Implementation of an alcohol tolerance prediction model using differential equations and Laplace transforms

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May 25, 2025

1 Introduction

1.1 Background: Blood Alcohol Level Model

We separate the alcohol concentration in the stomach $A(t)$ and the blood alcohol concentration $B(t)$ into two compartments, and assume a first-order kinetic model as follows.[1].

$$\begin{cases} \dfrac{dA}{dt} = -k_1 A(t), & A(0) = A_0, \\ \dfrac{dB}{dt} = k_1 A(t) - k_2 B(t), & B(0) = 0, \end{cases}$$

k_1 : Absorption rate of transfer from the stomach to the bloodstream
k_2 : Elimination rate from the bloodstream,
A_0 : Initial total amount of alcohol in the stomach

The solution of this system is given in a closed form as follows.[1]:

$$A(t) = A_0 e^{-k_1 t}, \qquad B(t) = \frac{k_1 A_0}{k_2 - k_1}\big(e^{-k_1 t} - e^{-k_2 t}\big).$$

1.2 Motivation: Blood Alcohol Level Model

Alcohol plays a significant role in modern society. It is a common element in social gatherings, meetings, and parties, often serving as a catalyst for interaction. However, alcohol consumption can cause various adverse effects such as headaches, confusion, fatigue, dizziness, drowsiness, sluggishness, lethargy, and loss of appetite. These symptoms frequently lead to accidents and dangerous situations.

From 2019 to 2023, an average of 42 drunk driving incidents occurred daily in South Korea. Over this five-year period, a total of 75,950 alcohol-related traffic accidents were reported, causing 1,161 fatalities and 122,566 injuries. These incidents most frequently occurred between 10:00 PM and midnight on Thursday and Friday nights, which is the time when social gatherings typically happen.

To reduce such accidents, this study proposes the development of a formula to estimate an individual's alcohol tolerance. By identifying personal limits more accurately, it may be possible to prevent the risks associated with excessive drinking and promote safer behavior in social contexts.[2].

1.3 Objective: Blood Alcohol Level Model

Many adolescents enter adulthood and university life without a clear understanding of their alcohol tolerance, leading to various incidents and accidents. To address this issue, individuals typically determine their own drinking tolerance through trial and error. However, this study aims to develop an algorithm that can estimate a person's alcohol tolerance mathematically, without the need for actual alcohol consumption. By using variables such as age, gender, body weight, drinking duration, and alcohol by volume (ABV), the algorithm predicts whether a person's blood alcohol concentration (BAC) would exceed 0.08%, which is the legal limit for driver's license revocation in South Korea. This threshold will be used as the criterion for defining an individual's alcohol tolerance.

1.4 Problem Statement: Blood Alcohol Level Model

The conventional first-order kinetic model commonly used to predict changes in an individual's blood alcohol concentration (BAC) assumes constant values for alcohol absorption rate (k1) and elimination rate (k2). However, this assumption poses significant limitations. In reality, the processes of alcohol absorption and elimination are not instantaneous reactions but are influenced by non-local memory effects, where past concentration changes affect the current rate of change. Traditional integer-order differential equation models fail to adequately capture these physiological memory phenomena. Also, alcohol elimination rates are not fixed constants; they vary nonlinearly depending on both the individual's physical condition and the current BAC level. Fixing the elimination rate as a constant makes it difficult to accurately model the body's actual physiological response. Therefore, there is a pressing need for a new modeling approach that integrates both the non-local memory effect and the dynamic variation in elimination rates. Such an approach would enable more precise and realistic predictions of an individual's alcohol tolerance.

2 Methodology

This section derives a BAC model using the Caputo fractional derivative operator and the Laplace transform. In particular, the ψ-Caputo fractional derivative is applied to effectively capture the non-local physiological memory effect observed during the processes of alcohol absorption and elimination.

By integrally accounting for how past concentration changes influence the current rate of change, the ψ-Caputo operator enables a more realistic representation of BAC dynamics than conventional integer-order models.

