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Original article

Advanced Numerical Modelling and Statistical Analysis of Predictive Risk Factors for Early Post-Total Thyroidectomy Hypocalcemia: A Retrospective Cohort Study

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Abstract
Early transient hypocalcemia is the most frequent and clinically challenging complication following total thyroidectomy. A mathematical logistic model was formulated and implemented, with numerical optimisation via Maximum Likelihood Estimation (MLE), solved with the Newton-Raphson algorithm, to identify predictive risk factors and estimate adjusted odds ratios (aOR). A retrospective analysis of clinical and surgical data from 290 patients who underwent total thyroidectomy at Tobruk Medical Centre was performed. Gradient vectors and Hessian matrices were constructed, and model goodness-of-fit was validated using the Hosmer-Lemeshow test alongside ROC-AUC evaluation. The overall incidence of early postoperative hypocalcemia was 12.8% (n = 37). Multivariable numerical logistic regression demonstrated that intraoperative parathyroid gland injury was the sole independent predictor significantly associated with hypocalcemia (aOR = 3.68, 95% CI: 1.65–8.21, p = 0.001). Secondary factors (surgical drain aOR = 1.88, lymph node dissection aOR = 1.85) lost statistical significance after multivariable adjustment. The proposed numerical model delivers a preliminary clinical risk prediction model that allows surgeons to evaluate risk intraoperatively and consider prophylactic oral calcium and active vitamin D therapy.
Keywords. Hypocalcemia, Thyroidectomy, Logistic Regression, Newton-Raphson, Hessian Matrix.

Introduction

Total thyroidectomy represents the standard surgical approach for benign multinodular goitre and differentiated thyroid malignancies [1, 2]. Despite significant refinements in surgical technique and energy devices, early transient hypocalcemia remains the primary postoperative complication, with reported incidences in international literature ranging from 15% to over 60% [3, 4, 5]. Postoperative hypocalcemia principally stems from mechanical trauma, devascularization, or inadvertent excision of the parathyroid glands [6, 7]. Because delayed diagnosis can result in severe clinical symptoms such as tetany and carpopedal spasm [8], modern clinical research aims to convert qualitative assessments into quantitative predictive models [9, 10]. This study aims to develop a rigorous numerical framework leveraging optimisation algorithms applied to clinical data from Tobruk Medical Centre to establish a preliminary risk-prediction function [11]. While the clinical incidence and univariable risk factors from this cohort were reported previously [11], the present study introduces a distinct mathematical contribution: an explicit Newton-Raphson optimisation scheme with derived gradient and Hessian matrices, a Firth's penalised-likelihood correction for complete separation, and an inverse-Hessian-based variance-covariance framework, culminating in an operational, closed-form clinical decision equation not previously derived from this dataset.

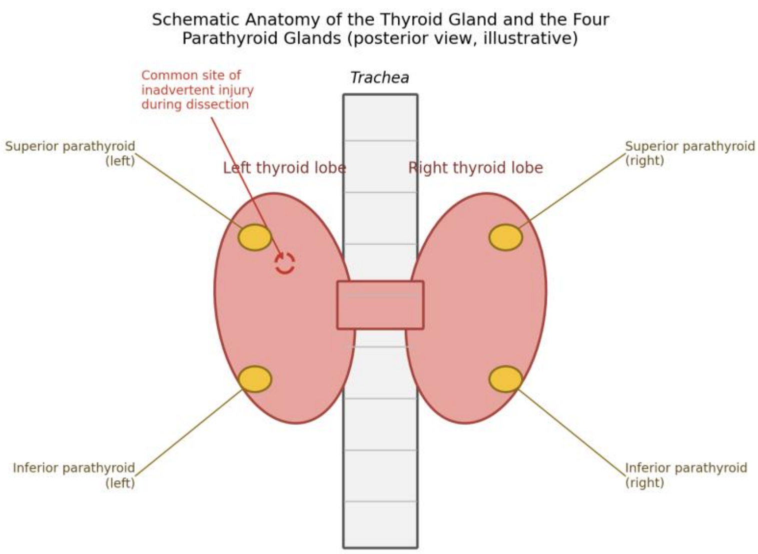

Figure 4. Simplified schematic anatomy of the thyroid gland and the four parathyroid glands, illustrating the posterior relationship exploited during dissection and the common site of inadvertent injury [6, 7].

