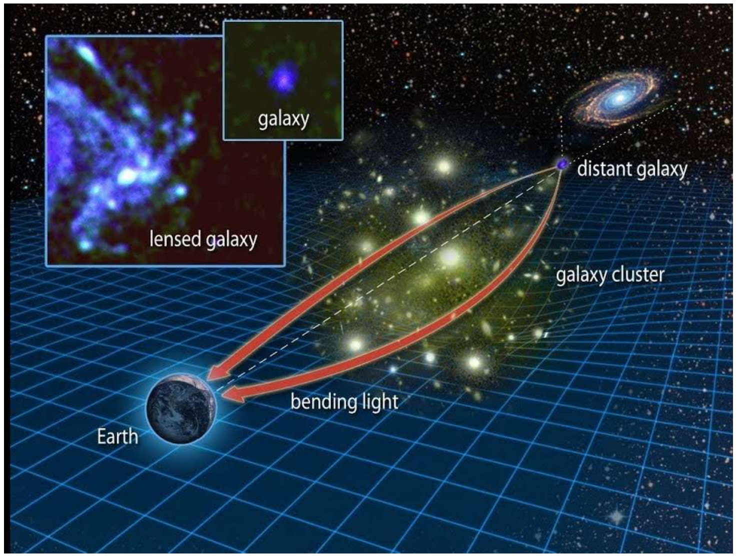
1. Classical Mechanics and Newtonian Gravity
Problem: By the late 19th century, Newton's laws and his law of universal gravitation were cornerstones of physics but couldn't explain certain observations, like the precession of Mercury's orbit.
Accomplishment: Provided a comprehensive framework for motion and gravity, but limitations suggested the need for a new theory.

2. Equivalence Principle (Einstein, 1907)
Key Idea: Einstein's thought experiment leading to the equivalence principle, suggesting that gravitational and inertial mass are equivalent.
Problem Solved: This principle challenged the Newtonian concept of gravity and set the stage for a new understanding of gravitation.

3. Special Theory of Relativity (Einstein, 1905)
Accomplishment: Overhauled the concepts of space and time, establishing that the laws of physics are the same for all non-accelerating observers and that the speed of light is constant.
Problem Solved: Addressed inconsistencies in electromagnetism and classical mechanics, laying the groundwork for General Relativity.

General relativity

4. General Relativity (Einstein, 1915)
Accomplishment: Einstein formulated General Relativity, describing gravity not as a force but as a curvature of spacetime caused by mass and energy.
Problem Solved: Explained the previously unresolved perihelion precession of Mercury's orbit and predicted phenomena like the bending of light by gravity.



https://www.syfy.com/syfy-wire/einstein-was-right-again-astronomers-watch-stars-gravity-bends-light-another-star

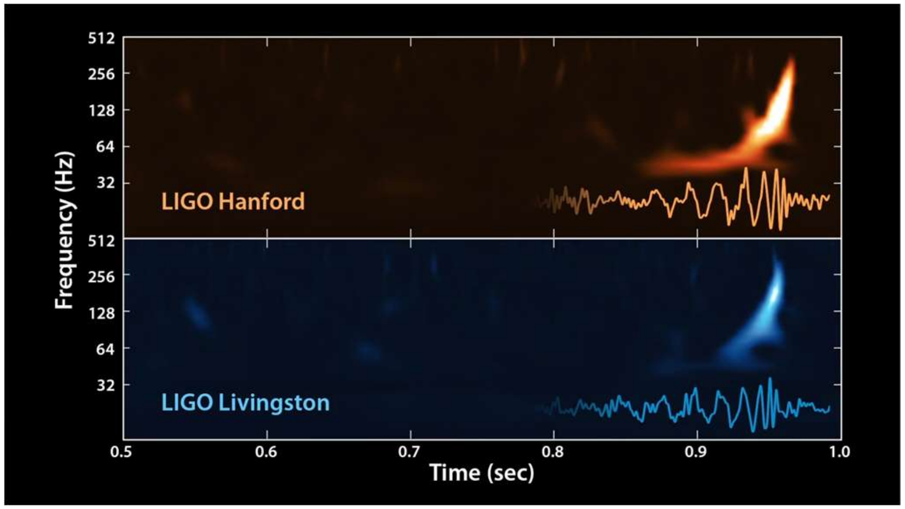
5. Experimental Confirmation: Light Bending (1919)
Event: The 1919 solar eclipse expedition led by Arthur Eddington.
Accomplishment: Confirmed Einstein's prediction that light bends in a gravitational field, providing strong evidence for General Relativity.

6. Expansion of the Universe (1920s-1930s)
Accomplishment: General Relativity led to the realization that the universe is expanding, as shown by Edwin Hubble's observations.
Problem Solved: Resolved discrepancies in cosmological observations, paving the way for modern cosmology.

General relativity

7. Black Holes and Singularities (1960s)
Theory Development: Theoretical work led to the prediction of black holes, objects with such strong gravity that not even light can escape.
Problem Solved: Explained extreme gravitational phenomena and laid the groundwork for studying objects like black holes and neutron stars.

8. Gravitational Waves Detection (2015)
Event: The first detection of gravitational waves by LIGO.
Accomplishment: Confirmed a major prediction of General Relativity, opening a new window into observing cosmic events.



