Cancer Prediction

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```
# 加载包
library(tidyverse)
```

```
Warning: package 'forcats' was built under R version 4.4.3
```

```
── Attaching core tidyverse packages ──────────────────────── tidyverse 2.0.0 ──
✓ dplyr     1.1.4     ✓ readr     2.1.5
✓ forcats   1.0.1     ✓ stringr   1.5.1
✓ ggplot2   3.5.1     ✓ tibble    3.2.1
✓ lubridate 1.9.3     ✓ tidyr     1.3.1
✓ purrr     1.0.2
── Conflicts ────────────────────────────────────────── tidyverse_conflicts() ──
✖ dplyr::filter() masks stats::filter()
✖ dplyr::lag()    masks stats::lag()
ℹ Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become
errors
```

```
library(caret)        # 用于模型训练和交叉验证
```

```
Warning: package 'caret' was built under R version 4.4.3
```

```
Loading required package: lattice
```

```
Attaching package: 'caret'
```

```
The following object is masked from 'package:purrr':

    lift
```

```
library(e1071)        # 用于SVM和Naive Bayes
```

```
Warning: package 'e1071' was built under R version 4.4.3
```

```
library(pROC)         # 用于ROC曲线和AUC
```

```
Warning: package 'pROC' was built under R version 4.4.3
```

```
Type 'citation("pROC")' for a citation.
```

```
Attaching package: 'pROC'
```

```
The following objects are masked from 'package:stats':
```

```
    cov, smooth, var
```

```
library(doParallel)   # 用于并行处理（可选，加速CV）
```

```
Warning: package 'doParallel' was built under R version 4.4.3
```

```
Loading required package: foreach
```

```
Warning: package 'foreach' was built under R version 4.4.3
```

```

Attaching package: 'foreach'
```

```
The following objects are masked from 'package:purrr':

    accumulate, when
```

```
Loading required package: iterators
```

```
Warning: package 'iterators' was built under R version 4.4.3
```

```
Loading required package: parallel
```

```
library(RColorBrewer) # 用于自定义颜色
# 加载集成模型包
library(xgboost)
```

```
Warning: package 'xgboost' was built under R version 4.4.3
```

```
library(lightgbm)
```

```
Warning: package 'lightgbm' was built under R version 4.4.3
```

```
library(reticulate)
```

```
Warning: package 'reticulate' was built under R version 4.4.3
```

```
# loaing
df <- read.csv("C:/Users/ouyan/OneDrive/文档/BIOSTAT625/The_Cancer_data_1500_V2.csv")
summary(df)
```

```
      Age            Gender            BMI           Smoking      
 Min.   :20.00   Min.   :0.0000   Min.   :15.00   Min.   :0.0000  
 1st Qu.:35.00   1st Qu.:0.0000   1st Qu.:21.48   1st Qu.:0.0000  
 Median :51.00   Median :0.0000   Median :27.60   Median :0.0000  
 Mean   :50.32   Mean   :0.4907   Mean   :27.51   Mean   :0.2693  
 3rd Qu.:66.00   3rd Qu.:1.0000   3rd Qu.:33.85   3rd Qu.:1.0000  
```

```
 Max.   :80.00   Max.   :1.0000   Max.   :39.96   Max.   :1.0000
  GeneticRisk     PhysicalActivity  AlcoholIntake      CancerHistory
 Min.   :0.0000   Min.   :0.00241   Min.   :0.001215   Min.   :0.000
 1st Qu.:0.0000   1st Qu.:2.43461   1st Qu.:1.210598   1st Qu.:0.000
 Median :0.0000   Median :4.83432   Median :2.382971   Median :0.000
 Mean   :0.5087   Mean   :4.89793   Mean   :2.417987   Mean   :0.144
 3rd Qu.:1.0000   3rd Qu.:7.40990   3rd Qu.:3.585624   3rd Qu.:0.000
 Max.   :2.0000   Max.   :9.99461   Max.   :4.987115   Max.   :1.000
   Diagnosis
 Min.   :0.0000
 1st Qu.:0.0000
 Median :0.0000
 Mean   :0.3713
 3rd Qu.:1.0000
 Max.   :1.0000
```

```r
print(head(df))
```

```
  Age Gender      BMI Smoking GeneticRisk PhysicalActivity AlcoholIntake
1  58      1 16.08531       0           1         8.146251      4.148219
2  71      0 30.82878       0           1         9.361630      3.519683
3  48      1 38.78508       0           2         5.135179      4.728368
4  34      0 30.04030       0           0         9.502792      2.044636
5  62      1 35.47972       0           0         5.356890      3.309849
6  27      0 37.10516       0           1         3.941905      2.324274
  CancerHistory Diagnosis
1             1         1
2             0         0
3             0         1
4             0         0
5             0         1
6             0         0
```