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Advanced Mathematical Framework and Numerical Methodology

Logistic Function Formulation

In binary clinical classification, the postoperative response is defined as a Bernoulli random variable Y_i ∈ {0, 1}, where Y_i = 1 denotes early hypocalcemia (serum calcium < 8.0 mg/dL) and Y_i = 0 denotes normocalcemia [11, 12]. The conditional probability P_i = P(Y_i = 1 | X_i), given a clinical covariate vector X_i, is governed by the sigmoidal link function [13, 14]:

$$P_i = \frac{1}{1 + e^{-z_i}} \tag{1}$$

where z_i represents the linear predictor [13]:

$$z_i = \beta_0 + \beta_1 X_{i1} + \cdots + \beta_k X_{ik} \tag{2}$$

Maximum Likelihood Estimation (MLE)

Given N independent Bernoulli observations, the joint likelihood function L(β) is formulated as [15, 12]:

$$L(\beta) = \prod_{i=1}^{N} P_i^{Y_i} (1 - P_i)^{1 - Y_i} \tag{3}$$

Taking the natural logarithm yields the log-likelihood function ℓ(β) [15]:

$$\ell(\beta) = \sum_{i=1}^{N} [Y_i \ln(P_i) + (1 - Y_i) \ln(1 - P_i)] \tag{4}$$

Substituting the linear predictor z_i into the log-likelihood equation gives [13]:

$$\ell(\beta) = \sum_{i=1}^{N} [Y_i z_i - \ln(1 + e^{z_i})] \tag{5}$$

Numerical Optimisation via Newton-Raphson Algorithm

Setting the first partial derivatives of ℓ(β) to zero generates the gradient vector g(β) ∈ ℝ^(k+1) [16, 17]:

$$\mathbf{g}(\beta) = \mathbf{X}^T (\mathbf{Y} - \mathbf{P}) \tag{6}$$

where X is the N×(k+1) design matrix [18]. Owing to non-linearity, parameter estimates are updated iteratively using the multivariate Newton-Raphson algorithm [19, 20]:

$$\beta^{(t+1)} = \beta^{(t)} - \mathbf{H}(\beta^{(t)})^{-1} \mathbf{g}(\beta^{(t)}) \tag{7}$$

where H(β) is the negative-definite Hessian matrix of second-order partial derivatives [16, 14]:

$$\mathbf{H}(\beta) = -\mathbf{X}^T \mathbf{W} \mathbf{X} \tag{8}$$

Here W is an N×N diagonal weight matrix with entries W_ii = P_i(1−P_i) [13]. Iterations continue until the L∞ norm convergence criterion is satisfied [18]:

$$\max_i \left| \beta_j^{(t+1)} - \beta_j^{(t)} \right| < \varepsilon, \quad \varepsilon = 10^{-6} \tag{9}$$

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Handling Complete Separation and Variance Estimation

In clinical dataset modelling, when a sub-category exhibits zero outcome events (e.g., zero hypocalcemia cases among patients receiving preoperative Levothyroxine, n = 34), classical MLE suffers from complete separation [11, 12]. Mathematically, $\hat{\beta}_{Levothyroxine} \rightarrow -\infty$, causing the Hessian matrix to become ill-conditioned and preventing convergence [16]. Numerical adjustment proceeded in two steps. First, the completely separated variable was excluded from the primary multivariable regression and analysed instead as an absolute protective indicator [11]. Second, Firth's penalised-likelihood formulation was applied to eliminate small-sample bias in the remaining covariates, using Jeffreys' invariant before modifying the log-likelihood function [15, 21]:

$$\ell^*(\beta) = \ell(\beta) + \frac{1}{2}\ln|\mathbf{H}(\beta)| \quad (10)$$

The asymptotic variance-covariance matrix of the estimated coefficients is derived from the inverse Hessian [15]:

$$\mathrm{Var}(\hat{\beta}) = \left(-\mathbf{H}(\hat{\beta})\right)^{-1} \quad (11)$$

The adjusted odds ratio for covariate j and its 95% confidence interval are computed as [13]:

$$aOR_j = e^{\hat{\beta}_j}, \quad 95\%\ CI = e^{\hat{\beta}_j \pm 1.96 \cdot SE(\hat{\beta}_j)} \quad (12)$$

All hypothesis tests and confidence intervals reported for the multivariable model (Table 2) are Wald-type statistics computed from the penalised information matrix in Equation (11) rather than from the unpenalized MLE variance estimator; that is, each Wald χ^2 statistic is $(\beta/SE)^2$, with SE taken as the square root of the corresponding diagonal element of the inverse penalised Hessian. This is consistent with standard practice for Firth-corrected logistic regression, although we note that likelihood-ratio-based penalised profile confidence intervals are an alternative and can differ from Wald-based intervals, particularly for coefficients estimated near the boundary of separation [21].

