

Data Science for Mathematicians

Lesson 6: Logistic Regression and Generalized Linear Models

Department of Mathematics and Computer Science

Outline

- 1 Beyond Linear Boundaries
- 2 Constructing the Logistic Model
- 3 Parameter Estimation via Maximum Likelihood
- 4 Gradient Descent for Logistic Regression
- 5 Worked Examples
- 6 Generalized Linear Models

Recap: The Linear Regression Model

So far we have modeled a continuous response $y \in \mathbb{R}$ via

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2).$$

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Key assumptions:

- Response is continuous and unbounded: $Y_i | \mathbf{x}_i \sim \mathcal{N}(\boldsymbol{\beta}^T \mathbf{x}_i, \sigma^2)$
- OLS solution: $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$
- Loss function: mean squared error, minimized by gradient descent (Week 5)

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Question: What happens when the response is not continuous?

The Classification Problem

In **binary classification**, the target is discrete: $y_i \in \{0, 1\}$.

Real-world examples:

- **Medical diagnosis:** malignant ($y = 1$) vs. benign ($y = 0$)
- **Spam detection:** spam ($y = 1$) vs. not spam ($y = 0$)
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Goal: Learn a function $\mathbf{x} \in \mathbb{R}^p \mapsto \hat{y} \in \{0, 1\}$.

Why Linear Regression Fails for Classification

Naive approach: fit $\hat{y} = \beta^T \mathbf{x}$ with OLS, then threshold at 0.5.

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Problem 2: Heteroscedasticity.

- $Y_i \sim \text{Bernoulli}(p_i) \implies \text{Var}(Y_i | \mathbf{x}_i) = p_i(1 - p_i)$.
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Problem 3: Non-Gaussian errors.

- Error $\epsilon_i = y_i - \beta^T \mathbf{x}_i$ takes only two values—cannot be Gaussian.

The Key Insight

These are not minor issues—they are **fundamental violations** of OLS assumptions.

Solution: Do not model y directly. Instead, model the **conditional probability**:

$$p(\mathbf{x}) \equiv \mathbb{P}(Y = 1 \mid X = \mathbf{x}).$$

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We need a function that:

- Takes the linear predictor $\eta = \boldsymbol{\beta}^T \mathbf{x} \in (-\infty, \infty)$
- Maps it to a valid probability $p(\mathbf{x}) \in [0, 1]$

This is precisely the role of **logistic regression**.

From Probability to Odds

We build the transformation in two steps.

Step 1: The **odds ratio** removes the upper bound.

$$\text{odds} = \frac{p}{1-p}, \quad p \in (0, 1) \implies \text{odds} \in (0, \infty).$$

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Example: Horse race

If $p = 0.8$, then $\text{odds} = \frac{0.8}{0.2} = 4$ ("4 to 1 in favor").

If $p = 0.2$, then $\text{odds} = \frac{0.2}{0.8} = 0.25$ ("4 to 1 against").

The Logit Function

Step 2: Take the logarithm to remove the lower bound.

Definition: Logit function

The logit function $\text{logit}: (0, 1) \rightarrow \mathbb{R}$ is defined by

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Key properties:

- Strictly increasing bijection $(0, 1) \rightarrow \mathbb{R}$
- $\text{logit}(1/2) = 0$ (maximum uncertainty maps to zero)
- $\text{logit}(p) \rightarrow -\infty$ as $p \rightarrow 0^+$; $\text{logit}(p) \rightarrow +\infty$ as $p \rightarrow 1^-$

Logit: Numerical Examples

Example

- $p = 0.9$: odds = 9, log-odds = $\log 9 \approx 2.197$
- $p = 0.1$: odds ≈ 0.111 , log-odds ≈ -2.197
- $p = 0.5$: odds = 1, log-odds = 0

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- $p = 0.5$: odds = 1, log-odds = 0

The **symmetry** $\text{logit}(p) = -\text{logit}(1-p)$ reflects that $p = 0.5$ is the point of maximum uncertainty.

Summary of the two-step transformation:

$$\underbrace{p \in (0, 1)}_{\text{probability}} \xrightarrow{\text{odds}} \underbrace{\frac{p}{1-p} \in (0, \infty)}_{\text{half-line}} \xrightarrow{\log} \underbrace{\log \frac{p}{1-p} \in \mathbb{R}}_{\text{real line}}$$

The Core Modeling Assumption

We assume that the **log-odds** is a **linear function of the predictors**:

$$\log \left(\frac{p(\mathbf{x})}{1 - p(\mathbf{x})} \right) = \boldsymbol{\beta}^T \mathbf{x}.$$

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Next step: Invert the logit to express $p(\mathbf{x})$ explicitly.