```r
colSums(is.na(df))
```

```
            Age           Gender              BMI          Smoking
              0                0                0                0
    GeneticRisk PhysicalActivity    AlcoholIntake    CancerHistory
              0                0                0                0
      Diagnosis
              0
```

```r
library(tidyverse)
df <- df %>%
  mutate(
    Gender = factor(as.character(Gender),
                    levels = c("0", "1"),
                    labels = c("Male","Female")),
```

```
    Smoking = factor(as.character(Smoking),
                     levels = c("0", "1"),
                     labels = c("No","Yes")),

    CancerHistory = factor(as.character(CancerHistory),
                           levels = c("0", "1"),
                           labels = c("No","Yes")),

    GeneticRisk = factor(as.character(GeneticRisk),
                         levels = c("0","1","2"),
                         labels = c("Low","Medium","High")),

    Diagnosis = factor(as.character(Diagnosis),
                       levels = c("0","1"),
                       labels = c("NoCancer","Cancer"))
  )

print(head(df))
```

```
  Age Gender      BMI Smoking GeneticRisk PhysicalActivity AlcoholIntake
1  58 Female 16.08531      No      Medium         8.146251      4.148219
2  71   Male 30.82878      No      Medium         9.361630      3.519683
3  48 Female 38.78508      No        High         5.135179      4.728368
4  34   Male 30.04030      No         Low         9.502792      2.044636
5  62 Female 35.47972      No         Low         5.356890      3.309849
6  27   Male 37.10516      No      Medium         3.941905      2.324274
  CancerHistory Diagnosis
1           Yes    Cancer
2            No  NoCancer
3            No    Cancer
4            No  NoCancer
5            No    Cancer
6            No  NoCancer
```

```
continuous_vars <- c("Age","BMI","PhysicalActivity","AlcoholIntake")
binary_vars <- c("Gender","Smoking","CancerHistory")
categorical_vars <- c("GeneticRisk")
target_var <- "Diagnosis"
```

```
# 定义用于划分和缩放的变量（确保这些变量已在你前面的代码中定义）
# continuous_vars <- c("Age","BMI","PhysicalActivity","AlcoholIntake")
# target_var <- "Diagnosis" # 假设这是你的目标变量

# 从你已经进行了因子转换的原始 df 开始
df_for_modeling <- df # 假设 'df' 是完成了因子转换后的数据框

# --- 1. 分割 X 和 y ---
X <- df_for_modeling %>% select(-all_of(target_var))
y <- df_for_modeling[[target_var]]
```

```r
# --- 2. 划分训练集和测试集 (80/20 stratified split) ---
set.seed(42)
# 使用目标变量 y 进行分层抽样
train_index <- createDataPartition(y, p = 0.8, list = FALSE)

X_train <- X[train_index, ]
X_test <- X[-train_index, ]
y_train <- y[train_index]
y_test <- y[-train_index]


# --- 3. 标准化 (仅在训练集上学习参数) ---
# 构建预处理步骤：仅对训练集的连续特征进行标准化 (fit)
preprocessor <- preProcess(X_train[, continuous_vars], method = c("center", "scale"))

# 应用预处理：将训练集和测试集进行转换 (transform)
X_train_processed <- predict(preprocessor, X_train)
X_test_processed <- predict(preprocessor, X_test)


# --- 4. 创建最终的训练/测试数据集 (合并 X 和 y) ---
# 注意：X_train_processed 已经包含了所有因子变量
train_data <- cbind(Diagnosis = y_train, X_train_processed)
test_data <- cbind(Diagnosis = y_test, X_test_processed)

# 最终检查：确保目标变量是两级因子（前面已完成，但这一步保证了数据完整性）
train_data$Diagnosis <- factor(train_data$Diagnosis, levels = c("NoCancer", "Cancer"))
test_data$Diagnosis <- factor(test_data$Diagnosis, levels = c("NoCancer", "Cancer"))

# 现在 train_data 和 test_data 已经准备好用于模型训练
cat("数据划分和标准化已完成，准备进入模型训练阶段。\n")
```

```
数据划分和标准化已完成，准备进入模型训练阶段。
```

```r
# 1. 定义交叉验证参数 (5-Fold Stratified CV)
control <- trainControl(
  method = "cv",
  number = 5,
  classProbs = TRUE,       # Accuracy 不依赖概率，可保留
  summaryFunction = defaultSummary,  # 改为默认 summary，这样会输出 Accuracy
  savePredictions = "final",
  verboseIter = FALSE
)