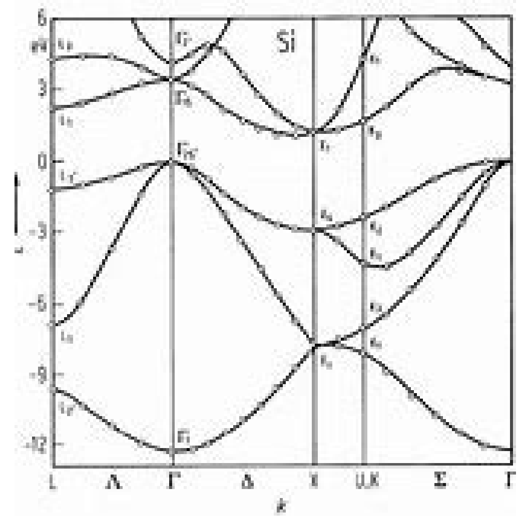
https://www.space.com/31894-gravitational-waves-ligo-search-complete-coverage.html

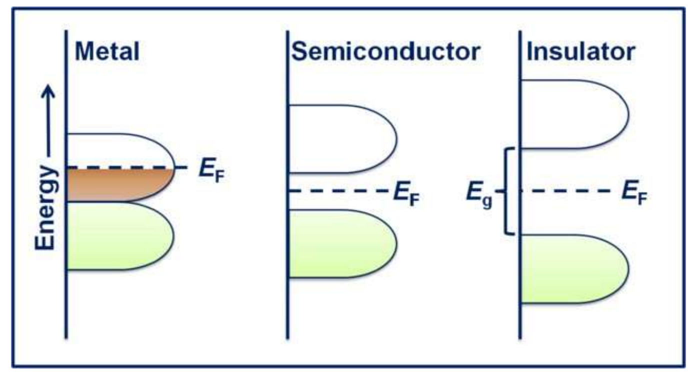
https://phys.org/news/2017-09-ligo-virgo-observatories-black-hole.html

Physics of semiconductors

1. Discovery of Semiconductors (Early 19th Century)
Problem: Early experiments showed that some materials had electrical conductivity between that of metals and insulators.
Accomplishment: Identification and classification of semiconductors.
Mathematical Formulation: Initial studies were more qualitative, focusing on the observation of conductivity behavior under different conditions.

2. Quantum Theory of Solids (Early 20th Century)
Problem: Classical physics couldn't explain the unique electrical properties of semiconductors.
Accomplishment: Application of quantum mechanics to the theory of solids, leading to a deeper understanding of band structures in materials.
Mathematical Formulation: Introduction of the band theory; energy bands are described by the electronic band structure $E(k)$, where E is energy and k is the wave vector.



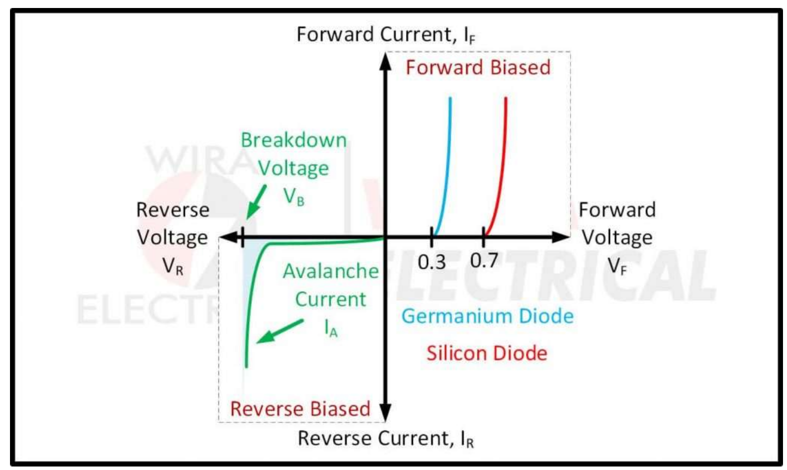


(14) (PDF) Metal-Insulator Transitions and non-Fermi Liquid Behaviors in 5d Perovskite Iridates (researchgate.net)

Physics of semiconductors

3. Semiconductor Diodes and Rectification (1930s)
Problem: Need for devices that allow current to flow in one direction.
Accomplishment: Development of semiconductor diodes, exploiting p-n junctions for rectification.
Mathematical Formulation: Shockley equation for the p-n junction: $I=I0(eqV/kT-1)$, where I is current, V is voltage, and $I0$ is reverse saturation current.

4. Transistor Effect and Invention (1947)
Problem: Requirement for better amplification and switching in electronics.
Accomplishment: Invention of the transistor by Bardeen, Brattain, and Shockley.
Mathematical Formulation: Transistor $I-V$ characteristics, described by similar equations to diodes but with additional terms for base current and amplification.



https://www.thoughtco.com/biography-of-william-shockley-4843200

Physics of semiconductors

5. Semiconductor Theory Development (1950s)
Problem: Need for comprehensive theory to design and optimize semiconductor devices.
Accomplishment: Development of detailed semiconductor theory, including doping, carrier concentration, and recombination.
Mathematical Formulation: Drift and diffusion equations, $J=q\mu nE+qD\nabla n$, where J is current density, n is carrier concentration, E is electric field, μ is mobility, and D is diffusivity.

