

02_prob2

September 6, 2025

1 Problem 2: Y-Chromosome Threshold Analysis - Implementation

Objective: Analyze the relationship between maternal BMI and timing of Y-chromosome concentration reaching 4% threshold using interval-censored survival analysis.

Key Approach: Use Accelerated Failure Time (AFT) models with proper interval censoring to handle multiple tests per mother and determine optimal testing weeks.

1.1 Implementation Plan

This notebook implements the complete analysis following the detailed implementation guide:

1. **Section 1:** Event Interval Construction (Per Mother)
2. **Section 2:** Feature Matrix Preparation
3. **Section 3:** AFT Modeling & Inference (Core Analysis)
4. **Section 4:** Turnbull Non-parametric Validation
5. **Section 5:** BMI Grouping & Group-specific Optimal Weeks
6. **Section 6:** Monte Carlo Measurement Error Testing
7. **Section 7:** Baseline Two-step ML Comparison (Optional)
8. **Section 8:** Validation & Final Policy Table

```
[1]: # Import libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from pathlib import Path
import warnings
import sys
import re
from scipy import stats

# Core survival analysis
from lifelines import WeibullAFTFitter, LogLogisticAFTFitter, KaplanMeierFitter

# Machine learning
from sklearn.tree import DecisionTreeRegressor
from sklearn.model_selection import KFold
```

```

from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier, RandomForestRegressor
from sklearn.metrics import roc_auc_score

# Add project root to Python path for imports
PROJECT_ROOT = Path("/home/richard/projects/cumcm")
if str(PROJECT_ROOT) not in sys.path:
    sys.path.insert(0, str(PROJECT_ROOT))

# Import our custom modules
from src.analysis.problem2 import (
    apply_qc_filters,
    construct_intervals,
    prepare_feature_matrix,
    perform_group_specific_analysis,
    create_group_optimal_weeks_summary,
    run_monte_carlo_robustness_test,
    create_monte_carlo_summary_table,
    run_ml_baseline_comparison,
    run_comprehensive_validation
)
from src.models.aft_models import (
    fit_aft_models,
    display_model_summary,
    predict_survival_curves,
    calculate_optimal_weeks,
    fit_turnbull_estimator,
    compare_aft_vs_turnbull,
    assess_aft_goodness_of_fit
)

# Configure environment
warnings.filterwarnings('ignore')
plt.style.use('seaborn-v0_8')
sns.set_palette("husl")
pd.set_option('display.max_columns', 50)
pd.set_option('display.width', 1000)

print(" Libraries imported successfully")
print(" Survival analysis tools ready")
print(" Machine learning tools ready")

```

```

Libraries imported successfully
Survival analysis tools ready
Machine learning tools ready

```

```
[2]: # Setup paths
DATA_PATH = PROJECT_ROOT / "src" / "data" / "data.xlsx"
OUTPUT_PATH = PROJECT_ROOT / "output"
OUTPUT_DATA_PATH = OUTPUT_PATH / "data"
OUTPUT_FIGURES_PATH = OUTPUT_PATH / "figures"
OUTPUT_RESULTS_PATH = OUTPUT_PATH / "results"

# Create output directories
OUTPUT_DATA_PATH.mkdir(parents=True, exist_ok=True)
OUTPUT_FIGURES_PATH.mkdir(parents=True, exist_ok=True)
OUTPUT_RESULTS_PATH.mkdir(parents=True, exist_ok=True)

print(f" Paths configured - Data: {DATA_PATH}")
print(f" Output paths ready")

# Load original male fetus data for interval construction
print(" Loading original male fetus data...")
male_data = pd.read_excel(DATA_PATH, sheet_name=' ')
print(f" Loaded {len(male_data)} rows and {len(male_data.columns)} columns")

print("\n Data structure preview:")
print(f" Columns: {list(male_data.columns[:10])}...")
print(f" Maternal IDs: {male_data[' '].nunique()} unique mothers")
print(f" Total tests: {len(male_data)} test records")
```

```

Paths configured - Data: /home/richard/projects/cumcm/src/data/data.xlsx
Output paths ready
Loading original male fetus data...
Loaded 1082 rows and 31 columns

```

```
Data structure preview:  
Columns: [' ', ' ', ' ', ' ', ' ', ' ', ' ', 'IVF ', ' ', ' ',  
          '']...  
Maternal IDs: 267 unique mothers  
Total tests: 1082 test records
```

1.2 Section 1: Event Interval Construction (Per Mother)

Goal: Convert multiple test records per mother into single interval-censored event records.

Event Definition: Y-chromosome concentration first reaches 4% threshold

Censoring Types: 1. **Left-censored:** First observation already 4% \rightarrow Event occurred before first test 2. **Interval-censored:** Threshold crossed between visits \rightarrow Event in interval (L, R] 3. **Right-censored:** Never reached threshold \rightarrow Event beyond last observation

```
[3]: ### Step 1.1: Data Preparation and QC Filtering

# Apply same QC as preprocessing to get df with individual tests
```

```

print(" Applying QC filters from preprocessing...")
df_tests, filter_stats = apply_qc_filters(male_data, verbose=True)

print(f"\n Individual test dataset ready:")
df_tests.head(10)

```

```

Applying QC filters from preprocessing...
Parsing variables and applying QC filters...
Variable parsing completed:
Gestational weeks: 1082/1082 valid
BMI: 1082/1082 valid
Y concentration: 1082/1082 valid
After gestational weeks filter (10-25): 1069 records
After GC content filter (40-60%): 620 records
After chromosome abnormality filter: 556 records
After missing data filter: 556 records
Applying IQR outlier detection...
gestational_weeks:
  IQR outliers: 0 (0.00%) - bounds: [3.500, 29.214]
  After IQR filtering: 556 records (removed 0)
bmi:
  IQR outliers: 13 (2.34%) - bounds: [24.982, 39.214]
  After IQR filtering: 543 records (removed 13)
y_concentration:
  IQR outliers: 5 (0.92%) - bounds: [-0.017, 0.168]
  After IQR filtering: 538 records (removed 5)

QC filtering completed: 538 records remaining (49.7% retention)
Unique mothers: 238
Tests per mother: 2.3 average

```

Individual test dataset ready:

```

[3]:  maternal_id  gestational_weeks      bmi  y_concentration
0      A002         13.857143  33.331832      0.059230
1      A003         13.000000  30.742188      0.065185
2      A003         20.285714  31.882812      0.052253
3      A004         11.000000  28.641243      0.049498
4      A004         15.857143  28.641243      0.066800
5      A004         23.571429  29.161993      0.082347
6      A005         15.285714  30.844444      0.081533
7      A006         12.142857  35.883634      0.069469
8      A007         12.285714  33.874064      0.021902
9      A007         16.000000  33.874064      0.038038

```

```

[4]: ### Step 1.2: Interval Construction Logic

```

```

# Generate interval-censored observations using module function

```

```
df_intervals = construct_intervals(df_tests, threshold=0.04, verbose=True)
```

Constructing interval-censored observations...
Interval construction completed: 238 mothers

Censoring type distribution:
left: 203 (85.3%)
interval: 22 (9.2%)
right: 13 (5.5%)

[5]: *### Step 1.3: Output Analysis*

```
print(f"\n Sample intervals:")
print(df_intervals.head(10)[['maternal_id', 'bmi', 'L', 'R', 'censor_type', 'n_tests', 'max_y_concentration']])
```

```
Sample intervals:
maternal_id      bmi      L      R censor_type  n_tests
max_y_concentration
0      A002  33.331832  0.000000  13.857143      left      1
0.059230
1      A003  30.742188  0.000000  13.000000      left      2
0.065185
2      A004  28.641243  0.000000  11.000000      left      3
0.082347
3      A005  30.844444  0.000000  15.285714      left      1
0.081533
4      A006  35.883634  0.000000  12.142857      left      1
0.069469
5      A007  33.874064  23.714286      inf      right      4
0.038038
6      A008  29.136316  0.000000  13.000000      left      2
0.060891
7      A009  33.333333  0.000000  13.857143      left      3
0.159267
8      A010  33.333333  20.857143      inf      right      2
0.031946
9      A011  36.250470  16.142857  20.571429  interval      4
0.068983
```

1.3 Section 2: Feature Matrix Preparation

Goal: Prepare covariate matrix for AFT modeling with proper standardization and quality checks.