# 2. 定义模型列表（使用caret支持的模型名称）
# 映射：Python名称 -> R caret 名称
# Logistic Regression -> glm (广义线性模型)
# Decision Tree -> rpart
```

```r
# Random Forest -> rf
# Gradient Boosting -> gbm
# SVM -> svmRadial (径向核SVM)
# k-NN -> knn
# Naive Bayes -> nb
# LightGBM -> gbm (需要特殊设置或使用专用包)
# CatBoost -> catboost (需要使用专用包)

models_to_run <- c("glm", "rpart", "rf", "gbm", "svmRadial", "knn", "nb")
results_cv <- list()

# 3. 运行交叉验证
# 注册并行后端（可选）
if (requireNamespace("doParallel", quietly = TRUE)) {
  cl <- makePSOCKcluster(detectCores() - 1)
  registerDoParallel(cl)
}

# 循环训练模型
for (model_name in models_to_run) {
  cat(paste("Training model:", model_name, "...\n"))

  # Rpart (决策树) 的调参网格
  if (model_name == "rpart") {
    tune_grid <- expand.grid(cp = seq(0.01, 0.1, 0.01))
  } else {
    tune_grid <- NULL # 使用默认调参网格
  }

  # 训练模型
  model_fit <- train(
    Diagnosis ~ .,
    data = train_data,
    method = model_name,
    trControl = control,
    metric = "Accuracy", # 使用准确率作为选择指标
    tuneGrid = tune_grid
  )

  results_cv[[model_name]] <- model_fit

  # 打印结果
  print(model_fit$results[order(model_fit$results$Accuracy, decreasing = TRUE), ][1, ])
}
```

```
Training model: glm ...
  parameter  Accuracy    Kappa AccuracySD    KappaSD
1      none 0.8792531 0.738078 0.02133139 0.04664393
Training model: rpart ...
    cp  Accuracy     Kappa AccuracySD   KappaSD
```

```
1 0.01 0.8509647 0.6745558 0.02448481 0.0489391
Training model: rf ...
  mtry  Accuracy     Kappa AccuracySD    KappaSD
2    5 0.9084094 0.8015616 0.02716388 0.05779453
Training model: gbm ...
Iter   TrainDeviance   ValidDeviance   StepSize   Improve
     1        1.2682             nan     0.1000    0.0266
     2        1.2253             nan     0.1000    0.0220
     3        1.1884             nan     0.1000    0.0164
     4        1.1617             nan     0.1000    0.0135
     5        1.1385             nan     0.1000    0.0102
     6        1.1173             nan     0.1000    0.0086
     7        1.0931             nan     0.1000    0.0114
     8        1.0763             nan     0.1000    0.0059
     9        1.0533             nan     0.1000    0.0104
    10        1.0343             nan     0.1000    0.0093
    20        0.8896             nan     0.1000    0.0053
    40        0.7116             nan     0.1000    0.0024
    60        0.6084             nan     0.1000    0.0015
    80        0.5477             nan     0.1000    0.0007
   100        0.5031             nan     0.1000    0.0008

  shrinkage interaction.depth n.minobsinnode n.trees  Accuracy     Kappa
5       0.1                 2             10     100 0.9492185 0.8901224
  AccuracySD    KappaSD
5 0.01537361 0.03309005
Training model: svmRadial ...
       sigma C Accuracy     Kappa AccuracySD    KappaSD
3 0.08401214 1 0.870121 0.7180163 0.01173217 0.02381047
Training model: knn ...
  k  Accuracy     Kappa AccuracySD    KappaSD
2 7 0.8110028 0.5645195 0.01555807 0.03740757
Training model: nb ...
  usekernel fL adjust  Accuracy     Kappa AccuracySD    KappaSD
1     FALSE  0      1 0.7935201 0.5255632 0.01201641 0.02750503
```

```r
# 停止并行后端（如果已注册）
if (exists("cl")) {
  stopCluster(cl)
  registerDoSEQ()
}

# 4. 汇总和选择最佳模型
results_summary <- data.frame(
    Model = character(),
    CV_Accuracy_Mean = numeric(),
    CV_Accuracy_Std = numeric(), # 修正此处的列名
    stringsAsFactors = FALSE
)
```