2.1 Data Preprocessing and Management

- Weight: m (kg)
- Total body water (TBW) distribution ratio: r (Male 0.68, Female 0.55)
- Alcohol volume consumed: V (mL)
- Alcohol by volume: ABV (%)
- Initial alcohol concentration in the stomach:

$$A(0) = A_0 = \frac{V \times (\text{ABV}/100) \times \rho_{\text{EtOH}}}{r\, m}, \quad \rho_{\text{EtOH}} = 0.789 \text{ g/mL}.$$

- Reference blood alcohol concentrations:

$$\text{BAC}_{\text{high}} = 0.08\%, \quad \text{BAC}_{\text{low}} = 0.01\%.$$

- ψ function: By default $\psi(t) = t$ (Standard Caputo), can be generalized

2.2 Theoretical Derivation of the Blood Alcohol Concentration Model

1. **Definition of the Caputo Fractional Derivative Operator**
   The Caputo fractional derivative ${}^{C}D^{\alpha}_{0+}$ of order alpha is defined as:

$$ {}^{C}D^{\alpha}_{0+} f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1}\, f^{(n)}(\tau)\, d\tau,$$

   where:

   - $n = \lceil \alpha \rceil$ (the smallest integer greater than or equal to α)
   - $\Gamma(\cdot)$is the gamma function: $\Gamma(z) = \int_0^{\infty} x^{z-1} e^{-x} dx$
   - $t$is time, $\tau$is the integration variable.

   The Caputo derivative is typically applied to initial-value problems and is advantageous because it naturally incorporates initial conditions expressed in terms of integer-order derivatives.

2. **Setting Up the Model Equations**
   $\psi(t) = t$ (Standard Caputo), compartment-compartment two models can be described by the following equations:

$$ {}^{C}D^{\alpha}_{0+} A(t) = -k_1\, A(t), \qquad A(0) = A_0, \tag{1}$$

$$ {}^{C}D^{\beta}_{0+} B(t) = k_1\, A(t) \; - \; k_2\, B(t), \qquad B(0) = 0. \tag{2}$$

   So,

   - $A(t)$: alcohol concentration in the stomach (or mass)

- $B(t)$: blood alcohol concentration (BAC)
- k_1: absorption rate constant, α fractional order of the derivative (typically $0 < \alpha \leq 1$)
- k_2: elimination rate constant, β fractional order of the derivative (typically $0 < \beta \leq 1$)

3. **Definition of the Laplace Transform**
   Laplace Transform $\mathcal{L}\{f(t)\}(s)$ is defined as:

$$\mathcal{L}\{f(t)\}(s) = \int_0^\infty e^{-st} f(t)\, dt$$

   This transform allows the fractional differential equations to be converted into algebraic equations for easier solution.

4. **Solving for Alcohol Concentration in the Stomach** $A(t)$
   Taking a Laplace transform of equation (1),

$$s^\alpha \big(\mathcal{L}\{A\}(s) - s^{-1} A_0\big) = -k_1\, \mathcal{L}\{A\}(s),$$

   Rearranging in terms of $\mathcal{L}\{A\}(s)$, we get:

$$\mathcal{L}\{A\}(s) = \frac{A_0\, s^{\alpha-1}}{s^\alpha + k_1}.$$

   Taking the inverse Laplace transform using the Mittag–Leffler function E_α:

$$A(t) = A_0\, E_\alpha\big(-k_1\, t^\alpha\big), \quad E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}. \tag{3}$$

5. **Solving for Blood Alcohol Concentration** $B(t)$
   Substitute the above obtained $\mathcal{L}\{A\}(s)$ into Equation (2),

$$\mathcal{L}\{B\}(s) = \frac{k_1\, \mathcal{L}\{A\}(s)}{s^\beta + k_2} = \frac{k_1\, A_0\, s^{\alpha-1}}{(s^\alpha + k_1)\,(s^\beta + k_2)}. \tag{4}$$