[6]: *### Step 2.1: Standardization and Feature Matrix Creation*

```
# Create feature matrix using module function
```

```
df_X = prepare_feature_matrix(df_intervals, verbose=True)
```

Preparing feature matrix for AFT modeling...

BMI standardization completed:

Mean BMI: 31.88

Std BMI: 2.59

BMI range: 26.6 - 39.2

All intervals are valid (L < R)

Feature matrix summary:

Observations: 238

Features: bmi, bmi_z

Interval bounds: L, R

Censoring types: ['left' 'right' 'interval']

Dataset statistics:

	bmi	bmi_z	L	R
count	238.000000	2.380000e+02	238.000000	238.000000
mean	31.879303	-5.747037e-16	2.337335	inf
std	2.587130	1.000000e+00	5.824886	NaN
min	26.619343	-2.033125e+00	0.000000	11.000000
25%	29.917696	-7.582176e-01	0.000000	12.571429
50%	31.632725	-9.530933e-02	0.000000	13.428571
75%	33.453780	6.085806e-01	0.000000	16.142857
max	39.159843	2.814138e+00	24.285714	inf

Quality checks:

Missing values: 0 total

Interval validity check:

Finite intervals: 225

Right-censored: 13

Left-censored: 203

Summary by censoring type:

	bmi			L	R
	count	mean	std	mean	<lambda>
interval	22	32.40	3.16	14.31	19.62
left	203	31.74	2.52	0.00	14.00
right	13	33.22	2.22	18.58	NaN

Feature matrix preparation completed - ready for AFT modeling

[7]: *### Step 2.2: Quality Checks*

Quality checks are included in the prepare_feature_matrix function above

```
print(" Feature matrix preparation completed with quality checks - ready for_AFT modeling")
```

Feature matrix preparation completed with quality checks - ready for AFT modeling

1.4 Section 3: AFT Modeling & Inference (Core Analysis)

Goal: Fit Accelerated Failure Time models to interval-censored data and derive BMI-specific survival functions.

Models: - Primary: Weibull AFT ($\log T = 'x + , \sim \text{Gumbel}$) - Alternative: Log-logistic AFT ($\sim \text{Logistic}$)

Key Output: Survival functions $S(t|x)$ for calculating optimal testing weeks

[8]: *### Step 3.1: Model Fitting*

```
# Fit AFT models using module function
primary_model, primary_name, all_models = fit_aft_models(df_X, formula='~_bmi_z', verbose=True)
```

Fitting AFT models to interval-censored data...

Fitting Weibull AFT model...

Weibull AFT model fitted successfully

Fitting Log-logistic AFT model...

Log-logistic AFT model fitted successfully

Using Weibull AFT as primary model

[9]: *### Step 3.2: Model Summary & Diagnostics*

```
# Display model summary and diagnostics using module function
display_model_summary(primary_model, primary_name, verbose=True)
```

Weibull AFT Model Summary:

```
=====
              coef exp(coef) se(coef)  coef lower 95%  coef upper 95%
exp(coef) lower 95% exp(coef) upper 95% cmp to      z      p
-log2(p)
param  covariate
lambda_ Intercept  2.018579   7.527618  0.146708      1.731035      2.306122
5.646497          10.035431      0.0  13.759117  4.489752e-43  140.676272
          bmi_z      0.167024   1.181783  0.072897      0.024149      0.309899
1.024443          1.363288      0.0   2.291235  2.194982e-02   5.509647
rho_ Intercept  0.122470   1.130286  0.179968     -0.230260      0.475201
0.794327          1.608338      0.0   0.680512  4.961806e-01   1.011063
```

Model Parameters:

```
('lambda_', 'Intercept'): 2.0186  
('lambda_', 'bmi_z'): 0.1670  
('rho_', 'Intercept'): 0.1225
```

BMI Effect Analysis:

```
BMI coefficient (standardized): 0.1670  
P-value: 0.0219  
Statistical significance: significant  
Interpretation: Higher BMI delays time to Y4% threshold  
AFT interpretation: 1-unit BMI increase → 16.7% change in log-time scale
```

Model Fit Statistics:

```
AIC: 253.54  
Log-likelihood: -123.77
```

[10]: *### Step 3.3: Survival Function Prediction*

```
# Generate survival curves using module function  
time_grid = np.linspace(10, 25, 100) # Gestational weeks 10-25  
survival_curves = predict_survival_curves(  
    primary_model,  
    df_intervals,  
    time_grid,  
    quartiles=[0.25, 0.5, 0.75],  
    verbose=True  
)
```

Generating survival curves for different BMI levels...

BMI quartiles for analysis:

```
Q25: 29.9  
Q50: 31.6  
Q75: 33.5
```

Computing survival functions...

```
Q25: BMI 29.9 (z=-0.76)  
Q50: BMI 31.6 (z=-0.10)  
Q75: BMI 33.5 (z=0.61)
```

Survival Probabilities at Key Weeks:

Week	BMI_Q25	BMI_Q50	BMI_Q75
12	0.142	0.179	0.222
14	0.099	0.130	0.167
16	0.066	0.091	0.123
18	0.045	0.065	0.091
20	0.031	0.046	0.068

Survival function prediction completed for 3 BMI levels

```
[11]: ### Step 3.4: Optimal Testing Week Calculation

# Calculate optimal testing weeks using module function
optimal_weeks_results = calculate_optimal_weeks(
    survival_curves,
    confidence_levels=[0.90, 0.95],
    verbose=True
)
```

Calculating optimal testing weeks for different confidence levels...

Optimal weeks for 90% confidence level:
(When 90% of mothers have reached Y 4% threshold)

Q25: BMI 29.9 → Week 13.9
Q50: BMI 31.6 → Week 15.6
Q75: BMI 33.5 → Week 17.6

Optimal weeks for 95% confidence level:
(When 95% of mothers have reached Y 4% threshold)

Q25: BMI 29.9 → Week 17.6
Q50: BMI 31.6 → Week 19.7
Q75: BMI 33.5 → Week 22.1

Optimal Testing Weeks Summary:

BMI Group	BMI Value	90% Conf	95% Conf
Q25	29.9	13.9	17.6
Q50	31.6	15.6	19.7
Q75	33.5	17.6	22.1

Optimal testing week calculation completed

1.5 Section 4: Turnbull Non-parametric Validation

Goal: Validate AFT assumptions using non-parametric Turnbull estimator.