6. Integrated Circuits and Microelectronics Revolution (1958)
Problem: Miniaturization and integration of electronic components were needed.
Accomplishment: Invention of the integrated circuit, leading to the microelectronics revolution.
Mathematical Formulation: Focus on fabrication processes and circuit design rather than new semiconductor physics.

7. Quantum Wells and Semiconductor Heterostructures (1970s)
Problem: Expanding the functionality and efficiency of semiconductor devices.
Accomplishment: Development of quantum wells and heterostructures, enhancing carrier mobility and confining carriers in two-dimensional layers.
Mathematical Formulation: Quantum well energy levels, $E_n=2m^*L^2\hbar^2\pi^2n^2$, where n is the quantum number, m^* is the effective mass, and L is the well width.

We have beautiful mathematical formulae describing physical phenomena, and sometimes can express solutions in simple form.

If not, we can use numerical methods to derive solutions and approximations.

Name	Law	Early Citation
Hubble's law	$v = H_0 D$	[79]
Kepler's Third Law	$P^2 \propto a^3$	[81]
Newton's law of universal gravitation	$\mathbf{F} = G\frac{m_1 m_2}{r^2}\hat{r}$	[82]
Planck's law	$B = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_B T}-1}$	[83]
Leavitt's Law	$M = \alpha \log_{10}(P) + \delta$	[84]
Schechter function	$n = \frac{\phi_*}{L_*}(\frac{L}{L_*})^\alpha e^{-\frac{L}{L_*}}$	[85]
Bode's law	$a = 0.4 + 0.3(2^n)$	[86]
Ideal gas law	$P = \frac{nRT}{V}$	[87]
Rydberg formula	$\frac{1}{\lambda} = R_H(\frac{1}{n_1^2} - \frac{1}{n_2^2})$	[88]

Table 2: Expressions in the EmpiricalBench and associated with the datasets in fig. 5. Each of these expressions was originally empirically discovered.

https://arxiv.org/pdf/2305.01582.pdf

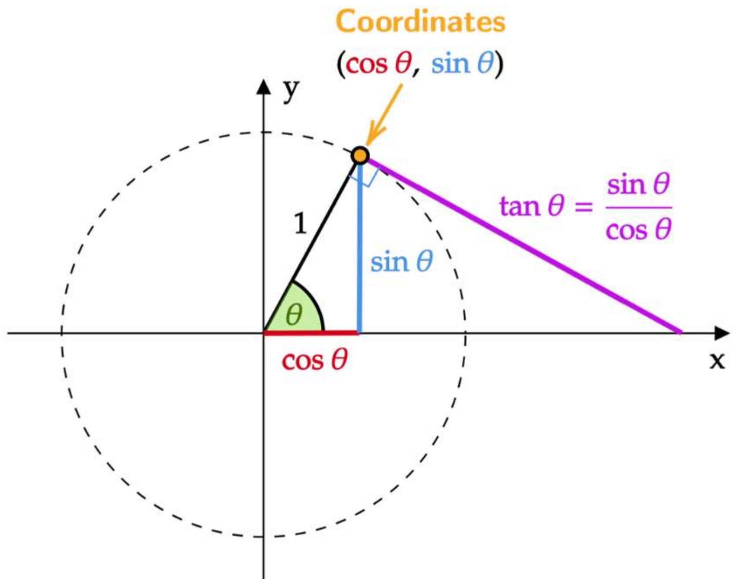
Where do mathematical functions come from?

Ancient to Early Medieval Period

•**Babylonians and Egyptians (2000 BCE - 300 BCE)**: Early uses of basic exponentiation and the beginnings of geometry.

•**Greek Mathematics (7th Century BCE - 5th Century CE)**: Development of geometric concepts, early foundations of trigonometry by Hipparchus.

•**Indian Mathematics (5th Century CE)**: Introduction of the sine function by Aryabhata.



https://matterofmath.com/trigonometry/unit-circle/

Medieval Period

•**Islamic Golden Age (8th - 14th Century)**: Expansion of trigonometry by Al-Khwarizmi and Al-Battani. Introduction of zero and negative numbers, influencing the concept of powers.

Renaissance to Early Modern Period

•**John Napier (1614)**: Invention of logarithms, leading to the development of logarithmic and exponential functions.

•**17th Century**: Formalization of trigonometric functions (sine, cosine) and further development of power functions as part of the rise of calculus by Newton and Leibniz.

Where do mathematical functions come from?

18th Century
•**Leonhard Euler (1707 - 1783)**: Significant contributions including formalizing the exponential function e(x), introducing the concept of the gamma function, and expanding the scope of trigonometric functions to complex numbers.
•**Bernoulli Family**: Development of Bernoulli polynomials.

19th Century
•**Gauss and Legendre**: Development of error functions, Legendre polynomials, and contributions to the theory of special functions.
•**Complex Analysis**: Mathematicians like Augustin-Louis Cauchy and Bernhard Riemann formalized complex analysis, further expanding the understanding and use of trigonometric and exponential functions.

Early 20th Century
•**Special Functions in Physics**: With the advent of quantum mechanics, special functions like Bessel functions, Hermite polynomials, and spherical harmonics became integral in solving complex physical problems.

One function family, many origins

Ancient Astronomy and Navigation: Trigonometry, the study of relationships between angles and lengths in triangles, originated from practical needs in astronomy, navigation, and surveying. The Babylonians and Greeks, especially Hipparchus and Ptolemy, made significant contributions to early trigonometry.