Inverting the Logit: Deriving the Sigmoid

Let $\eta = \beta^T \mathbf{x}$. Starting from $\log\left(\frac{p}{1-p}\right) = \eta$:

$$\frac{p}{1-p} = e^\eta$$

$$p = e^\eta(1-p) = e^\eta - e^\eta p$$

$$p(1 + e^\eta) = e^\eta$$

$$p = \frac{e^\eta}{1 + e^\eta} = \frac{1}{1 + e^{-\eta}}.$$

Substituting $\eta = \beta^T \mathbf{x}$:

$$p(\mathbf{x}) = \frac{1}{1 + e^{-\beta^T \mathbf{x}}}.$$

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The Sigmoid Function

Definition: Sigmoid function

The sigmoid function $\sigma: \mathbb{R} \rightarrow (0, 1)$ is defined as

$$\sigma(z) = \frac{1}{1 + e^{-z}}.$$

The logistic regression model: $p(\mathbf{x}) = \sigma(\boldsymbol{\beta}^T \mathbf{x})$.

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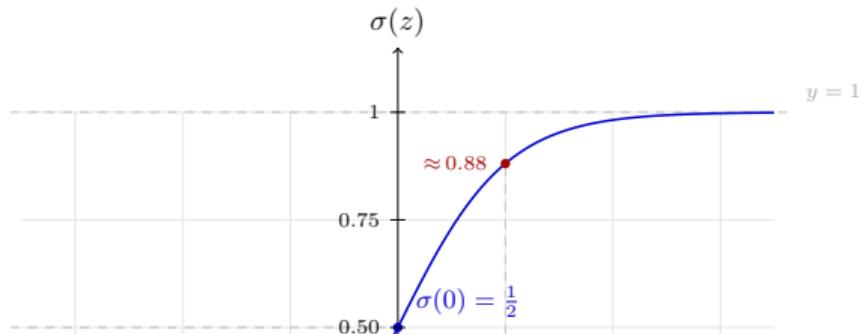
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Properties:

- $\sigma(z) \rightarrow 0$ as $z \rightarrow -\infty$
- $\sigma(0) = 1/2$
- $\sigma(z) \rightarrow 1$ as $z \rightarrow +\infty$
- Anti-symmetry: $\sigma(-z) = 1 - \sigma(z)$



Sigmoid: Numerical Examples

Example

- $\sigma(0) = \frac{1}{1 + e^0} = 0.5$ (maximum uncertainty)
- $\sigma(2) = \frac{1}{1 + e^{-2}} \approx 0.880$
- $\sigma(-2) \approx 0.119$

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In a logistic regression model, if $\beta^T \mathbf{x} = 2$, the model assigns probability $\approx 88\%$ to class 1.

The bounded range $(0, 1)$ ensures outputs are always valid probabilities—resolving the central flaw of linear regression.

The Derivative of the Sigmoid

Theorem: Sigmoid derivative

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Proof sketch.

By the quotient rule with $u = 1$, $v = 1 + e^{-z}$:

$$\sigma'(z) = \frac{e^{-z}}{(1 + e^{-z})^2} = \frac{1}{1 + e^{-z}} - \left(\frac{1}{1 + e^{-z}}\right)^2 = \sigma(z) - [\sigma(z)]^2.$$

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Why this matters: The derivative is expressed entirely in terms of $\sigma(z)$ itself. This will produce an elegant cancellation in the gradient of the loss function.

The Bernoulli Likelihood

Since $Y_i \sim \text{Bernoulli}(p_i)$ with $p_i = \sigma(\boldsymbol{\beta}^T \mathbf{x}_i)$, the probability of a single observation is

$$\mathbb{P}(Y_i = y_i \mid \mathbf{x}_i; \boldsymbol{\beta}) = p_i^{y_i} (1 - p_i)^{1-y_i}.$$

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The **log-likelihood**:

$$\ell(\boldsymbol{\beta}) = \sum_{i=1}^n [y_i \log p_i + (1 - y_i) \log(1 - p_i)].$$

Binary Cross-Entropy Loss

Negating the log-likelihood converts maximization to minimization.