1.5.1 Overview

- Fit Turnbull estimator to same interval-censored data
- Compare Turnbull vs AFT survival curves
- Assess goodness of fit for parametric assumptions

```
[12]: ### Step 4.1: Turnbull Fitting
```

```
# Fit Turnbull non-parametric estimator using module function  
turnbull_model = fit_turnbull_estimator(df_X, verbose=True)
```

```
Fitting Turnbull non-parametric estimator...  
Iteration 0  
  delta log-likelihood: 113.6900846918  
  log-like:           -153.399751  
Iteration 1  
  delta log-likelihood: -101.1526863254  
  log-like:           -132.911080  
Iteration 2  
  delta log-likelihood:  2.9231947109  
  log-like:           -129.987885  
Iteration 3  
  delta log-likelihood: -1.0849443151  
  log-like:           -126.598301  
Iteration 4  
  delta log-likelihood:  1.0252113341  
  log-like:           -125.573090  
Iteration 5  
  delta log-likelihood: -0.0043090313  
  log-like:           -124.052893  
Iteration 6  
  delta log-likelihood:  0.6773956086  
  log-like:           -122.989866  
Iteration 7  
  delta log-likelihood: -0.1124386356  
  log-like:           -122.198954  
Iteration 8  
  delta log-likelihood:  0.4953306406  
  log-like:           -121.587947  
Iteration 9  
  delta log-likelihood: -0.1470470728  
  log-like:           -121.106272  
Iteration 10  
  delta log-likelihood:  0.3827816919  
  log-like:           -120.719448  
Iteration 11  
  delta log-likelihood: -0.1542395080  
  log-like:           -120.405148  
Iteration 12  
  delta log-likelihood:  0.1367757006  
  log-like:           -120.268372  
Iteration 13  
  delta log-likelihood:  0.0208871686  
  log-like:           -120.033195
```

```
Iteration 14
  delta log-likelihood: 0.1034543726
  log-like:            -119.837019
Iteration 15
  delta log-likelihood: 0.0060184068
  log-like:            -119.672051
Iteration 16
  delta log-likelihood: 0.0806968021
  log-like:            -119.532256
Iteration 17
  delta log-likelihood: -0.0024361723
  log-like:            -119.412988
Iteration 18
  delta log-likelihood: 0.0645611503
  log-like:            -119.310564
Iteration 19
  delta log-likelihood: -0.0071565792
  log-like:            -119.222084
Iteration 20
  delta log-likelihood: 0.0527439360
  log-like:            -119.145206
Iteration 21
  delta log-likelihood: -0.0096519134
  log-like:            -119.078056
Iteration 22
  delta log-likelihood: 0.0438424917
  log-like:            -119.019097
Iteration 23
  delta log-likelihood: -0.0108040344
  log-like:            -118.967082
Iteration 24
  delta log-likelihood: 0.0369699499
  log-like:            -118.920976
Iteration 25
  delta log-likelihood: -0.0111424797
  log-like:            -118.879927
Iteration 26
  delta log-likelihood: 0.0315475596
  log-like:            -118.843224
Iteration 27
  delta log-likelihood: -0.0109919317
  log-like:            -118.810273
Iteration 28
  delta log-likelihood: 0.0271871201
  log-like:            -118.780573
Iteration 29
  delta log-likelihood: -0.0105545888
  log-like:            -118.753704
```

```
Iteration 30
  delta log-likelihood: 0.0236217730
  log-like:            -118.729309
Iteration 31
  delta log-likelihood: -0.0099576962
  log-like:            -118.707084
Iteration 32
  delta log-likelihood: 0.0106061086
  log-like:            -118.696478
Iteration 33
  delta log-likelihood: 0.0006978986
  log-like:            -118.677050
Iteration 34
  delta log-likelihood: 0.0091457544
  log-like:            -118.659209
Iteration 35
  delta log-likelihood: 0.0003370091
  log-like:            -118.642779
Iteration 36
  delta log-likelihood: 0.0079509036
  log-like:            -118.627607
Iteration 37
  delta log-likelihood: 0.0000994209
  log-like:            -118.613559
Iteration 38
  delta log-likelihood: 0.0069607969
  log-like:            -118.600520
Iteration 39
  delta log-likelihood: -0.0000524145
  log-like:            -118.588390
Iteration 40
  delta log-likelihood: 0.0061306498
  log-like:            -118.577081
Iteration 41
  delta log-likelihood: -0.0001447958
  log-like:            -118.566515
Iteration 42
  delta log-likelihood: 0.0054272447
  log-like:            -118.556625
Iteration 43
  delta log-likelihood: -0.0001961852
  log-like:            -118.547351
Iteration 44
  delta log-likelihood: 0.0048256315
  log-like:            -118.538639
Iteration 45
  delta log-likelihood: -0.0002195820
  log-like:            -118.530442
```

Iteration 46
delta log-likelihood: 0.0043068240
log-like: -118.522719
Iteration 47
delta log-likelihood: -0.0002241542
log-like: -118.515431
Iteration 48
delta log-likelihood: 0.0038561881
log-like: -118.508545
Iteration 49
delta log-likelihood: -0.0002163672
log-like: -118.502032
Iteration 50
delta log-likelihood: 0.0034623036
log-like: -118.495863
Iteration 51
delta log-likelihood: -0.0002007698
log-like: -118.490014
Iteration 52
delta log-likelihood: 0.0031161494
log-like: -118.484464
Iteration 53
delta log-likelihood: -0.0001805473
log-like: -118.479191
Iteration 54
delta log-likelihood: 0.0028105148
log-like: -118.474178
Iteration 55
delta log-likelihood: -0.0001579131
log-like: -118.469407
Iteration 56
delta log-likelihood: 0.0025395697
log-like: -118.464863
Iteration 57
delta log-likelihood: -0.0001343867
log-like: -118.460533
Iteration 58
delta log-likelihood: 0.0022985469
log-like: -118.456403
Iteration 59
delta log-likelihood: -0.0001109930
log-like: -118.452461
Iteration 60
delta log-likelihood: 0.0020835073
log-like: -118.448697
Iteration 61
delta log-likelihood: -0.0000884053
log-like: -118.445099

Iteration 62
delta log-likelihood: 0.0018911621
log-like: -118.441660
Iteration 63
delta log-likelihood: -0.0000670477
log-like: -118.438369
Iteration 64
delta log-likelihood: 0.0017187401
log-like: -118.435218
Iteration 65
delta log-likelihood: -0.0000471686
log-like: -118.432201
Iteration 66
delta log-likelihood: 0.0015638854
log-like: -118.429310
Iteration 67
delta log-likelihood: -0.0000288944
log-like: -118.426539
Iteration 68
delta log-likelihood: 0.0014245792
log-like: -118.423880
Iteration 69
delta log-likelihood: -0.0000122670
log-like: -118.421329
Iteration 70
delta log-likelihood: 0.0012990789
log-like: -118.418880
Iteration 71
delta log-likelihood: 0.0000027290
log-like: -118.416528
Iteration 72
delta log-likelihood: 0.0011858715
log-like: -118.414268
Iteration 73
delta log-likelihood: 0.0000161462
log-like: -118.412095
Iteration 74
delta log-likelihood: 0.0010836352
log-like: -118.410006
Iteration 75
delta log-likelihood: 0.0000280613
log-like: -118.407996
Iteration 76
delta log-likelihood: 0.0009912102
log-like: -118.406061
Iteration 77
delta log-likelihood: 0.0000385649
log-like: -118.404199