```r
for (name in names(results_cv)) {
    best_tune <- results_cv[[name]]$results[order(results_cv[[name]]$results$Accuracy, decreasing
    results_summary <- results_summary %>%
        add_row(
            Model = name,
            CV_Accuracy_Mean = best_tune$Accuracy,
            CV_Accuracy_Std = best_tune$AccuracySD #关键修正：使用 AccuracySD
        )
}

# 3. 打印 CV 汇总
print("=== Cross-Validation Results ===")
```

```
[1] "=== Cross-Validation Results ==="
```

```r
print(results_summary)
```

```
      Model CV_Accuracy_Mean CV_Accuracy_Std
1       glm        0.8792531      0.02133139
2     rpart        0.8509647      0.02448481
3        rf        0.9084094      0.02716388
4       gbm        0.9492185      0.01537361
5 svmRadial        0.8701210      0.01173217
6       knn        0.8110028      0.01555807
7        nb        0.7935201      0.01201641
```

```r
# 4. 选择最佳模型（Accuracy 最大）
best_model_name <- results_summary$Model[which.max(results_summary$CV_Accuracy_Mean)]
best_model <- results_cv[[best_model_name]]
cat(paste("\nBest model:", best_model_name, "with mean CV Accuracy=",
          max(results_summary$CV_Accuracy_Mean), "\n"))
```

```
Best model: gbm with mean CV Accuracy= 0.949218533886584
```

```r
# 1. 测试集评估
test_results_list <- list()

for (model_name in names(results_cv)) {
  model_fit <- results_cv[[model_name]]

  # 预测
  y_pred <- predict(model_fit, newdata = test_data)

  # 计算混淆矩阵
  cm <- confusionMatrix(y_pred, test_data$Diagnosis, positive = "Cancer")

  # 提取指标
```

```
  acc <- cm$overall['Accuracy']
  prec <- cm$byClass['Pos Pred Value'] # Precision
  rec <- cm$byClass['Recall']         # Recall
  f1 <- cm$byClass['F1']

  test_results_list[[model_name]] <- data.frame(
    Model = model_name,
    Test_Accuracy = acc,
    Test_Precision = prec,
    Test_Recall = rec,
    Test_F1 = f1
  )

  # 打印混淆矩阵（对应Python中的 ConfusionMatrixDisplay plot）
  if (model_name == best_model_name) {
    cat(paste("\n=== Confusion Matrix -", model_name, "===\n"))
    print(cm$table)

    # 混淆矩阵可视化
    cm_df <- as.data.frame(cm$table)

    # 使用 ggplot2 绘制热图形式的混淆矩阵
    ggplot(cm_df, aes(x = Prediction, y = Reference, fill = Freq)) +
      geom_tile(color = "white") +
      scale_fill_gradient(low = "white", high = "#336699") +
      geom_text(aes(label = Freq), vjust = 1, fontface = "bold", size = 5) +
      labs(title = paste("Confusion Matrix -", model_name),
           x = "Predicted Label", y = "True Label") +
      theme_minimal() +
      theme(plot.title = element_text(face = "bold", size = 14), legend.position = "none")
  }
}
```

```
=== Confusion Matrix - gbm ===
          Reference
Prediction NoCancer Cancer
  NoCancer      185     11
  Cancer          3    100
```

```
# 2. 汇总测试结果
test_results_df <- do.call(rbind, test_results_list)

print("\n=== Test Set Results ===")
```

```
[1] "\n=== Test Set Results ==="
```

```
print(test_results_df)
```

```
             Model Test_Accuracy Test_Precision Test_Recall   Test_F1
glm            glm     0.8829431      0.8584906   0.8198198 0.8387097
rpart        rpart     0.8762542      0.8557692   0.8018018 0.8279070
rf              rf     0.9230769      0.9150943   0.8738739 0.8940092
gbm            gbm     0.9531773      0.9708738   0.9009009 0.9345794
svmRadial svmRadial     0.8829431      0.8800000   0.7927928 0.8341232
knn            knn     0.8193980      0.9130435   0.5675676 0.7000000
nb              nb     0.7892977      0.8428571   0.5315315 0.6519337
```

```r
# 3. 保存结果
#write.csv(results_summary, 'cross_validation_results_R.csv', row.names = FALSE)
#write.csv(test_results_df, 'test_set_results_R.csv', row.names = FALSE)
#cat("\nResults saved to 'cross_validation_results_R.csv' and 'test_set_results_R.csv'.\n")
```