Definition: Binary cross-entropy loss

The **binary cross-entropy (BCE)** loss is

$$J(\boldsymbol{\beta}) = - \sum_{i=1}^n [y_i \log p_i + (1 - y_i) \log(1 - p_i)],$$

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Example

True label $y_i = 1$:

- $p_i = 0.9 \implies J_i = -\log(0.9) \approx 0.105$ (small loss)
- $p_i = 0.1 \implies J_i = -\log(0.1) \approx 2.303$ (severe penalty)

Information-Theoretic Interpretation

The name *cross-entropy* comes from information theory.

For observation i with true label y_i :

- Empirical distribution P : deterministic ($P(Y = y_i) = 1$)
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Minimizing BCE \iff minimizing the information-theoretic dissimilarity between the model's predictions and the observed labels.

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Theorem

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Proof sketch.

The Hessian is

$$\nabla^2 J(\beta) = \sum_{i=1}^n \underbrace{\sigma_i(1 - \sigma_i)}_{\geq 0} \mathbf{x}_i \mathbf{x}_i^T.$$

For any $\mathbf{v} \in \mathbb{R}^{p+1}$:

$$\mathbf{v}^T \nabla^2 J(\beta) \mathbf{v} = \sum_{i=1}^n \sigma_i(1 - \sigma_i) (\mathbf{x}_i^T \mathbf{v})^2 \geq 0.$$

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Implication: No local minima. Gradient descent converges to the **unique global minimum**.

The Optimization Problem

We seek the parameter vector that minimizes the convex BCE loss:

$$\boldsymbol{\beta}^* = \arg \min_{\boldsymbol{\beta}} \left\{ - \sum_{i=1}^n [y_i \log p_i + (1 - y_i) \log(1 - p_i)] \right\}.$$

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We must use iterative optimization—gradient descent:

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We need the gradient $\nabla J(\boldsymbol{\beta})$.

Deriving the Gradient: Chain Rule

For a single sample, apply the chain rule:

$$\frac{\partial J_i}{\partial \beta_j} = \frac{\partial J_i}{\partial p_i} \cdot \frac{\partial p_i}{\partial z_i} \cdot \frac{\partial z_i}{\partial \beta_j},$$

where $z_i = \beta^T \mathbf{x}_i$ and $p_i = \sigma(z_i)$.

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③ $\frac{\partial z_i}{\partial \beta_j} = x_{ij}$

The Elegant Cancellation

Multiplying the three terms:

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Summing over all observations:

$$\frac{\partial J}{\partial \beta_j} = \sum_{i=1}^n (\sigma(\boldsymbol{\beta}^T \mathbf{x}_i) - y_i) x_{ij}.$$

The Vectorized Gradient

The full gradient vector in compact form:

$$\nabla J(\boldsymbol{\beta}) = \mathbf{X}^T(\mathbf{p} - \mathbf{y}),$$

where $\mathbf{p} = (\sigma(\boldsymbol{\beta}^T \mathbf{x}_1), \dots, \sigma(\boldsymbol{\beta}^T \mathbf{x}_n))^T$.

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Both share the structure $\mathbf{X}^T(\text{prediction} - \text{truth})$.

This is not a coincidence—it arises from using a canonical link function with an exponential family distribution.

Gradient Descent Update Rule

The complete gradient descent algorithm for logistic regression:

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- ② **Repeat** until convergence:

- ① Compute predictions: $\mathbf{p} = \sigma(\mathbf{X}\beta^{(t)})$
- ② Compute gradient: $\nabla J = \mathbf{X}^T(\mathbf{p} - \mathbf{y})$
- ③ Update parameters: $\beta^{(t+1)} = \beta^{(t)} - \eta \nabla J$

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 - ① Compute predictions: $\mathbf{p} = \sigma(\mathbf{X}\beta^{(t)})$
 - ② Compute gradient: $\nabla J = \mathbf{X}^T(\mathbf{p} - \mathbf{y})$
 - ③ Update parameters: $\beta^{(t+1)} = \beta^{(t)} - \eta \nabla J$

Convergence is guaranteed by the convexity of $J(\beta)$, provided η is sufficiently small.

Example 1: Medical Screening (Setup)

Example

Single predictor x (standardized biomarker), binary outcome y (disease).

i	1	2	3	4	5	6
x_i	-2	-1	0	1	2	3
y_i	0	0	0	1	1	1

Model: $p(x) = \sigma(\beta_0 + \beta_1 x)$. Initialize $\boldsymbol{\beta}^{(0)} = (0, 0)^T$, $\eta = 0.1$.

Example 1: Iteration 0

With $\beta^{(0)} = (0, 0)^T$: every $z_i = 0$, so $p_i = 0.5$ for all i .