Iteration 78
delta log-likelihood: 0.0009075743
log-like: -118.402405
Iteration 79
delta log-likelihood: 0.0000477548
log-like: -118.400676
Iteration 80
delta log-likelihood: 0.0008318235
log-like: -118.399010
Iteration 81
delta log-likelihood: 0.0000557313
log-like: -118.397404
Iteration 82
delta log-likelihood: 0.0007631560
log-like: -118.395854
Iteration 83
delta log-likelihood: 0.0000625942
log-like: -118.394359
Iteration 84
delta log-likelihood: 0.0007008586
log-like: -118.392916
Iteration 85
delta log-likelihood: 0.0000684401
log-like: -118.391523
Iteration 86
delta log-likelihood: 0.0006442956
log-like: -118.390177
Iteration 87
delta log-likelihood: 0.0000733618
log-like: -118.388876
Iteration 88
delta log-likelihood: 0.0005928995
log-like: -118.387619
Iteration 89
delta log-likelihood: 0.0000774467
log-like: -118.386404
Iteration 90
delta log-likelihood: 0.0005461627
log-like: -118.385228
Iteration 91
delta log-likelihood: 0.0000807770
log-like: -118.384091
Iteration 92
delta log-likelihood: 0.0005036305
log-like: -118.382990
Iteration 93
delta log-likelihood: 0.0000834292
log-like: -118.381925

Iteration 94
delta log-likelihood: 0.0004648954
log-like: -118.380893
Iteration 95
delta log-likelihood: 0.0000854739
log-like: -118.379894
Iteration 96
delta log-likelihood: 0.0004295915
log-like: -118.378926
Iteration 97
delta log-likelihood: 0.0000869767
log-like: -118.377987
Iteration 98
delta log-likelihood: 0.0003973903
log-like: -118.377077
Iteration 99
delta log-likelihood: 0.0000879973
log-like: -118.376195
Iteration 100
delta log-likelihood: 0.0003679962
log-like: -118.375339
Iteration 101
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log-like: -118.337633
Iteration 644
delta log-likelihood: 0.0000003053
log-like: -118.337632
Iteration 645
delta log-likelihood: 0.0000003032
log-like: -118.337631
Iteration 646
delta log-likelihood: 0.0000003011
log-like: -118.337630
Iteration 647
delta log-likelihood: 0.0000002990
log-like: -118.337629
Iteration 648
delta log-likelihood: 0.0000002970
log-like: -118.337628
Iteration 649
delta log-likelihood: 0.0000002950
log-like: -118.337626
Iteration 650
delta log-likelihood: 0.0000002929
log-like: -118.337625
Iteration 651
delta log-likelihood: 0.0000002909
log-like: -118.337624
Iteration 652
delta log-likelihood: 0.0000002890
log-like: -118.337623
Iteration 653
delta log-likelihood: 0.0000002870
log-like: -118.337622

```
Iteration 654
  delta log-likelihood: 0.0000002850
  log-like:            -118.337621
Iteration 655
  delta log-likelihood: 0.0000002831
  log-like:            -118.337620
Iteration 656
  delta log-likelihood: 0.0000002812
  log-like:            -118.337619
Iteration 657
  delta log-likelihood: 0.0000002793
  log-like:            -118.337618
Iteration 658
  delta log-likelihood: 0.0000002774
  log-like:            -118.337617
Iteration 659
  delta log-likelihood: 0.0000002755
  log-like:            -118.337616
Iteration 660
  delta log-likelihood: 0.0000002736
  log-like:            -118.337615
Iteration 661
  delta log-likelihood: 0.0000002717
  log-like:            -118.337614
Iteration 662
  delta log-likelihood: 0.0000002699
  log-like:            -118.337613
Iteration 663
  delta log-likelihood: 0.0000002681
  log-like:            -118.337612
Iteration 664
  delta log-likelihood: 0.0000002662
  log-like:            -118.337611
Iteration 665
  delta log-likelihood: 0.0000002644
  log-like:            -118.337610
Iteration 666
  delta log-likelihood: 0.0000002627
  log-like:            -118.337609
Iteration 667
  delta log-likelihood: 0.0000002609
  log-like:            -118.337608
Iteration 668
  delta log-likelihood: 0.0000002591
  log-like:            -118.337607
Iteration 669
  delta log-likelihood: 0.0000002574
  log-like:            -118.337606
```

Iteration 670
delta log-likelihood: 0.0000002556
log-like: -118.337605
Iteration 671
delta log-likelihood: 0.0000002539
log-like: -118.337604
Iteration 672
delta log-likelihood: 0.0000002522
log-like: -118.337603
Iteration 673
delta log-likelihood: 0.0000002505
log-like: -118.337602
Iteration 674
delta log-likelihood: 0.0000002488
log-like: -118.337601
Iteration 675
delta log-likelihood: 0.0000002471
log-like: -118.337600
Iteration 676
delta log-likelihood: 0.0000002455
log-like: -118.337599
Iteration 677
delta log-likelihood: 0.0000002438
log-like: -118.337598
Iteration 678
delta log-likelihood: 0.0000002422
log-like: -118.337598
Iteration 679
delta log-likelihood: 0.0000002406
log-like: -118.337597
Iteration 680
delta log-likelihood: 0.0000002389
log-like: -118.337596
Iteration 681
delta log-likelihood: 0.0000002373
log-like: -118.337595
Iteration 682
delta log-likelihood: 0.0000002358
log-like: -118.337594
Iteration 683
delta log-likelihood: 0.0000002342
log-like: -118.337593
Iteration 684
delta log-likelihood: 0.0000002326
log-like: -118.337592
Iteration 685
delta log-likelihood: 0.0000002311
log-like: -118.337591

```
Iteration 686
  delta log-likelihood: 0.0000002295
  log-like:            -118.337591
Iteration 687
  delta log-likelihood: 0.0000002280
  log-like:            -118.337590
Iteration 688
  delta log-likelihood: 0.0000002265
  log-like:            -118.337589
Iteration 689
  delta log-likelihood: 0.0000002249
  log-like:            -118.337588
Iteration 690
  delta log-likelihood: 0.0000002234
  log-like:            -118.337587
Iteration 691
  delta log-likelihood: 0.0000002220
  log-like:            -118.337586
Iteration 692
  delta log-likelihood: 0.0000002205
  log-like:            -118.337586
Iteration 693
  delta log-likelihood: 0.0000002190
  log-like:            -118.337585
Iteration 694
  delta log-likelihood: 0.0000002176
  log-like:            -118.337584
Iteration 695
  delta log-likelihood: 0.0000002161
  log-like:            -118.337583
Iteration 696
  delta log-likelihood: 0.0000002147
  log-like:            -118.337582
Iteration 697
  delta log-likelihood: 0.0000002132
  log-like:            -118.337581
Iteration 698
  delta log-likelihood: 0.0000002118
  log-like:            -118.337581
Iteration 699
  delta log-likelihood: 0.0000002104
  log-like:            -118.337580
Iteration 700
  delta log-likelihood: 0.0000002090
  log-like:            -118.337579
Iteration 701
  delta log-likelihood: 0.0000002076
  log-like:            -118.337578
```

Iteration 702
delta log-likelihood: 0.0000002063
log-like: -118.337578
Iteration 703
delta log-likelihood: 0.0000002049
log-like: -118.337577
Iteration 704
delta log-likelihood: 0.0000002036
log-like: -118.337576
Iteration 705
delta log-likelihood: 0.0000002022
log-like: -118.337575
Iteration 706
delta log-likelihood: 0.0000002009
log-like: -118.337575
Iteration 707
delta log-likelihood: 0.0000001995
log-like: -118.337574
Iteration 708
delta log-likelihood: 0.0000001982
log-like: -118.337573
Iteration 709
delta log-likelihood: 0.0000001969
log-like: -118.337572
Iteration 710
delta log-likelihood: 0.0000001956
log-like: -118.337572
Iteration 711
delta log-likelihood: 0.0000001943
log-like: -118.337571
Iteration 712
delta log-likelihood: 0.0000001931
log-like: -118.337570
Iteration 713
delta log-likelihood: 0.0000001918
log-like: -118.337569
Iteration 714
delta log-likelihood: 0.0000001905
log-like: -118.337569
Iteration 715
delta log-likelihood: 0.0000001893
log-like: -118.337568
Iteration 716
delta log-likelihood: 0.0000001880
log-like: -118.337567
Iteration 717
delta log-likelihood: 0.0000001868
log-like: -118.337567