```r
library(dplyr)

df %>%
  group_by(Diagnosis) %>%
  summarise(
    Count = n(),
    Percentage = n() / nrow(df) * 100
  ) %>%
  ungroup() %>%
  mutate(
    # 格式化百分比为两位小数
    Percentage_Formatted = paste0(round(Percentage, 2), "%")
  )
```

```
# A tibble: 2 × 4
  Diagnosis Count Percentage Percentage_Formatted
  <fct>     <int>      <dbl> <chr>
1 NoCancer    943       62.9 62.87%
2 Cancer      557       37.1 37.13%
```

```r
set.seed(42)

K <- 5
folds <- createFolds(train_data$Diagnosis, k = K, list = TRUE)

# 用来存放 OOF stacking 特征
oof_rf_prob  <- rep(NA, nrow(train_data))
oof_gbm_prob <- rep(NA, nrow(train_data))

# 5-fold stacking
for (i in 1:K) {
  cat("Processing fold", i, "\n")

  idx_valid <- folds[[i]]
  idx_train <- setdiff(seq_len(nrow(train_data)), idx_valid)
```

```
  train_fold <- train_data[idx_train, ]
  valid_fold <- train_data[idx_valid, ]

  # RF
  rf_model <- train(
    Diagnosis ~ ., data = train_fold, method = "rf",
    trControl = trainControl(method = "cv", number = 3),
    tuneLength = 5
  )

  # GBM
  gbm_model <- train(
    Diagnosis ~ ., data = train_fold, method = "gbm",
    trControl = trainControl(method = "cv", number = 3),
    verbose = FALSE
  )

  # OOF predictions
  oof_rf_prob[idx_valid]  <- predict(rf_model,  valid_fold, type = "prob")[, "Cancer"]
  oof_gbm_prob[idx_valid] <- predict(gbm_model, valid_fold, type = "prob")[, "Cancer"]
}
```

```
Processing fold 1
Processing fold 2
Processing fold 3
Processing fold 4
Processing fold 5
```

```
# 生成无泄漏 stacked 特征
stacked_train <- data.frame(
  rf_prob  = oof_rf_prob,
  gbm_prob = oof_gbm_prob,
  y = as.numeric(train_data$Diagnosis == "Cancer")
)
```

```
library(glmnet)
```

```
Warning: package 'glmnet' was built under R version 4.4.3

Loading required package: Matrix

Warning: package 'Matrix' was built under R version 4.4.3


Attaching package: 'Matrix'

The following objects are masked from 'package:tidyr':
```

```
    expand, pack, unpack
Loaded glmnet 4.1-10
```

```r
X_stack <- as.matrix(stacked_train[, c("rf_prob", "gbm_prob")])
y_stack <- stacked_train$y

stack_lr <- cv.glmnet(
  X_stack, y_stack,
  family = "binomial",
  alpha = 1,       # LASSO: prevent over fitting
  nfolds = 5
)

cat("Selected lambda:", stack_lr$lambda.min, "\n")
```

```
Selected lambda: 0.003861134
```

```r
coef(stack_lr, s = "lambda.min")
```

```
3 x 1 sparse Matrix of class "dgCMatrix"
            lambda.min
(Intercept) -5.1876271
rf_prob      0.6420093
gbm_prob    10.9185016
```

```r
rf_full <- train(
  Diagnosis ~ ., data = train_data, method = "rf",
  trControl = trainControl(method = "none"),
  tuneGrid = data.frame(mtry = floor(sqrt(ncol(train_data) - 1))),
  ntree = 500
)

gbm_full <- train(
  Diagnosis ~ ., data = train_data, method = "gbm",
  trControl = trainControl(method = "none"),
  verbose = FALSE,
  tuneGrid = data.frame(
    n.trees = 200,
    interaction.depth = 3,
    shrinkage = 0.05,
    n.minobsinnode = 10
  )
)
```

```r
rf_test_prob  <- predict(rf_full, newdata = test_data, type = "prob")[, "Cancer"]
gbm_test_prob <- predict(gbm_full, newdata = test_data, type = "prob")[, "Cancer"]

stacked_test <- as.matrix(data.frame(
```

```
  rf_prob  = rf_test_prob,
  gbm_prob = gbm_test_prob
))

final_probs <- predict(stack_lr, newx = stacked_test, s = "lambda.min", type = "response")
final_pred  <- ifelse(final_probs > 0.5, "Cancer", "NoCancer")
final_pred  <- factor(final_pred, levels = c("NoCancer","Cancer"))
```