Residual vector: $\mathbf{p} - \mathbf{y} = (0.5, 0.5, 0.5, -0.5, -0.5, -0.5)^T$.

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Update:

$$\beta^{(1)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} - 0.1 \begin{pmatrix} 0 \\ -4.5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0.45 \end{pmatrix}.$$

The zero first component reflects the balanced dataset; β_1 increases as expected.

Example 1: Iteration 1

With $\beta^{(1)} = (0, 0.45)^T$, the linear predictors are $z_i = 0.45x_i$:

$$\mathbf{p} \approx (0.289, 0.389, 0.500, 0.611, 0.711, 0.794)^T.$$

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$$\nabla J \approx \begin{pmatrix} 0.294 \\ -2.334 \end{pmatrix}.$$

Update:

$$\beta^{(2)} = \begin{pmatrix} 0 \\ 0.45 \end{pmatrix} - 0.1 \begin{pmatrix} 0.294 \\ -2.334 \end{pmatrix} = \begin{pmatrix} -0.029 \\ 0.683 \end{pmatrix}.$$

β_1 continues to grow, sharpening discrimination between classes.

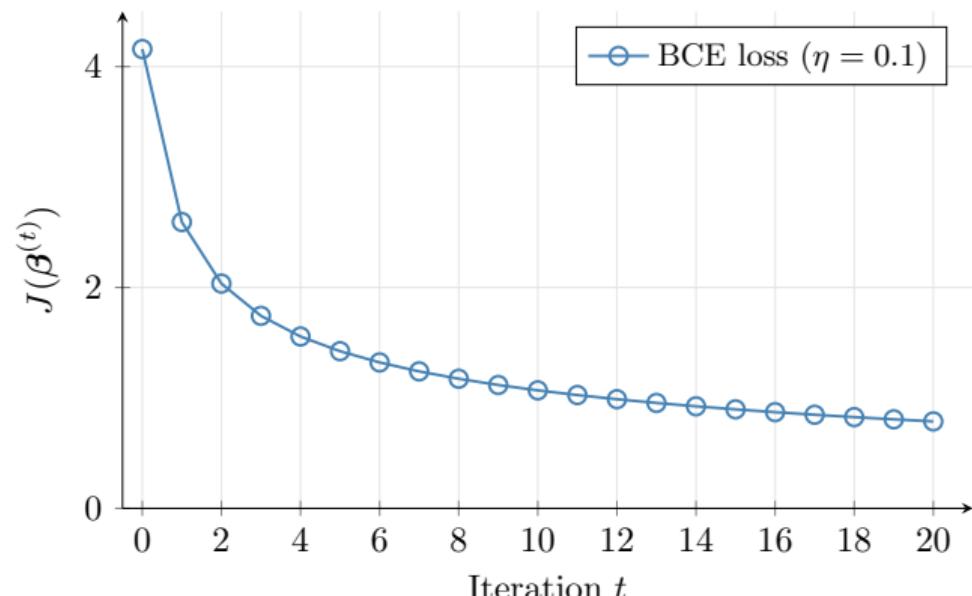
Example 1: Convergence

t	0	1	2	3	4	5	10
$J(\beta^{(t)})$	4.159	2.592	2.035	1.743	1.556	1.423	1.068

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Monotone decrease,
consistent with convexity.
Parameters stabilize near
 $\hat{\beta} \approx (-0.41, 1.55)^T$.



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Fitted model: $\hat{p}(x) = \sigma(-0.41 + 1.55 x)$.

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Perfect classification: Accuracy = 1.0, Precision = 1.0, Recall = 1.0, $F_1 = 1.0$.

Example 2: Loan Approval (Setup)

Example

Two predictors: income (x_1) and credit history (x_2). Outcome: approval (y).

i	1	2	3	4	5	6
x_{1i}	-2	-1	0	1	0	2
x_{2i}	-1	-2	-1	1	2	1
y_i	0	0	0	1	1	1

Model: $p(\mathbf{x}) = \sigma(\beta_0 + \beta_1 x_1 + \beta_2 x_2)$. Initialize $\boldsymbol{\beta}^{(0)} = \mathbf{0}$, $\eta = 0.1$.