   For the inverse transform, we use the two-parameter Mittag-Leffler function $E^{(2)}_{\alpha,\beta}$:

$$B(t) = k_1\, A_0\, t^{\beta-1}\, E^{(2)}_{\alpha,\beta}\big(-k_1\, t^\alpha,\, -k_2\, t^\beta\big),$$

   where:

$$E^{(2)}_{\alpha,\beta}(x, y) = \sum_{m,n\geq 0} \frac{x^m\, y^n}{\Gamma(\alpha m + \beta n + 1)}.$$

6. **Definition of Tolerance (ΔT)**

- Intoxication threshold: For t_i, where $B(t_i) = 0.08\%$
- Recovery threshold: For t_f, where $B(t_f) = 0.01\%$
- Tolerance is defined as $\Delta T = t_f - t_i$.

2.3 Time-Dependent Analysis of BAC Variation

1. **Definition of Time Grid**

$$t_j = j\,\Delta t, \quad j = 0, 1, 2, \ldots, J, \quad \Delta t = \frac{T_{\max}}{J},$$

Here, $T_{\max}$is the total simulation time of the model (e.g., 8 hours), and J is the number of intervals.

2. **Calculating concentration time series**

$$A_j = A(t_j), \quad B_j = B(t_j), \quad j = 0, \ldots, J,$$

Evaluate the expressions (3), (4) for each unit time step Δt to get the vector $\{B_j\}$.

3. **Time of Maximum Concentration**

$$t_{\max} = \arg\max_{0 \le j \le J} B_j.$$

Find the index where $\{B_j\}$ reaches its maximum value and record the corresponding $t_{\max}$.

4. **Numerical Solution for Threshold Times**

- $\mathrm{BAC}_{\mathrm{high}}$ passing time t_i:
$$B(t_i) = \mathrm{BAC}_{\mathrm{high}}.$$
- $\mathrm{BAC}_{\mathrm{low}}$ passing time t_f:
$$B(t_f) = \mathrm{BAC}_{\mathrm{low}}.$$

To solve these equations, the bisection method or the Newton-Raphson method can be used. For example, in the case of the bisection method:

$$\text{Initial interval: } [t_a, t_b], If the signs of \quad B(t_a) - C \text{ and } B(t_b) - C \text{ are different,}$$

$$t_{\mathrm{mid}} = \tfrac{1}{2}(t_a + t_b), \quad \text{Repeat: } \begin{cases} t_b = t_{\mathrm{mid}}, & \text{if } B(t_{\mathrm{mid}}) > C, \\ t_a = t_{\mathrm{mid}}, & \text{otherwise,} \end{cases}$$

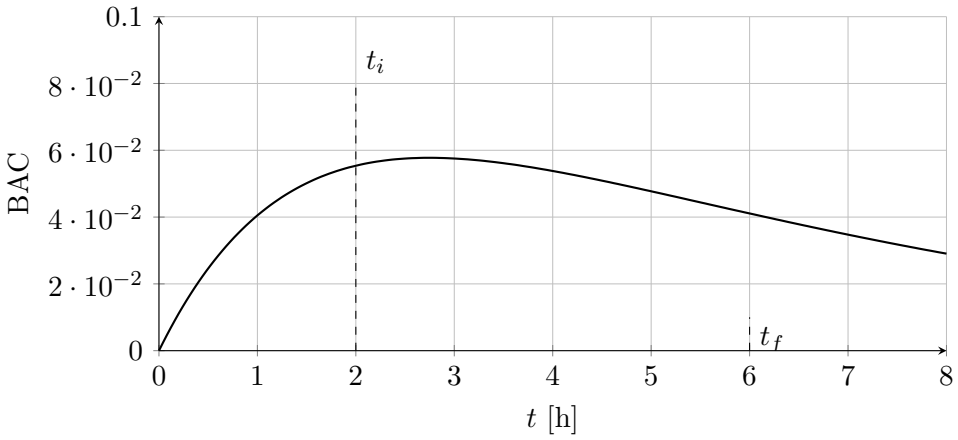
Repeat until the error tolerance is satisfied to calculate t_i and t_f

5. **Definition of Tolerance**

$$\Delta T = t_f - t_i.$$

This value is defined as the "tolerance time," i.e., the time it takes from intoxication to recovery.