```
# Confusion Matrix
confusionMatrix(final_pred, test_data$Diagnosis)
```

```
Confusion Matrix and Statistics

          Reference
Prediction NoCancer Cancer
  NoCancer      181     10
  Cancer          7    101

               Accuracy : 0.9431
                 95% CI : (0.9105, 0.9665)
    No Information Rate : 0.6288
    P-Value [Acc > NIR] : <2e-16

                  Kappa : 0.8775

 Mcnemar's Test P-Value : 0.6276

            Sensitivity : 0.9628
            Specificity : 0.9099
         Pos Pred Value : 0.9476
         Neg Pred Value : 0.9352
             Prevalence : 0.6288
         Detection Rate : 0.6054
   Detection Prevalence : 0.6388
      Balanced Accuracy : 0.9363

       'Positive' Class : NoCancer
```

```
train_pred <- predict(stack_lr, newx = X_stack, s = "lambda.min", type = "response")
# Convert matrix into vector
train_pred_vector <- as.numeric(train_pred[, 1])  # 提取第一列并转为 numeric 向量
final_probs_vector <- as.numeric(final_probs[, 1])

# ROC curve
roc_curve <- roc(test_data$Diagnosis, final_probs_vector)
```

```
Setting levels: control = NoCancer, case = Cancer
```

```
Setting direction: controls < cases
```

```
auc(roc_curve)
```

```
Area under the curve: 0.9492
```

```
library(MLmetrics)
```

```
Warning: package 'MLmetrics' was built under R version 4.4.3
```

```

Attaching package: 'MLmetrics'

The following objects are masked from 'package:caret':

    MAE, RMSE

The following object is masked from 'package:base':

    Recall
```

```
# 将 factor 转成 numeric (1 = Cancer, 0 = NoCancer)
y_true <- ifelse(test_data$Diagnosis == "Cancer", 1, 0)
y_pred <- ifelse(final_pred == "Cancer", 1, 0)

Precision <- Precision(y_pred, y_true)
Recall    <- Recall(y_pred, y_true)
F1        <- F1_Score(y_pred, y_true)

cat("Precision:", Precision, "\n")
```

```
Precision: 0.962766
```

```
cat("Recall:", Recall, "\n")
```

```
Recall: 0.947644
```

```
cat("F1 Score:", F1, "\n")
```

```
F1 Score: 0.9551451
```

```
# (i) Evaluate over fitting
train_pred <- predict(stack_lr, newx = X_stack, s = "lambda.min", type = "response")

auc_train <- auc(roc(train_data$Diagnosis, train_pred_vector))
```

```
Setting levels: control = NoCancer, case = Cancer
```

```
Setting direction: controls < cases
```

```
auc_test  <- auc(roc(test_data$Diagnosis, final_probs_vector))
```

```
Setting levels: control = NoCancer, case = Cancer
Setting direction: controls < cases
```

```
cat("Train AUC:", auc_train, "\n")
```

```
Train AUC: 0.961824
```

```
cat("Test  AUC:", auc_test, "\n")
```

```
Test  AUC: 0.9492045
```

```
cat("Gap =", auc_train - auc_test, "\n")
```

```
Gap = 0.01261949
```

```
# 1. 确保 Stacked Train Vector 已转换
# train_pred <- predict(stack_lr, newx = X_stack, s = "lambda.min", type = "response")
# train_pred_vector <- as.numeric(train_pred[, 1])

# 2. 获取 GLM 在测试集上的概率预测
glm_model <- results_cv[["glm"]]
glm_test_probs <- predict(glm_model, newdata = test_data, type = "prob")[, "Cancer"]