Example 2: First Two Iterations

Iteration 0 ($\beta^{(0)} = \mathbf{0}$, all $p_i = 0.5$):

$$\nabla J = \begin{pmatrix} 0 \\ -3.0 \\ -4.0 \end{pmatrix}, \quad \beta^{(1)} = \begin{pmatrix} 0 \\ 0.30 \\ 0.40 \end{pmatrix}.$$

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$$\nabla J \approx \begin{pmatrix} 0.009 \\ -1.657 \\ -2.391 \end{pmatrix}, \quad \beta^{(2)} = \begin{pmatrix} -0.001 \\ 0.466 \\ 0.639 \end{pmatrix}.$$

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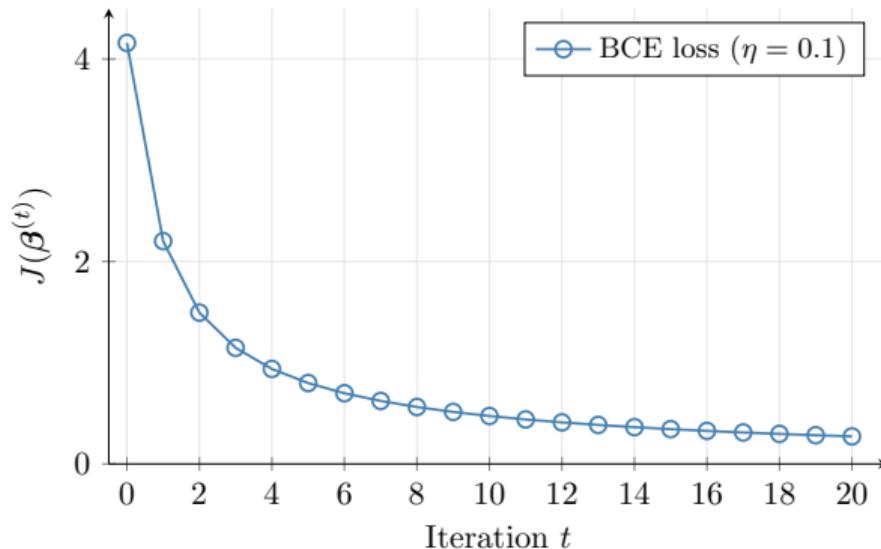
Both β_1 and β_2 grow, sharpening discrimination. The larger gradient component for x_2 suggests credit history has stronger influence.

Example 2: Convergence

t	0	1	2	3	4	5	10
$J(\beta^{(t)})$	4.159	2.201	1.495	1.146	0.938	0.799	0.473

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Parameters stabilize near $\hat{\beta} \approx (-0.10, 1.10, 1.80)^T$.

Example 2: Coefficient Interpretation

Fitted model: $\hat{p}(\mathbf{x}) = \sigma(-0.10 + 1.10x_1 + 1.80x_2)$.

Odds ratio interpretation:

- Income: $e^{1.10} \approx 3.00$ — a one-unit increase in income multiplies the odds of approval by ≈ 3

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Both positive \implies higher income and longer credit history increase approval odds.

$|\hat{\beta}_2| > |\hat{\beta}_1| \implies$ credit history has a stronger influence.

Example 2: Test Set Evaluation

Applying the model to 8 new applicants:

i	1	2	3	4	5	6	7	8
\hat{p}_i	0.07	0.21	0.56	0.87	0.90	0.89	0.97	0.48
\hat{y}_i	0	0	1	1	1	1	1	0
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Confusion matrix: $TP = 4$, $TN = 2$, $FP = 1$, $FN = 1$.

$$\text{Accuracy} = 0.75, \quad \text{Precision} = 0.80, \quad \text{Recall} = 0.80, \quad F_1 = 0.80.$$

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Borderline cases ($\hat{p}_3 = 0.56$, $\hat{p}_8 = 0.48$) motivate threshold tuning.

Interpreting Logistic Regression Coefficients

In OLS: β_j is the additive change in y per unit increase in x_j .

In logistic regression: β_j is the additive change in the **log-odds**.

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- $\beta_j > 0 \implies e^{\beta_j} > 1$: increased odds
- $\beta_j < 0 \implies e^{\beta_j} < 1$: decreased odds
- $\beta_j = 0 \implies e^{\beta_j} = 1$: no effect

Odds Ratio: Clinical Example

Example: Heart disease risk

Logistic regression predicts 10-year heart disease risk.

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The link function determines coefficient interpretation:

- Logit link → multiplicative effects on odds
- Identity link → additive effects on the mean

The Exponential Family

Definition: One-parameter exponential family

A distribution belongs to the **exponential family** if its density can be written as

$$f(y; \theta, \phi) = \exp\left\{ \frac{y\theta - b(\theta)}{\phi} + c(y, \phi) \right\},$$

where θ is the natural parameter, $b(\theta)$ is the log-partition function, and $\phi > 0$ is the dispersion parameter.