Circular Functions: The trigonometric functions we are familiar with today (sine, cosine, tangent, etc.) evolved from the study of circles. The unit circle (a circle with radius 1) is central to understanding these functions. For example, in the unit circle, the sine and cosine of an angle correspond to the coordinates of a point on the circle.

From Lines and Circles to Functions: The transition from geometric lines and circles to functions occurred through the work of mathematicians in the Hellenistic world, Islamic Golden Age, and Renaissance Europe. They created tables of values that were effectively early versions of sine and cosine functions.

Analytic Trigonometry: With the development of calculus, trigonometric functions were described analytically, leading to their modern form. They became defined not just for angles in triangles but for all real numbers, and their properties were studied as functions.

One function family, many origins

Symmetry and Periodicity: Trigonometric functions are inherently linked to symmetry and periodicity, two concepts important in group theory. For instance, the periodic nature of these functions (e.g., sine and cosine repeating every 2π radians) is a manifestation of rotational symmetry.

Groups in Mathematics: In group theory, certain groups called “rotation groups” describe rotations in space. The sine and cosine functions are related to these groups because they describe the coordinates of points after rotation. For example, in 2D space, the rotation group SO(2) can be related to the circular functions.

Euler's Formula: Euler’s formula, $e^{ix}=\cos(x)+i\sin(x)$, where i is the imaginary unit, connects trigonometric functions with exponential functions in the complex plane. This formula is fundamental in complex analysis and has far-reaching implications in various fields of mathematics and physics.

- **Wave Phenomena**: In physics, trigonometric functions describe wave phenomena, including sound and light waves.
- **Fourier Analysis**: Trigonometric functions are essential in Fourier analysis, which decomposes general functions into sums of simpler trigonometric functions. This is crucial in signal processing, quantum mechanics, and heat transfer.

Bessel functions

Bessel's Differential Equation: Bessel functions arise as solutions to Bessel's differential equation: $x^2\, dx^2/d^2y + x\, dx/dy + (x2 - n2)y = 0$, where n is a real or complex number, known as the order of the Bessel function.

Friedrich Bessel (1784-1846): Bessel initially studied these functions in the context of astronomical problems related to Kepler's problem of planetary motion.

Connection to Circular and Cylindrical Problems

•**Circular and Cylindrical Symmetry**: Bessel functions are particularly significant in problems with circular or cylindrical symmetry. This includes heat conduction in cylindrical objects, vibrations of circular membranes, and electromagnetic waves in cylindrical structures.

•**Orthogonality**: Bessel functions of different orders are orthogonal to each other, a property useful in solving boundary value problems.

Why do scientists invent special functions?

They have distinctive properties and structures that make them particularly useful in various areas of physics and engineering. Some special functions are derived from physical problems:

1. Legendre Polynomials

•**Origin**: Arise from solving the Legendre differential equation, which itself emerges in the process of solving Laplace's equation in spherical coordinates.
•**Physical Problem**: In physics, they frequently appear in problems involving spherical symmetry, such as the gravitational potential outside a sphere or the electric field of a charge distribution with spherical symmetry.
•**Derivation**: Legendre polynomials $Pn(x)$ are derived when solving the Legendre differential equation, typically in the context of expanding a function over a sphere (spherical harmonics).

2. Bessel Functions

•**Origin**: Solutions to Bessel's differential equation.
•**Physical Problem**: Common in problems with cylindrical symmetry, like heat conduction in a cylinder, vibrations of circular membranes, or electromagnetic waves in cylindrical structures.
•**Derivation**: Derived when solving wave equations or heat equations in cylindrical coordinates.

Why do scientists invent special functions?

3. Hermite Polynomials
•**Origin**: Arise from the solution of the Hermite differential equation.
•**Physical Problem**: Prominent in quantum mechanics, especially in solving the Schrödinger equation for the quantum harmonic oscillator.
•**Derivation**: When the Schrödinger equation for a harmonic oscillator is solved, the solution involves the Hermite polynomials, which describe the wavefunctions of the oscillator's quantum states.

4. Laguerre Polynomials
•**Origin**: Solutions to the Laguerre differential equation.
•**Physical Problem**: Appear in quantum mechanics, particularly in the radial part of the wavefunction for a hydrogen atom.
•**Derivation**: When solving the radial part of the Schrödinger equation for the hydrogen atom, Laguerre polynomials emerge naturally in the solution.

Why do scientists invent special functions?

5. Hypergeometric Functions

•**Origin**: Solutions to the hypergeometric differential equation.

•**Physical Problem**: Occur in various contexts, including quantum field theory and statistical mechanics.

•**Derivation**: These functions appear when solving differential equations that cannot be solved using elementary functions, providing generalizations of simpler special functions.

- **Hypergeometric Differential Equation:**

  $x(1-x)\frac{d^2y}{dx^2} + [c-(a+b+1)x]\frac{dy}{dx} - aby = 0$

  Where a, b, and c are parameters.