6. **Visualization of Concentration Curve**
   Using the dataset
   $$\{(t_j,\, B_j)\}_{j=0}^{J}$$
   plot a graph and indicate $t_i, t_{\max}, t_f$ with vertical lines. Example:



7. **Slope Correction and Residual Analysis**

   - Log-linear regression: In the second interval (post-peak) of $\ln B_j$ vs. t_j, perform linear regression on the log-transformed values to estimate the elimination rate $\tilde{k}_2$:
     $$\ln B_j \approx -\tilde{k}_2\, t_j + c.$$
   - Residuals: Calculate the residuals $\varepsilon_j = B_j - \widehat{B}(t_j)$ to assess model fit quality.

8. **Sensitivity Analysis**
   For each parameter $\theta \in \{k_1, k_2, \alpha, \beta\}$, evaluate the sensitivity of the outcome with respect to tolerance time:
   $$S_\theta = \frac{\Delta T(\theta + \delta) - \Delta T(\theta)}{\delta},$$
   This quantifies how changes in model parameters affect the resulting tolerance time.

2.4 Model Validation and Performance Evaluation

1. **Parameter Estimation (Nonlinear Least Squares)**
   For the model solution
   $$B(t;\theta) = A_0 \frac{k_1}{k2 - k_1}(e^{-k_1 t} - e^{-k_2 t})$$
   ,
   $$\hat{\theta} = \arg\min_{\theta=(k_1,k_2)} S(\theta), \quad S(\theta) = \sum_{j=1}^{N} \big(B_{\text{obs}}(t_j) - B(t_j;\theta)\big)^2.$$
   (where A_0 is a pre-calculated value from alcohol consumption-weight).

2. **Goodness-of-Fit Metrics**
   Define the following metrics with the estimated $\hat{\theta}$

$$\begin{aligned} \mathrm{SSE} &= \sum_{j=1}^{N} \big(B_{\mathrm{obs}}(t_j) - B(t_j;\hat{\theta})\big)^2, \\ \mathrm{RMSE} &= \sqrt{\tfrac{1}{N}\mathrm{SSE}}, \\ R^2 &= 1 - \frac{\displaystyle\sum_{j=1}^{N} \big(B_{\mathrm{obs}}(t_j) - B(t_j;\hat{\theta})\big)^2}{\displaystyle\sum_{j=1}^{N} \big(B_{\mathrm{obs}}(t_j) - \bar{B}_{\mathrm{obs}}\big)^2}, \end{aligned}$$

   where $\bar{B}_{\mathrm{obs}} = \frac{1}{N}\sum_j B_{\mathrm{obs}}(t_j)$.

3. **Residual Analysis**
   For residuals $\varepsilon_j = B_{\mathrm{obs}}(t_j) - B(t_j;\hat{\theta})$

   - *residuals vs. time* Scatterplot: Checking for structural errors
   - *residual histogram*: Review normality (distribution symmetry)

4. **Validate alcohol consumption (ΔT) prediction**
   From the drunkenness-passage time t_i, t_f

$$\Delta T_{\mathrm{pred}} = t_f - t_i, \quad \Delta T_{\mathrm{obs}} = t_f^{\mathrm{obs}} - t_i^{\mathrm{obs}},$$

   Calculate the $\mathrm{MAE}_{\Delta T}$ and $\mathrm{RMSE}_{\Delta T}$ of the two values to further check the accuracy of the stock forecast.

References

[1] Ricardo Almeida, Nuno R. O. Bastos, and M. Teresa T. Monteiro, *Modelling some real phenomena by fractional differential equations*, **39**, no. 16, 4846–4855.

[2] KOROAD, *Drunk Driving Traffic Accidents Occur 42 Times a Day... December is the Month with the Most Traffic Accidents*, `https://www.koroad.or.kr/main/board/6/301735/board_view.do?&cp=1&listType=list&bdOpenYn=Y&bdNoticeYn=N`, [Accessed 25-04-2025].