Iteration 718
delta log-likelihood: 0.0000001856
log-like: -118.337566
Iteration 719
delta log-likelihood: 0.0000001844
log-like: -118.337565
Iteration 720
delta log-likelihood: 0.0000001832
log-like: -118.337565
Iteration 721
delta log-likelihood: 0.0000001820
log-like: -118.337564
Iteration 722
delta log-likelihood: 0.0000001808
log-like: -118.337563
Iteration 723
delta log-likelihood: 0.0000001796
log-like: -118.337563
Iteration 724
delta log-likelihood: 0.0000001784
log-like: -118.337562
Iteration 725
delta log-likelihood: 0.0000001772
log-like: -118.337561
Iteration 726
delta log-likelihood: 0.0000001761
log-like: -118.337561
Iteration 727
delta log-likelihood: 0.0000001749
log-like: -118.337560
Iteration 728
delta log-likelihood: 0.0000001738
log-like: -118.337559
Iteration 729
delta log-likelihood: 0.0000001727
log-like: -118.337559
Iteration 730
delta log-likelihood: 0.0000001715
log-like: -118.337558
Iteration 731
delta log-likelihood: 0.0000001704
log-like: -118.337557
Iteration 732
delta log-likelihood: 0.0000001693
log-like: -118.337557
Iteration 733
delta log-likelihood: 0.0000001682
log-like: -118.337556

Iteration 734
delta log-likelihood: 0.0000001671
log-like: -118.337555
Iteration 735
delta log-likelihood: 0.0000001660
log-like: -118.337555
Iteration 736
delta log-likelihood: 0.0000001650
log-like: -118.337554
Iteration 737
delta log-likelihood: 0.0000001639
log-like: -118.337554
Iteration 738
delta log-likelihood: 0.0000001628
log-like: -118.337553
Iteration 739
delta log-likelihood: 0.0000001618
log-like: -118.337552
Iteration 740
delta log-likelihood: 0.0000001607
log-like: -118.337552
Iteration 741
delta log-likelihood: 0.0000001597
log-like: -118.337551
Iteration 742
delta log-likelihood: 0.0000001587
log-like: -118.337551
Iteration 743
delta log-likelihood: 0.0000001576
log-like: -118.337550
Iteration 744
delta log-likelihood: 0.0000001566
log-like: -118.337549
Iteration 745
delta log-likelihood: 0.0000001556
log-like: -118.337549
Iteration 746
delta log-likelihood: 0.0000001546
log-like: -118.337548
Iteration 747
delta log-likelihood: 0.0000001536
log-like: -118.337548
Iteration 748
delta log-likelihood: 0.0000001526
log-like: -118.337547
Iteration 749
delta log-likelihood: 0.0000001516
log-like: -118.337547


```
Iteration 750
  delta log-likelihood: 0.0000001507
  log-like:            -118.337546
Iteration 751
  delta log-likelihood: 0.0000001497
  log-like:            -118.337545
Iteration 752
  delta log-likelihood: 0.0000001487
  log-like:            -118.337545
Iteration 753
  delta log-likelihood: 0.0000001478
  log-like:            -118.337544
Iteration 754
  delta log-likelihood: 0.0000001468
  log-like:            -118.337544
Iteration 755
  delta log-likelihood: 0.0000001459
  log-like:            -118.337543
Iteration 756
  delta log-likelihood: 0.0000001449
  log-like:            -118.337543
Iteration 757
  delta log-likelihood: 0.0000001440
  log-like:            -118.337542
Iteration 758
  delta log-likelihood: 0.0000001431
  log-like:            -118.337542
Iteration 759
  delta log-likelihood: 0.0000001422
  log-like:            -118.337541
Iteration 760
  delta log-likelihood: 0.0000001413
  log-like:            -118.337541
Iteration 761
  delta log-likelihood: 0.0000001404
  log-like:            -118.337540
Iteration 762
  delta log-likelihood: 0.0000001395
  log-like:            -118.337540
Iteration 763
  delta log-likelihood: 0.0000001386
  log-like:            -118.337539
Iteration 764
  delta log-likelihood: 0.0000001377
  log-like:            -118.337539
Iteration 765
  delta log-likelihood: 0.0000001368
  log-like:            -118.337538
```

Iteration 766
delta log-likelihood: 0.0000001359
log-like: -118.337538
Iteration 767
delta log-likelihood: 0.0000001351
log-like: -118.337537
Iteration 768
delta log-likelihood: 0.0000001342
log-like: -118.337536
Iteration 769
delta log-likelihood: 0.0000001334
log-like: -118.337536
Iteration 770
delta log-likelihood: 0.0000001325
log-like: -118.337536
Iteration 771
delta log-likelihood: 0.0000001317
log-like: -118.337535
Iteration 772
delta log-likelihood: 0.0000001308
log-like: -118.337535
Iteration 773
delta log-likelihood: 0.0000001300
log-like: -118.337534
Iteration 774
delta log-likelihood: 0.0000001292
log-like: -118.337534
Iteration 775
delta log-likelihood: 0.0000001284
log-like: -118.337533
Iteration 776
delta log-likelihood: 0.0000001276
log-like: -118.337533
Iteration 777
delta log-likelihood: 0.0000001267
log-like: -118.337532
Iteration 778
delta log-likelihood: 0.0000001259
log-like: -118.337532
Iteration 779
delta log-likelihood: 0.0000001251
log-like: -118.337531
Iteration 780
delta log-likelihood: 0.0000001244
log-like: -118.337531
Iteration 781
delta log-likelihood: 0.0000001236
log-like: -118.337530

Iteration 782
delta log-likelihood: 0.0000001228
log-like: -118.337530
Iteration 783
delta log-likelihood: 0.0000001220
log-like: -118.337529
Iteration 784
delta log-likelihood: 0.0000001212
log-like: -118.337529
Iteration 785
delta log-likelihood: 0.0000001205
log-like: -118.337528
Iteration 786
delta log-likelihood: 0.0000001197
log-like: -118.337528
Iteration 787
delta log-likelihood: 0.0000001190
log-like: -118.337528
Iteration 788
delta log-likelihood: 0.0000001182
log-like: -118.337527
Iteration 789
delta log-likelihood: 0.0000001175
log-like: -118.337527
Iteration 790
delta log-likelihood: 0.0000001167
log-like: -118.337526
Iteration 791
delta log-likelihood: 0.0000001160
log-like: -118.337526
Iteration 792
delta log-likelihood: 0.0000001153
log-like: -118.337525
Iteration 793
delta log-likelihood: 0.0000001146
log-like: -118.337525
Iteration 794
delta log-likelihood: 0.0000001138
log-like: -118.337525
Iteration 795
delta log-likelihood: 0.0000001131
log-like: -118.337524
Iteration 796
delta log-likelihood: 0.0000001124
log-like: -118.337524
Iteration 797
delta log-likelihood: 0.0000001117
log-like: -118.337523