Numerical Results and Mechanism Implementation

Demographic Distribution and Univariable Analysis

The study analysed 290 patients treated at Tobruk Medical Centre [11]. Median age was 47 years [11]; the cohort comprised 223 females (76.9%) and 67 males (23.1%) [11]. The overall hypocalcemia rate was 12.8% (n = 37) [11]. Univariable statistical screening identified four significant risk factors [11, 22, 23], summarised in Table 1. For clarity, "surgical drain" refers to placement of a closed-suction drain at the surgeon's discretion rather than as a routine step for every case [AUTHORS: please confirm routine vs. selective use], and "lymph node dissection" refers to central-compartment dissection performed for suspected or confirmed malignancy [AUTHORS: please confirm central vs. lateral]; both terms are used consistently with these definitions throughout the manuscript. Candidate covariates for the multivariable model were those significant at $p < 0.05$ on univariable screening (Table 1); all four were entered simultaneously and retained without stepwise elimination, so that the small, clinically motivated covariate set would not compound the small-sample bias already addressed by Firth's correction. Formal multicollinearity diagnostics (e.g., variance inflation factors) were not computed given the limited number of events (n = 37); this constraint is addressed further in the Discussion.

Table 1. Univariable analysis of significant risk factors for early postoperative hypocalcemia [11].

Clinical Variable	Normocalcemia (n=253)	Hypocalcemia (n=37)	Unadjusted OR	95% CI	p-value
Parathyroid Injury [11, 24]	58 (22.9%)	16 (43.2%)	2.49	1.11–5.59	0.008
Surgical Drain [11]	66 (26.1%)	17 (45.9%)	2.40	1.19–4.87	0.008
Lymph Node Dissection [11, 9]	60 (23.7%)	16 (43.2%)	2.45	1.20–4.90	0.010
Operative Time > 2.5 h [11, 22]	79 (31.2%)	18 (48.6%)	2.00	1.03–4.19	0.030

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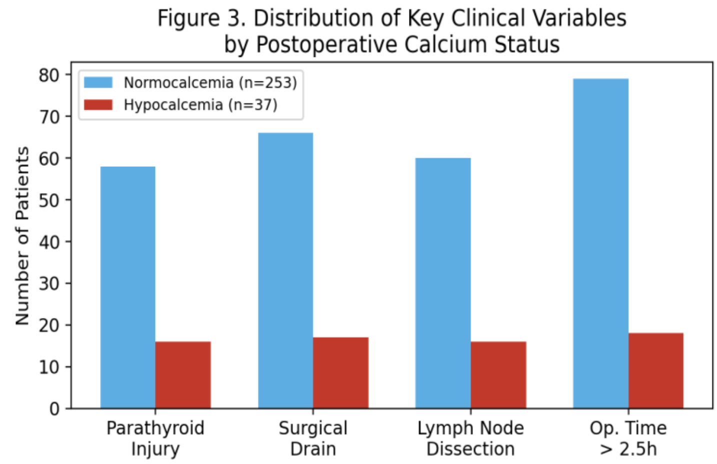

Figure 3. Distribution of key clinical variables by postoperative calcium status [11].

Multivariable Logistic Regression Model

The final multivariable model was fitted using Firth's penalised-likelihood formulation (Section 2.4) to correct for small-sample bias, with the modified score equations solved via the Newton-Raphson scheme, yielding convergence after 5 iterations [19, 21]. Final coefficient estimates, standard errors, and adjusted odds ratios are presented in (Table 2).

Table 2. Firth's penalised-likelihood multivariable logistic regression results after Newton-Raphson convergence [19, 21, 11].