# 3. 计算 GLM 的 ROC 曲线
roc_glm <- roc(test_data$Diagnosis, glm_test_probs)
```

```
Setting levels: control = NoCancer, case = Cancer

Setting direction: controls < cases
```

```
# --- 绘图 ---
# 绘制 Stacked Train ROC (作为基础图)
plot(roc(train_data$Diagnosis, train_pred_vector),
     col = "blue",
     main = "Stacked vs. Logistic Regression ROC Comparison",
     # 设置 y 轴和 x 轴标签
     xlab = "False Positive Rate (1 - Specificity)",
     ylab = "True Positive Rate (Sensitivity)")
```

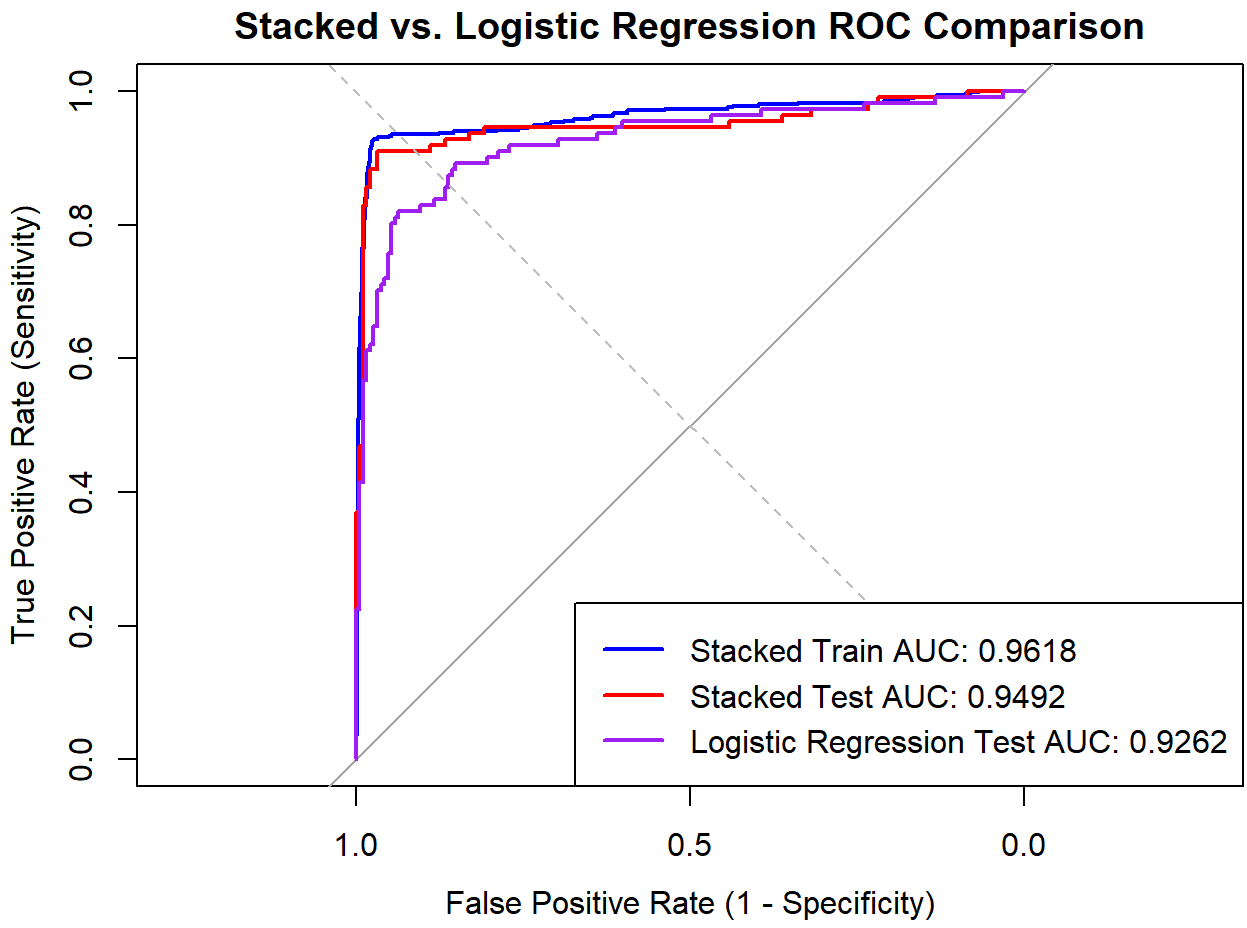
```
Setting levels: control = NoCancer, case = Cancer
Setting direction: controls < cases
```

```r
# 叠加 Stacked Test ROC
plot(roc(test_data$Diagnosis, final_probs_vector),
     col = "red",
     add = TRUE)
```

```
Setting levels: control = NoCancer, case = Cancer
Setting direction: controls < cases
```

```r
# 叠加 GLM Test ROC
plot(roc_glm,
     col = "purple",
     add = TRUE)

# 4. 添加图例和随机猜测线
abline(a = 0, b = 1, lty = 2, col = "gray") # 随机猜测线

legend("bottomright",
       legend = c(
         paste("Stacked Train AUC:", round(auc(roc(train_data$Diagnosis, train_pred_vector)), 4)),
         paste("Stacked Test AUC:", round(auc(roc(test_data$Diagnosis, final_probs_vector)), 4)),
         paste("Logistic Regression Test AUC:", round(auc(roc_glm), 4))
       ),
       col = c("blue", "red", "purple"),
       lwd = 2)
```