- **Hypergeometric Function:** The standard solution to this equation is given by the hypergeometric series:

  ${}_2F_1(a,b;c;x) = 1 + \frac{ab}{c\cdot 1}x + \frac{a(a+1)b(b+1)}{c(c+1)\cdot 1\cdot 2}x^2 + \cdots$

Properties

- **Convergence:** For $|x| < 1$, the hypergeometric series converges absolutely. At $x = 1$, it converges if $\Re(c-a-b) > 0$.
- **Special Cases:** Many common functions are special cases of the hypergeometric function. For example, when $a = b = 1$ and $c = 2$, ${}_2F_1(1,1;2;x)$ reduces to $-\ln(1-x)/x$.

Special functions are not arbitrary constructs; they naturally arise from the process of solving differential equations encountered in physical problems. Their utility in describing complex physical systems and phenomena highlights the intertwined nature of mathematics and physics. Each of these functions encapsulates a wealth of information about the behavior of systems under study and serves as a powerful tool in theoretical and applied physics.

What are other sources of special functions?

1. Series Solutions and Summations
Power Series: Functions defined by power series that cannot be expressed in terms of elementary functions often become special functions.
Infinite Series and Products: Some special functions arise as the sum or product of an infinite series. The Riemann zeta function, defined by an infinite series, is a notable example.

2. Integral Transforms
Fourier and Laplace Transforms: These transforms are crucial in solving differential equations and are used in signal processing and physics. The resulting functions, like the Fourier transform of simple functions, can be considered special functions in their own right.
Mellin and Hilbert Transforms: Integral transforms can lead to functions that are essential in various applications, particularly in complex analysis and number theory.

3. Combinatorics and Number Theory
Generating Functions: In combinatorics, generating functions encapsulate sequences of numbers (like binomial coefficients) and can be considered special functions.
Elliptic Functions: Arising in number theory and algebraic geometry, these functions are linked to elliptic curves and have numerous applications in cryptography and complex analysis.

What are other sources of special functions?

4. Orthogonal Polynomials
Sturm-Liouville Theory: This theory in differential equations leads to orthogonal polynomials like Legendre, Laguerre, and Hermite polynomials, which are vital in mathematical physics, particularly in solving partial differential equations.

5. Optimization and Variational Problems
Calculus of Variations: Solutions to variational problems often lead to functions that describe optimal states or configurations, such as the brachistochrone curve in mechanics.

6. Geometric and Topological Considerations
Spherical Harmonics: These arise in solving Laplace's equation in spherical coordinates and are used in quantum mechanics, geophysics, and computer graphics.
Elliptic Integrals: Originating in the calculation of arc lengths of ellipses and hyperellipses, these integrals cannot be expressed in terms of elementary functions.

7. Statistical Distributions and Stochastic Processes
Probability Distributions: Gaussian (normal distribution) and Gamma distribution are crucial in statistics and probability theory.
Green's Functions: In stochastic processes and quantum field theory, Green's functions, which describe the evolution of physical systems, are considered special functions.

To summarize:

1. Solving Differential Equations
2. Modeling Physical Phenomena
3. Summarizing Complex Relationships
4. Generalizing Existing Functions
5. Orthogonality and Completeness in Function Spaces
6. Convenience in Mathematical and Numerical Analysis
7. Addressing Abstract Mathematical Concepts
8. Statistical Applications

The justification for introducing a special function typically hinges on its utility in simplifying complex problems, generalizing existing mathematical constructs, providing deeper insights into physical phenomena, or encapsulating intricate relationships in a tractable form. These functions often become indispensable tools in both applied and theoretical domains.

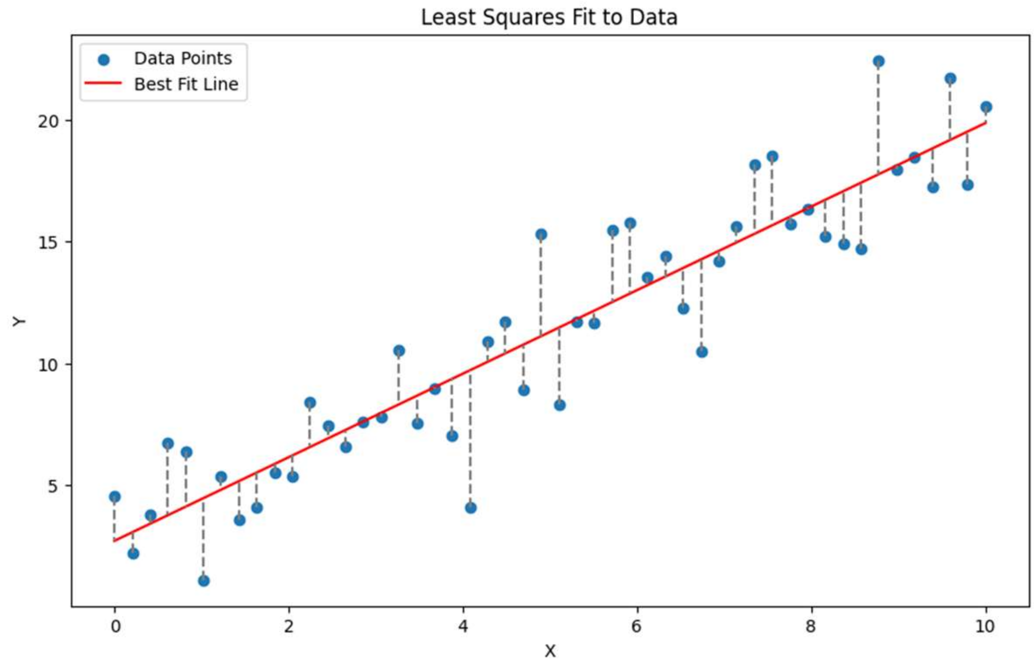
Now, imagine we have language in which we can express physical laws.
Several immediate questions become:

1. How do we know that this language is complete?
2. Is it always sufficient?
3. Can we go from data to equations?

Let's start linear!