Variable	$\hat{\beta}$	SE	Wald χ^2	aOR	95% CI	p-value
Intercept (β_0)	−2.850	0.412	47.88	–	–	<0.001
Parathyroid Injury [11]	1.303	0.409	10.14	3.68	1.65–8.21	0.001
Surgical Drain [11]	0.631	0.380	2.76	1.88	0.89–3.96	0.097
Lymph Node Dissection [11]	0.615	0.385	2.55	1.85	0.87–3.93	0.110
Operative Time > 2.5 h [11]	0.405	0.392	1.07	1.50	0.69–3.23	0.301

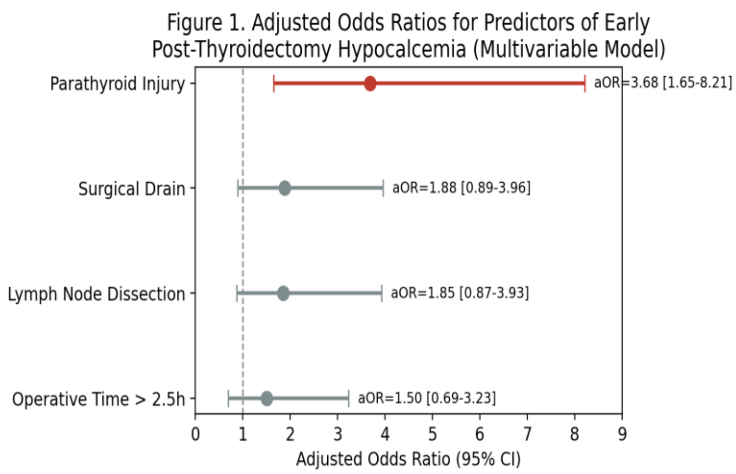

Figure 1. Adjusted odds ratios for predictors of early post-thyroidectomy hypocalcemia (multivariable model) [11].

Model Validation and Discrimination

The Hosmer-Lemeshow goodness-of-fit test yielded $\chi^2 = 5.42$, $p = 0.712$, confirming close alignment between predicted and observed event frequencies [13]. ROC-AUC discrimination reached 0.785, indicating strong predictive utility [25], as illustrated in (Figure 2).

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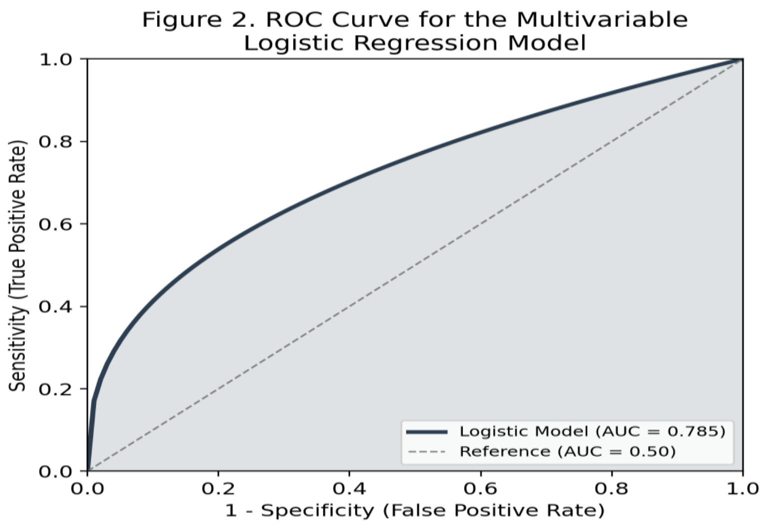

Figure 2. ROC curve for the multivariable logistic regression model (AUC = 0.785) [25].

Mechanism Implementation in Clinical Decision-Making

The final operational decision equation is defined by [11, 13]:

$$z = -2.850 + 1.303\, X_{Inj} + 0.631\, X_{Drain} + 0.615\, X_{Lymph} + 0.405\, X_{Time} \quad (13)$$