Iteration 798
delta log-likelihood: 0.0000001110
log-like: -118.337523
Iteration 799
delta log-likelihood: 0.0000001103
log-like: -118.337522
Iteration 800
delta log-likelihood: 0.0000001096
log-like: -118.337522
Iteration 801
delta log-likelihood: 0.0000001090
log-like: -118.337522
Iteration 802
delta log-likelihood: 0.0000001083
log-like: -118.337521
Iteration 803
delta log-likelihood: 0.0000001076
log-like: -118.337521
Iteration 804
delta log-likelihood: 0.0000001069
log-like: -118.337520
Iteration 805
delta log-likelihood: 0.0000001063
log-like: -118.337520
Iteration 806
delta log-likelihood: 0.0000001056
log-like: -118.337520
Iteration 807
delta log-likelihood: 0.0000001049
log-like: -118.337519
Iteration 808
delta log-likelihood: 0.0000001043
log-like: -118.337519
Iteration 809
delta log-likelihood: 0.0000001036
log-like: -118.337518
Iteration 810
delta log-likelihood: 0.0000001030
log-like: -118.337518
Iteration 811
delta log-likelihood: 0.0000001024
log-like: -118.337518
Iteration 812
delta log-likelihood: 0.0000001017
log-like: -118.337517
Iteration 813
delta log-likelihood: 0.0000001011
log-like: -118.337517

```

Iteration 814
  delta log-likelihood: 0.0000001005
  log-like:           -118.337517
Iteration 815
  delta log-likelihood: 0.0000000999
  log-like:           -118.337516
Turnbull estimator fitted successfully
Timeline range: 0.0 - 24.4
Number of intervals: 27

```

[13]: *### Step 4.2: Model Comparison*

```

# Compare AFT vs Turnbull using median BMI as representative
median_bmi = df_intervals['bmi'].median()
comparison_results = compare_aft_vs_turnbull(
    primary_model,
    turnbull_model,
    time_grid,
    median_bmi,
    df_intervals,
    verbose=True
)

```

Comparing AFT model vs Turnbull non-parametric estimator...
 Restricting comparison to clinically meaningful range: 12.0 - 24.7 weeks
 Using 84 time points (avoids unreliable early extrapolation)
 Model comparison completed

Population-Level Survival Curve Comparison:
 Turnbull: Non-parametric estimate using all 238 observations
 AFT: Parametric prediction averaged across all observations

Comparison Metrics:
 Mean Absolute Error: 0.0141
 Root Mean Square Error: 0.0186
 Maximum Absolute Error: 0.0559
 KS Statistic: 0.0559
 Excellent agreement (MAE < 0.05)

Survival Probabilities at Key Weeks:

Week	Turnbull	AFT	Difference

12	0.195	0.184	0.011
14	0.108	0.139	0.031
16	0.108	0.100	0.008
18	0.066	0.074	0.007
20	0.049	0.054	0.005

```
[14]: ### Step 4.3: Goodness of Fit Assessment

# Assess overall AFT model adequacy using module function
fit_assessment = assess_aft_goodness_of_fit(comparison_results, verbose=True)
```

AFT Model Goodness of Fit Assessment:

=====

Fit Quality Metrics:

MAE: 0.0141 (threshold: < 0.1)
 RMSE: 0.0186 (threshold: < 0.15)
 KS: 0.0559 (threshold: < 0.2)

Criteria Assessment:

MAE: PASS
 RMSE: PASS
 KS: PASS

Overall Assessment:

Criteria met: 3/3

Overall fit quality: Good

Recommendation: AFT model provides adequate fit to data
 The parametric AFT assumptions appear reasonable.

Validation Summary:

- Turnbull provides the non-parametric gold standard
- AFT model offers interpretable covariate effects
- Model agreement suggests good parametric fit

1.6 Section 5: BMI Grouping & Group-specific Optimal Weeks

Goal: Create BMI groups and calculate optimal testing weeks for each group.

1.6.1 Overview

- Calculate predicted median times for CART-based grouping
- Apply multiple BMI grouping strategies (clinical, tertile, CART)
- Evaluate grouping strategies using risk-based scoring
- Calculate group-specific optimal weeks for different confidence levels
- Generate final policy recommendations by BMI group

```
[15]: ### Step 5.1: Comprehensive Group-specific Analysis
```

```
# Perform group-specific analysis including:
# - Predicted median time calculation
# - Multiple BMI grouping strategies
# - Grouping strategy evaluation
# - Group-specific optimal weeks calculation
```

```

group_analysis_results = perform_group_specific_analysis(
    df_intervals,
    primary_model,
    confidence_levels=[0.90, 0.95],
    time_grid=time_grid,
    grouping_methods=['clinical', 'tertile', 'cart'], # Include CART if data
↳allows
    verbose=True
)

```

Performing group-specific optimal weeks analysis...
 Calculating individual predicted median survival times...
 Predicted median times calculated: 238/238 valid

Predicted Median Time Statistics:

Mean: 5.52 weeks
 Std: 0.98 weeks
 Range: 3.88 - 8.71 weeks

Evaluating 4 grouping strategies...

Evaluating grouping strategy: bmi_group_cart

Number of groups: 6
 Risk score: 11.522
 Weighted median: 5.522 weeks
 Complexity penalty: 6.000
 Between-group variance: 1.187
 Within-group variance: 0.083

Group sizes:

CART_G2: 58 (24.4%)
 CART_G5: 46 (19.3%)
 CART_G1: 38 (16.0%)
 CART_G3: 35 (14.7%)
 CART_G4: 31 (13.0%)
 CART_G6: 30 (12.6%)

Evaluating grouping strategy: bmi_group_clinical

Number of groups: 3
 Risk score: 8.522
 Weighted median: 5.522 weeks
 Complexity penalty: 3.000
 Between-group variance: 2.240
 Within-group variance: 0.227

Group sizes:

Obese I (30-35): 147 (61.8%)
 Overweight (25-30): 61 (25.6%)
 Obese II+ (35): 30 (12.6%)

Evaluating grouping strategy: bmi_group_tertile

Number of groups: 3
 Risk score: 8.522
 Weighted median: 5.522 weeks
 Complexity penalty: 3.000
 Between-group variance: 1.068
 Within-group variance: 0.240

Group sizes:
 Low BMI (T1): 80 (33.6%)
 High BMI (T3): 79 (33.2%)
 Medium BMI (T2): 79 (33.2%)

Best grouping strategy: clinical
 Risk score: 8.522

Calculating optimal weeks for 3 BMI groups...

Analyzing group: Obese I (30-35)
 90% confidence: Week 15.9
 95% confidence: Week 20.2

Analyzing group: Overweight (25-30)
 90% confidence: Week 13.3
 95% confidence: Week 16.7

Analyzing group: Obese II+ (35)
 90% confidence: Week 21.1
 95% confidence: Week Never

Group-specific analysis completed for 3 groups

```
[16]: ### Step 5.2: Generate Group-specific Optimal Weeks Summary

# Create comprehensive summary table for group-specific recommendations
group_summary_table = □
↪create_group_optimal_weeks_summary(group_analysis_results, verbose=True)
```

Group-Specific Optimal Testing Weeks Summary:

```
=====
      BMI_Group  n_mothers  representative_BMI  BMI_range  optimal_week_90
optimal_week_95
      Obese I (30-35)      147      32.017138  30.0-34.9      15.9
20.2
Overweight (25-30)      61      29.136316  26.6-30.0      13.3
16.7
      Obese II+ ( 35)      30      36.326687  35.1-39.2      21.1
Never
```


Summary Statistics:
Total mothers: 238
Number of BMI groups: 3
Grouping method: clinical

1.7 Section 6: Monte Carlo Measurement Error Testing

Goal: Assess robustness to Y-chromosome concentration measurement errors.