Least Squares Fitting: a method to determine the best-fitting line through a set of points.

Objective: Minimize the sum of the squares of the differences (residuals) between observed and predicted values.

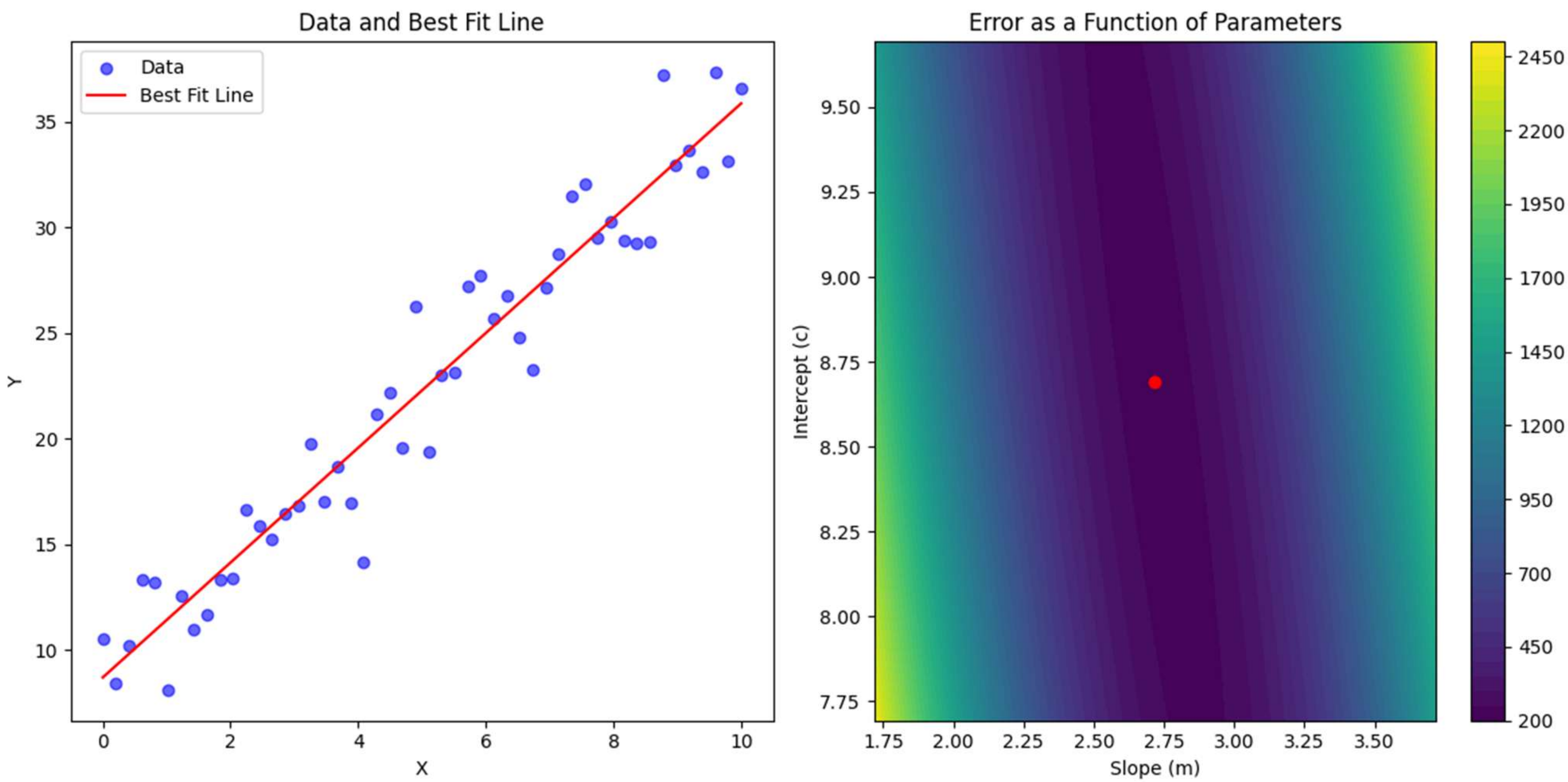


• Developed by Carl Friedrich Gauss and Adrien-Marie Legendre