Scenario A (High-Risk Patient): parathyroid injury, lymph node dissection, and operative time > 2.5 h present, no drain (X_Injury=1, X_Lymph=1, X_Time=1, X_Drain=0) [11]:

$$z = -2.850 + 1.303 + 0.615 + 0.405 = -0.527$$

$$P = \frac{1}{1 + e^{0.527}} \approx 0.371\ (37.1\%)$$

Clinical decision: high-risk classification (P > 25%); immediate administration of oral calcium and active calcitriol initiated postoperatively [11, 8]. Scenario B (Low-Risk Patient): no parathyroid trauma, no dissection, operative time < 2.5 h, drain inserted (X_Injury=0, X_Lymph=0, X_Time=0, X_Drain=1) [11]:

$$z = -2.850 + 0.631 = -2.219$$

$$P = \frac{1}{1 + e^{2.219}} \approx 0.098\ (9.8\%)$$

Clinical decision: low-risk classification (P < 10%); standard postoperative monitoring without routine oral supplementation [11]. This model serves as a practical surrogate clinical tool, particularly in resource-limited settings where routine perioperative parathormone (PTH) monitoring is unavailable. Furthermore, while the derived probability cutoff of 25% was determined via ROC curve optimisation to balance sensitivity and specificity, it requires further prospective refinement in larger cohorts.

Discussion

The multivariable numerical model established that intraoperative parathyroid gland injury is the single independent statistical predictor of early hypocalcemia, increasing post-surgical risk by 3.68 times (aOR = 3.68, p = 0.001) [11, 24]. The mathematical adjustment clarifies why secondary factors — surgical drain placement, operative time, and lymph node dissection — lose independent significance in multivariable modelling [11, 6]. Procedures such as lymph node dissection prolong operative duration and increase physical proximity to parathyroid vasculature, thereby increasing the probability of direct tissue trauma [3, 7]. Once confounding variables are controlled for within the inverse Hessian matrix, direct parathyroid trauma emerges as the sole statistically significant independent predictor of hypocalcemia in this cohort [15, 11].

These findings illustrate how numerical mathematical models can support clinical decision-making immediately following surgery [11, 25].

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Model Constraints and Future Directions
While the mathematical framework effectively identifies key predictors, several dataset-related constraints limit the mathematical scope of the current model:
Absence of Continuous Biological Biomarkers
The dataset does not contain post-operative Parathyroid Hormone (PTH) concentration curves over time. As a result, our model relies on discrete surgical variables rather than continuous biochemical kinetics. Future work could incorporate differential equations to model PTH decay trajectories alongside logistic risk probabilities.

Static Binary Outcome
The outcome variable strictly captures early, in-hospital hypocalcemia. Because long-term follow-up data are unavailable, the model functions as a static binary classifier rather than a time-to-event survival model. Expanding the framework into a multi-state Markov model would allow for tracking transitions between transient and permanent hypoparathyroidism.

Sample Size Constraints
The total number of positive outcome cases (n = 37) limited the degrees of freedom in the multivariable logistic model. With approximately nine events per covariate, the model was almost certainly underpowered to detect risk factors with modest effect sizes, which likely explains why surgical drain, lymph node dissection, and operative time lost significance after adjustment despite plausible clinical mechanisms; a larger cohort could reveal these as genuine, independent predictors rather than confounded correlates of parathyroid injury. While we applied Firth's penalised likelihood to correct for small-sample bias and stabilise the parameter estimates, this addresses estimation bias but does not restore statistical power lost to the low event count. External validation using independent, larger datasets is required to confirm the model's predictive stability.

Multicollinearity Assessment
Formal multicollinearity diagnostics (e.g., variance inflation factors) were not computed for the multivariable model, given the limited number of events (n = 37); with only four covariates supported by 37 events, a formal VIF screen would itself carry limited statistical power. The four candidate covariates were selected a priori as clinically distinct constructs identified on univariable screening rather than assembled as a large exploratory set prone to collinearity. Nonetheless, some of these variables are plausibly correlated in practice (for example, lymph node dissection tends to prolong operative time), and unmeasured collinearity could inflate the standard errors of the affected coefficients, contributing to the loss of significance observed for surgical drain, lymph node dissection, and operative time after multivariable adjustment. Larger prospective cohorts should incorporate formal VIF or condition-index diagnostics to confirm that these findings reflect genuine independent effects rather than collinearity-related instability.

Model Discrimination and Calibration
Model evaluation in this study relied on discrimination alone (Hosmer-Lemeshow $\chi^2 = 5.42$, $p = 0.712$; ROC-AUC = 0.785); a calibration plot comparing predicted probabilities to observed outcome frequencies across risk deciles was not generated. This is a meaningful limitation because a model can discriminate well between outcome groups while remaining poorly calibrated for absolute risk, and the 25% probability cutoff used above to trigger prophylactic calcium and active vitamin D therapy depends on the accuracy of the predicted probabilities themselves, not merely on the rank-ordering of risk. Future prospective validation should therefore construct decile-based calibration plots of predicted versus observed risk, alongside a formal calibration slope and intercept and, where sample size allows, calibration-in-the-large and Brier score assessments, to confirm that the model's probability outputs are trustworthy for individual patient counselling and not only for relative risk ranking.