1.7.1 Overview

- Model measurement error as Gaussian noise: $y_{\text{observed}} = y_{\text{true}} + \epsilon$, $\epsilon \sim N(0, \sigma^2)$
- Run Monte Carlo simulations with noisy measurements
- Refit AFT models and recalculate group-specific optimal weeks
- Assess stability and provide uncertainty quantification
- Generate robustness summary with confidence intervals

```
[17]: ### Step 6.1: Monte Carlo Robustness Testing

# Run Monte Carlo simulation to assess robustness to measurement errors
# Use smaller sample size for demonstration (increase for production)
print(" Starting Monte Carlo robustness testing...")
print(" Note: Using reduced simulation count for demonstration")

mc_results = run_monte_carlo_robustness_test(
    df_tests, # Original test data
    construct_intervals, # Function to construct intervals
    fit_aft_models, # Function to fit AFT models
    perform_group_specific_analysis, # Function for group analysis
    n_simulations=300, # Production setting for smooth CI and stable assessment
    sigma_error=0.002, # 0.2% absolute concentration error
    confidence_levels=[0.90, 0.95],
    random_seed=42,
    n_workers=1, # Single-threaded for stability
    verbose=True
)
```

```
Starting Monte Carlo robustness testing..
Note: Using reduced simulation count for demonstration
Running Monte Carlo robustness test...
Simulations: 300
Measurement error : 0.0020 (0.20%)
Confidence levels: ['90%', '95%']
Running simulations (single-threaded)...
Progress: 30/300 (10.0%)
Progress: 60/300 (20.0%)
Progress: 90/300 (30.0%)
Progress: 120/300 (40.0%)
Progress: 150/300 (50.0%)
```

Progress: 180/300 (60.0%)
Progress: 210/300 (70.0%)
Progress: 240/300 (80.0%)
Progress: 270/300 (90.0%)
Progress: 300/300 (100.0%)
Analyzing Monte Carlo results...
Monte Carlo Analysis:
Successful iterations: 300/300 (100.0%)

Group: Obese I (30-35)

90% confidence:

Mean: 15.90 \pm 0.38 weeks

Median: 15.91 weeks

95% CI: [15.15, 16.52]

CV: 0.024

95% confidence:

Mean: 20.03 \pm 0.56 weeks

Median: 20.00 weeks

95% CI: [19.09, 21.21]

CV: 0.028

Group: Overweight (25-30)

90% confidence:

Mean: 13.55 \pm 0.67 weeks

Median: 13.48 weeks

95% CI: [12.12, 14.85]

CV: 0.049

95% confidence:

Mean: 17.05 \pm 0.78 weeks

Median: 16.97 weeks

95% CI: [15.45, 18.64]

CV: 0.046

Group: Obese II+ (35)

90% confidence:

Mean: 20.27 \pm 1.08 weeks

Median: 20.15 weeks

95% CI: [18.33, 22.42]

CV: 0.053

95% confidence:

Mean: 24.06 \pm 0.80 weeks

Median: 24.24 weeks

95% CI: [22.18, 25.00]

CV: 0.033

Group: High BMI (T3)

90% confidence:

Mean: 18.24 \pm 0.56 weeks

Median: 18.33 weeks
95% CI: [16.89, 19.24]
CV: 0.031
95% confidence:
Mean: 23.03 \pm 0.92 weeks
Median: 23.18 weeks
95% CI: [20.98, 24.48]
CV: 0.040

Group: Medium BMI (T2)

90% confidence:
Mean: 15.62 \pm 0.39 weeks
Median: 15.61 weeks
95% CI: [14.92, 16.36]
CV: 0.025
95% confidence:
Mean: 19.75 \pm 0.59 weeks
Median: 19.70 weeks
95% CI: [18.71, 20.91]
CV: 0.030

Group: Low BMI (T1)

90% confidence:
Mean: 13.78 \pm 0.60 weeks
Median: 13.79 weeks
95% CI: [12.58, 14.70]
CV: 0.044
95% confidence:
Mean: 17.40 \pm 0.73 weeks
Median: 17.42 weeks
95% CI: [15.91, 18.56]
CV: 0.042

Robustness Assessment:

Obese I (30-35) (90%): Good stability
CV: 0.024 (Excellent)
95% CI width: 1.37 weeks (Good)
Obese I (30-35) (95%): Good stability
CV: 0.028 (Excellent)
95% CI width: 2.12 weeks (Moderate)
Overweight (25-30) (90%): Good stability
CV: 0.049 (Excellent)
95% CI width: 2.73 weeks (Moderate)
Overweight (25-30) (95%): Good stability
CV: 0.046 (Excellent)
95% CI width: 3.18 weeks (Moderate)
Obese II+ (35) (90%): Poor stability
CV: 0.053 (Good)

95% CI width: 4.09 weeks (Poor)
 Obese II+ (35) (95%): Good stability
 CV: 0.033 (Excellent)
 95% CI width: 2.82 weeks (Moderate)
 High BMI (T3) (90%): Good stability
 CV: 0.031 (Excellent)
 95% CI width: 2.35 weeks (Moderate)
 High BMI (T3) (95%): Good stability
 CV: 0.040 (Excellent)
 95% CI width: 3.50 weeks (Moderate)
 Medium BMI (T2) (90%): Good stability
 CV: 0.025 (Excellent)
 95% CI width: 1.44 weeks (Good)
 Medium BMI (T2) (95%): Good stability
 CV: 0.030 (Excellent)
 95% CI width: 2.20 weeks (Moderate)
 Low BMI (T1) (90%): Good stability
 CV: 0.044 (Excellent)
 95% CI width: 2.12 weeks (Moderate)
 Low BMI (T1) (95%): Good stability
 CV: 0.042 (Excellent)
 95% CI width: 2.66 weeks (Moderate)

Overall Stability: Good
 Good: 11
 Moderate: 0
 Poor: 1

[18]: *### Step 6.2: Robustness Summary & Uncertainty Quantification*

```
# Generate comprehensive robustness summary table
mc_summary_table = create_monte_carlo_summary_table(mc_results, verbose=True)
```

Monte Carlo Robustness Summary:

```
=====
      BMI_Group optimal_week_90_mean optimal_week_90_std optimal_week_90_ci
stability_90 optimal_week_95_mean optimal_week_95_std optimal_week_95_ci
stability_95
      Obese I (30-35)          15.90          ±0.38      [15.15, 16.52]
Good      20.03          ±0.56      [19.09, 21.21]      Good
Overweight (25-30)          13.55          ±0.67      [12.12, 14.85]
Good      17.05          ±0.78      [15.45, 18.64]      Good
      Obese II+ (35)          20.27          ±1.08      [18.33, 22.42]
Poor      24.06          ±0.80      [22.18, 25.00]      Good
      High BMI (T3)          18.24          ±0.56      [16.89, 19.24]
Good      23.03          ±0.92      [20.98, 24.48]      Good
      Medium BMI (T2)          15.62          ±0.39      [14.92, 16.36]
Good      19.75          ±0.59      [18.71, 20.91]      Good
```

	Low BMI (T1)	13.78	± 0.60	[12.58, 14.70]
Good	17.40	± 0.73	[15.91, 18.56]	Good

Monte Carlo Test Summary:

Measurement error : 0.0020 (0.20%)

Simulations: 300

Success rate: 100.0%

Overall stability: Good

1.8 Section 7: Baseline Two-step ML Comparison (Optional)

Goal: Compare AFT survival approach against traditional machine learning methods.