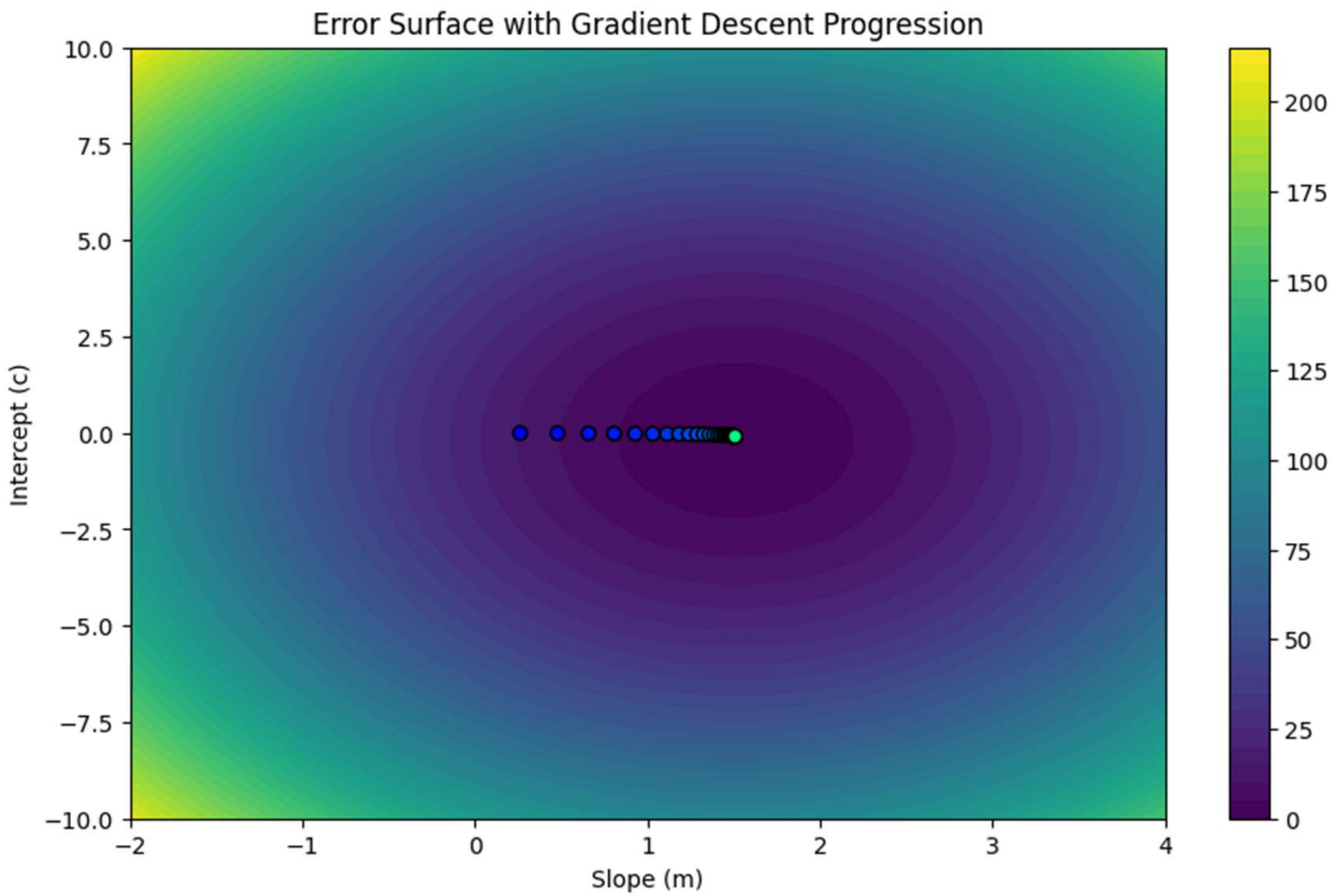
• Initially used for astronomical data to predict planetary movements.

- We have data, meaning collection of points (x_i, y_i)
- We choose function, here $y = a + b\,x$
- We calculate total error, $L(a,b) = \sum((y_i - (a + b\,x_i))^2)$
- We find parameters a, b for which L(a,b) is minimal