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Key properties from the log-partition function:

$$\mathbb{E}[Y] = b'(\theta), \quad \text{Var}(Y) = \phi b''(\theta).$$

Members of the Exponential Family

Example: Bernoulli

$$p^y(1-p)^{1-y} = \exp\left\{y \log \frac{p}{1-p} + \log(1-p)\right\}.$$

Natural parameter: $\theta = \log(p/(1-p))$ (the log-odds).

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Both distributions we have used—Bernoulli for classification, Gaussian for regression—are members of the exponential family.

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The link maps the range of μ_i to \mathbb{R} :

- Identity: $\mathbb{R} \rightarrow \mathbb{R}$ (Gaussian)
- Logit: $(0, 1) \rightarrow \mathbb{R}$ (Bernoulli)
- Log: $(0, \infty) \rightarrow \mathbb{R}$ (Poisson)

The Canonical Link

Each exponential family distribution has a distinguished **canonical link**:

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Since $\mu = b'(\theta)$, the canonical link is $g = (b')^{-1}$.

Why canonical links are special:

- The sufficient statistic $\mathbf{X}^T \mathbf{y}$ appears directly in the likelihood
- Score equations take a clean form
- This explains the elegant gradient $\nabla J = \mathbf{X}^T (\mathbf{p} - \mathbf{y})$

Three Instances of the GLM Framework

Component	Linear Regression	Logistic Regression	Poisson Regression
Distribution	$Y_i \sim \mathcal{N}(\mu_i, \sigma^2)$	$Y_i \sim \text{Bernoulli}(p_i)$	$Y_i \sim \text{Poisson}(\lambda_i)$
Mean range	\mathbb{R}	$(0, 1)$	$(0, \infty)$
Canonical link	$g(\mu) = \mu$	$g(p) = \log \frac{p}{1-p}$	$g(\lambda) = \log \lambda$
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All three share the same systematic component $\eta_i = \beta^T \mathbf{x}_i$.

Changing the distribution \implies changing the link \implies changing the loss.

Example: Poisson Regression

Example: Circuit board defects

Model: $Y_i \sim \text{Poisson}(\lambda_i)$ with log link:

$$\log \lambda_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}.$$

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Fitted: $\hat{\beta}_0 = -1.386$, $\hat{\beta}_1 = 0.030$, $\hat{\beta}_2 = 0.008$.

Interpretation: $e^{0.030} \approx 1.03$, so each additional cm^2 of board area multiplies the expected defect count by 1.03 (3% increase).

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For $x_1 = 50 \text{ cm}^2$, $x_2 = 250^\circ\text{C}$:

$$\hat{\lambda} = \exp(-1.386 + 0.030 \times 50 + 0.008 \times 250) \approx 8.28.$$

Key Formulas

Logistic regression model:

$$p(\mathbf{x}) = \sigma(\boldsymbol{\beta}^T \mathbf{x}) = \frac{1}{1 + e^{-\boldsymbol{\beta}^T \mathbf{x}}}.$$

Binary cross-entropy loss:

$$J(\boldsymbol{\beta}) = - \sum_{i=1}^n [y_i \log p_i + (1 - y_i) \log(1 - p_i)].$$

Gradient:

$$\nabla J(\boldsymbol{\beta}) = \mathbf{X}^T (\mathbf{p} - \mathbf{y}).$$

Classification rule: Predict $\hat{y} = 1$ if $\sigma(\boldsymbol{\beta}^T \mathbf{x}) \geq \tau$.

Key Takeaways

- Linear regression fails for binary classification due to unbounded predictions, heteroscedasticity, and non-Gaussian errors.
- The sigmoid function $\sigma(z) = 1/(1 + e^{-z})$ maps the linear predictor to a valid probability, with the elegant derivative $\sigma'(z) = \sigma(z)(1 - \sigma(z))$.
- Maximum likelihood estimation on Bernoulli data yields the convex binary cross-entropy loss, guaranteeing gradient descent converges to the global optimum.
- The gradient $\nabla J = \mathbf{X}^T(\mathbf{p} - \mathbf{y})$ shares the same structure as the OLS gradient—a consequence of using the canonical link.
- Coefficients have an odds ratio interpretation: e^{β_j} is the multiplicative change in odds per unit increase in x_j .
- The GLM framework unifies linear, logistic, and Poisson regression through the choice of distribution and link function.