1.8.1 Overview

- **Classification Component:** Binary outcome (ever reached 4% threshold)
- **Regression Component:** Time to threshold (interval midpoint approximation)
- **Feature Engineering:** BMI + derived features (squared, log-transformed)
- **Model Comparison:** Logistic Regression, Random Forest for both components
- **Group Mapping:** Map ML predictions to group-level recommendations
- **Benchmarking:** Compare AFT vs ML optimal weeks side-by-side

```
[19]: ### Step 7.1: Complete ML Baseline Comparison Pipeline

# Run comprehensive ML baseline comparison including:
# - Binary classification (ever reached threshold)
# - Time-to-event regression (interval midpoint approximation)
# - Group-level recommendation mapping
# - Side-by-side comparison with AFT results

print(" Running ML baseline comparison against AFT survival analysis...")

ml_comparison_results = run_ml_baseline_comparison(
    df_X, # Use feature matrix with standardized BMI (bmi_z)
    group_analysis_results, # AFT group-specific results from Section 5
    confidence_levels=[0.90, 0.95],
    cv_folds=5,
    random_state=42,
    verbose=True
)
```

Running ML baseline comparison against AFT survival analysis...

Running ML baseline comparison pipeline...

Preparing dataset for ML baseline comparison...

ML dataset prepared:

Samples: 238

Features: 4 (bmi, bmi_z, bmi_squared, bmi_log)

Ever reached threshold: 0.945

Mean time approximation: 8.66 weeks
Training classification models for binary outcome...

Training Logistic Regression...

AUC (CV): 0.657 \pm 0.207

AUC (full): 0.677

Brier score: 0.051

Training Random Forest...

AUC (CV): 0.565 \pm 0.229

AUC (full): 0.998

Brier score: 0.015

Best classification model: Logistic Regression

Cross-validation AUC: 0.657

Training regression models for time to threshold...

Training Random Forest...

MAE (CV): 3.499 \pm 0.280 weeks

RMSE (CV): 5.323 \pm 0.470 weeks

MAE (full): 1.575 weeks

R²: 0.677

Best regression model: Random Forest

Cross-validation MAE: 3.499 weeks

Mapping ML predictions to group-level recommendations...

Group: Obese I (30-35)

n = 147, BMI = 32.1

Threshold prob: 0.945

Predicted time: 8.74 \pm 2.80

ML optimal week (90%): 6.40

ML optimal week (95%): 6.22

Group: Overweight (25-30)

n = 61, BMI = 29.0

Threshold prob: 0.973

Predicted time: 7.53 \pm 1.93

ML optimal week (90%): 6.18

ML optimal week (95%): 6.00

Group: Obese II+ (35)

n = 30, BMI = 36.7

Threshold prob: 0.889

Predicted time: 10.46 \pm 3.27

ML optimal week (90%): 7.05

ML optimal week (95%): 6.82

Comparing AFT vs ML baseline recommendations...

Comparing 3 common BMI groups...

AFT vs ML Comparison:

=====						
BMI_Group		n_mothers_AFT	n_mothers_ML	bmi_mean_AFT	bmi_mean_ML	
AFT_week_90	ML_week_90	diff_90	AFT_week_95	ML_week_95	diff_95	
Overweight (25-30)		61	61	29.136316	28.991183	
13.33	6.18	+7.15	16.67	6.00	+10.66	
Obese I (30-35)		147	147	32.017138	32.087644	
15.91	6.40	+9.51	20.15	6.22	+13.93	
Obese II+ (35)		30	30	36.326687	36.730942	
21.06	7.05	+14.01	Never	6.82	N/A	

Comparison Summary:

90% confidence level:

Mean difference (AFT - ML): +10.22 ± 2.85 weeks

Agreement: Poor

95% confidence level:

Mean difference (AFT - ML): +12.29 ± 1.63 weeks

Agreement: Poor

ML baseline comparison completed

1.9 Section 8: Validation & Final Policy Table

Goal: Generate final recommendations with comprehensive validation and uncertainty quantification.

1.9.1 Overview

- **Cross-validation:** K-fold validation for model robustness assessment
- **Sensitivity Analysis:** Test different confidence levels and model assumptions
- **Final Policy Table:** Comprehensive recommendations with uncertainty bounds
- **Results Export:** Save final policy table for clinical implementation
- **Quality Assurance:** Complete validation summary with confidence metrics

```
[20]: ### Step 8.1: Comprehensive Validation & Final Policy Generation

# Run complete validation pipeline including:
# - K-fold cross-validation for model robustness
# - Sensitivity analysis across confidence levels
# - Final policy table with uncertainty quantification
# - Automatic export to CSV for clinical use

print(" Running comprehensive validation and final policy generation...")

final_validation_results = run_comprehensive_validation(
    df_intervals, # Interval-censored dataset
    group_analysis_results, # AFT group-specific results
```

```

    construct_intervals, # Function to construct intervals
    fit_aft_models, # Function to fit AFT models
    perform_group_specific_analysis, # Function for group analysis
    mc_results=mc_results, # Monte Carlo robustness results
    k_folds=5, # Cross-validation folds
    confidence_levels=[0.90, 0.95],
    export_results=True, # Export to CSV
    output_path=None, # Use default path
    verbose=True
)

```

Running comprehensive validation and final policy generation...

Running comprehensive validation and final policy generation...

Performing 5-fold cross-validation of AFT pipeline...

Fold 1/5

Train: 190 intervals from 190 mothers

Test: 48 intervals from 48 mothers

Fold completed: 48 test predictions

Fold 2/5

Train: 190 intervals from 190 mothers

Test: 48 intervals from 48 mothers

Fold completed: 48 test predictions

Fold 3/5

Train: 190 intervals from 190 mothers

Test: 48 intervals from 48 mothers

Fold completed: 48 test predictions

Fold 4/5

Train: 191 intervals from 191 mothers

Test: 47 intervals from 47 mothers

Fold completed: 47 test predictions

Fold 5/5

Train: 191 intervals from 191 mothers

Test: 47 intervals from 47 mothers

Fold completed: 47 test predictions

Cross-validation Summary:

Successful folds: 5/5

Performing sensitivity analysis...

Testing different confidence levels...

Variant 1: ['85%', '90%', '95%']

Success

Variant 2: ['90%', '95%']

Success
 Variant 3: ['80%', '90%', '95%']
 Success

Testing AFT model robustness...
 Weibull: AIC = 253.54
 LogLogistic: AIC = 254.20

Sensitivity analysis completed
 Creating final policy recommendation table...
 Final Policy Recommendation Table:

```
=====
```

BMI_Range	n_mothers	representative_BMI	bmi_range	optimal_week_90
threshold_prob_at_optimal_90	optimal_week_95	threshold_prob_at_optimal_95	mc_ci_90	mc_ci_95
cv_success_rate				
Obese I (30-35)	147	32.017138	30.0-34.9	15.9
0.900	20.2	0.951	[15.1, 16.5]	[19.1, 21.2]
1.00				
Overweight (25-30)	61	29.136316	26.6-30.0	13.3
0.903	16.7	0.950	[12.1, 14.8]	[15.5, 18.6]
1.00				
Obese II+ (35)	30	36.326687	35.1-39.2	21.1
0.901	Never	N/A	[18.3, 22.4]	[22.2, 25.0]
1.00				

Policy Summary:
 Analysis method: clinical
 Total mothers: 238
 BMI groups: 3
 Confidence levels: ['90%', '95%']
 Monte Carlo stability: Good
 Cross-validation success rate: 1.00
 Final policy table exported to:
 /home/richard/projects/cumcm/output/results/prob2_policy_recommendations.csv
 File size: 0.5 KB

Comprehensive validation completed
 Cross-validation success: 1.00
 Final policy groups: 3
 Results exported to:
 /home/richard/projects/cumcm/output/results/prob2_policy_recommendations.csv