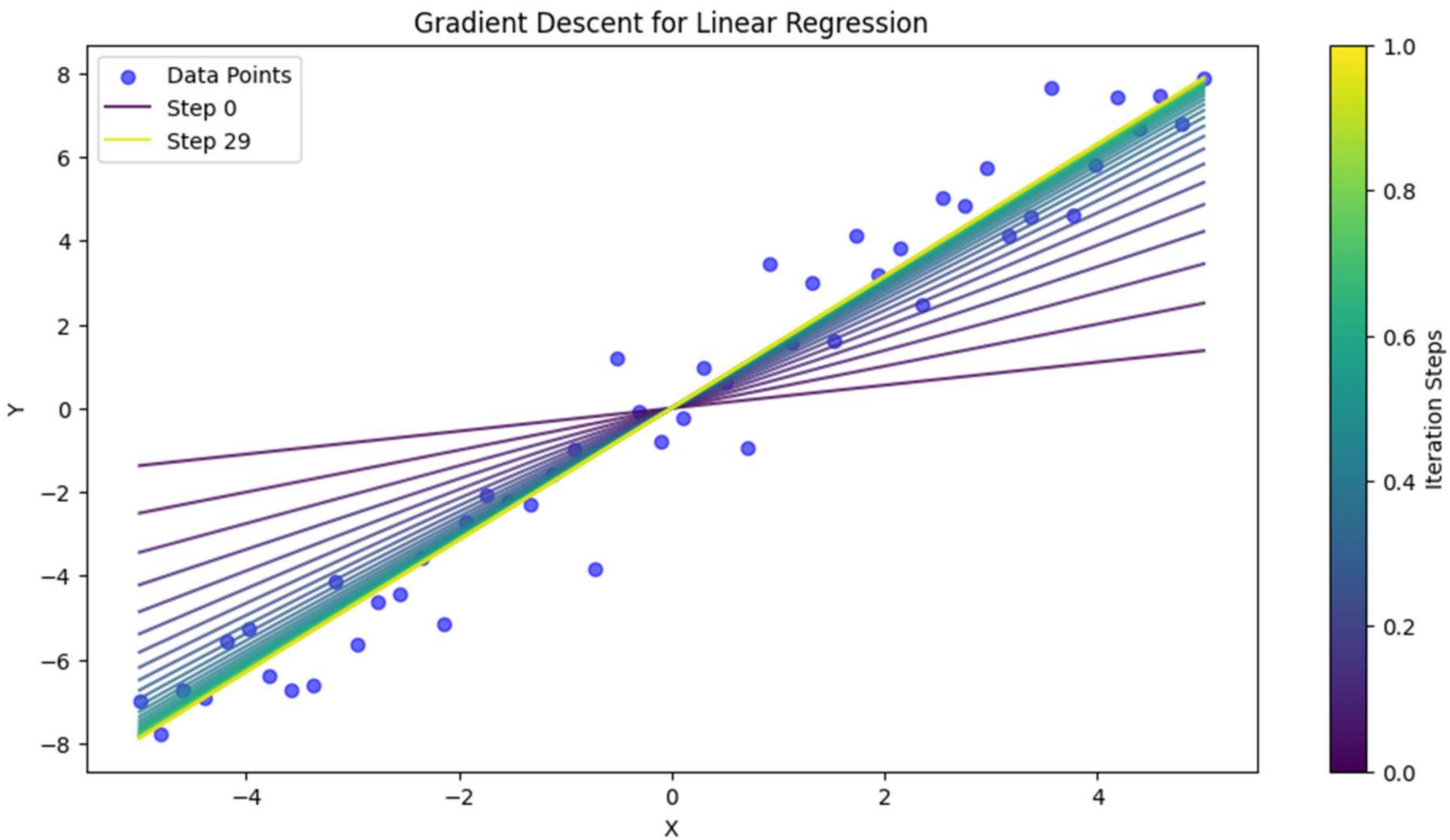
Let’s start linear!



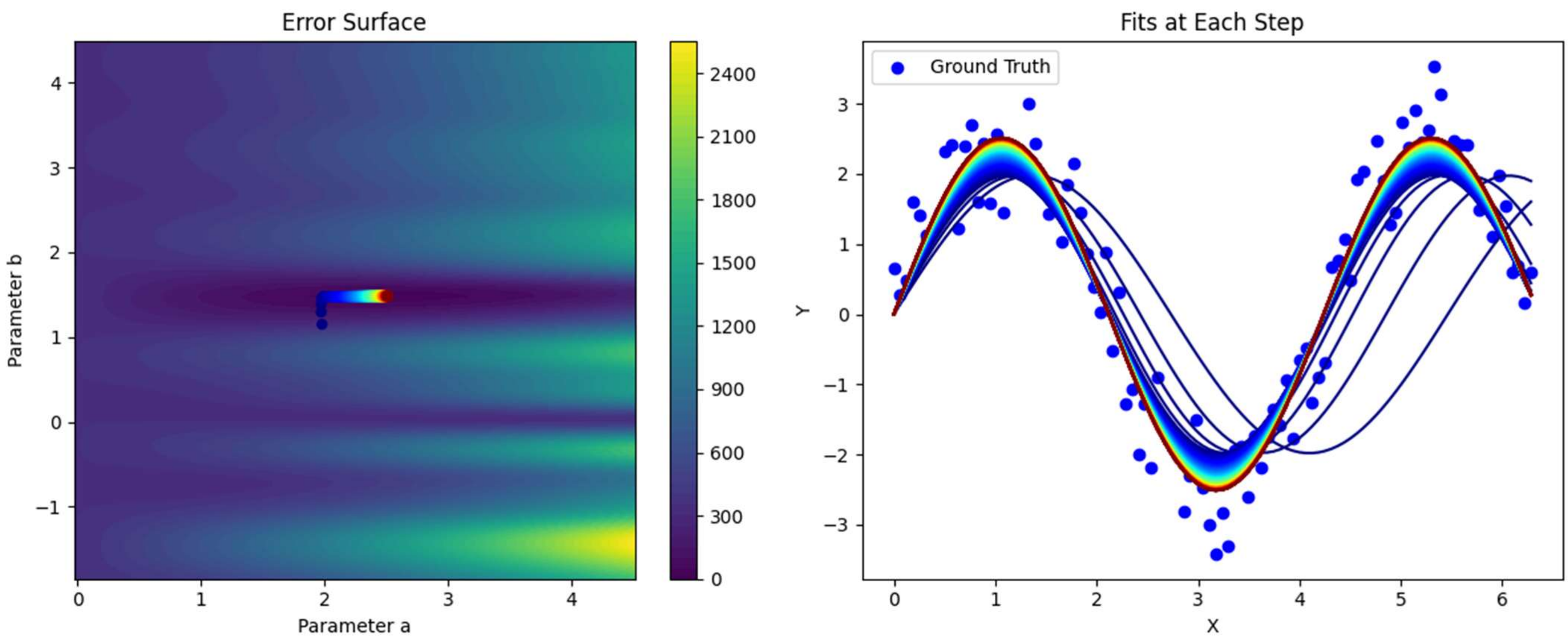
Finding minimum with gradient descent



Finding minimum with gradient descent



The sine that works



The sine that doesn't