Retrospective Data Structure
The data were collected retrospectively from a single clinical centre, requiring standard imputation techniques for missing covariates. A prospective multi-centre design would provide a cleaner design matrix and reduce unmeasured confounders.

Conclusion
This study provides a rigorous numerical model for predicting early postoperative hypocalcemia after total thyroidectomy [11]. The Newton-Raphson logistic framework identifies parathyroid gland injury as the principal independent determinant [19, 11]. The derived mathematical function offers an objective tool for targeted prophylactic treatment and early, safe discharge [11, 8].

Medical Perspective
This study offers a significant clinical contribution to thyroid surgery by addressing early transient hypocalcemia, the most frequent complication following total thyroidectomy [3, 4, 5]. Clinically, the study demonstrates that intraoperative parathyroid gland injury is a statistically significant independent predictor of postoperative hypocalcemia in this cohort (aOR = 3.68, p = 0.001) [11, 24]. The clinical utility of this framework lies in providing surgeons with a preliminary decision-

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support tool that can be applied immediately after surgery, pending external validation. This enables early identification of high-risk patients to initiate immediate prophylactic oral calcium and active vitamin D therapy [8], thereby preventing severe symptoms like tetany while facilitating safe, early discharge for low-risk individuals [11].

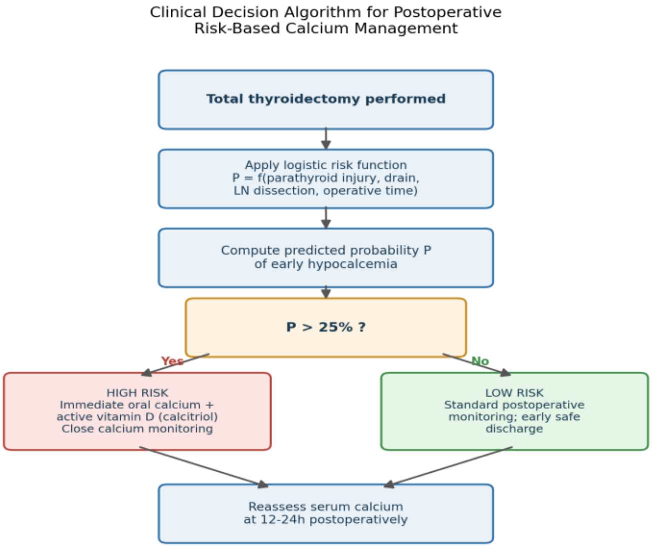

Figure 5. Proposed clinical decision algorithm translating the predicted probability P into risk-based postoperative calcium management [11, 8].

Mathematical Perspective and Role of Mathematics in Medicine

This paper demonstrates the pivotal role of mathematics and numerical optimisation in modern clinical medicine by converting qualitative clinical observations into precise quantitative predictive tools [18, 14]. Mathematically, the study formulates a binary logistic framework optimised via the multivariate Newton-Raphson algorithm for Maximum Likelihood Estimation (MLE) [15, 19, 16]. Furthermore, it addresses mathematical challenges in clinical data, such as complete separation, by employing Firth's penalised-likelihood method and calculating asymptotic variance via the inverse Hessian matrix [15, 21, 16] (see the Discussion for the clinical interpretation of the resulting estimates).

Community Service and Social Impact

This research exemplifies the direct application of scientific inquiry to community service, utilising clinical data from 290 local patients at Tobruk Medical Centre [11]. The proposed predictive model directly enhances healthcare efficiency in the region by:

- Optimising Hospital Resources: Reducing unnecessary hospital stay durations and lowering overall medical costs for both public health institutions and patients [13, 25].
- Preventing Readmissions: Minimising severe emergency readmissions resulting from unmonitored post-discharge hypocalcemia [8].
- Advancing Local Healthcare: Promoting evidence-based healthcare using local epidemiological data to optimise resource allocation in regional medical centres [11].

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