```
Setting levels: control = NoCancer, case = Cancer
Setting direction: controls < cases

Setting levels: control = NoCancer, case = Cancer

Setting direction: controls < cases
```




```
cat("\nLogistic Regression Test AUC:", auc(roc_glm), "\n")
```

```
Logistic Regression Test AUC: 0.9261549
```

```
# (ii) Evaluate the stratified split
prop.table(table(train_data$Diagnosis))
```

```
 NoCancer    Cancer 
0.6286428 0.3713572 
```

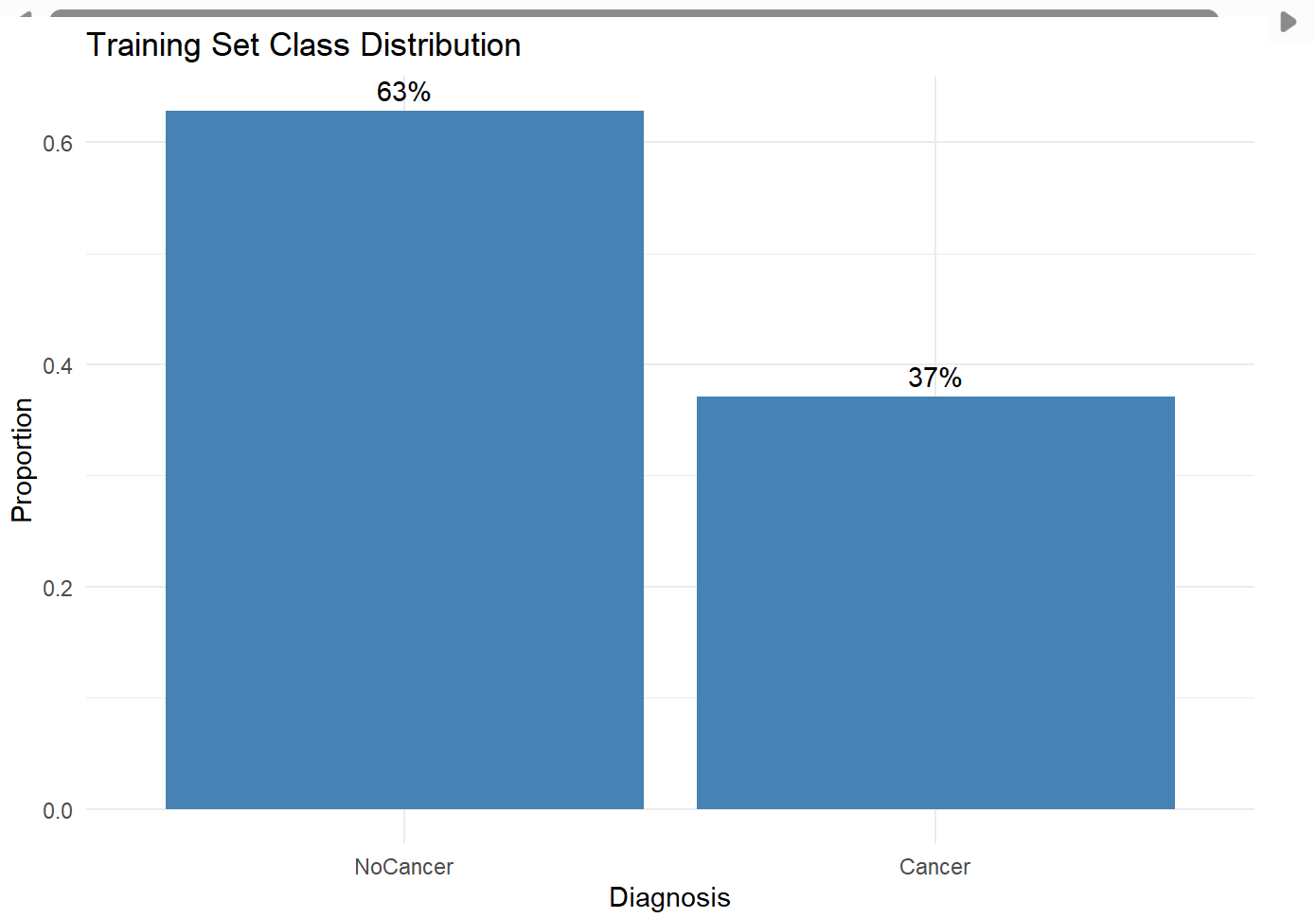
```
prop.table(table(test_data$Diagnosis))
```

```
 NoCancer    Cancer 
0.6287625 0.3712375 
```

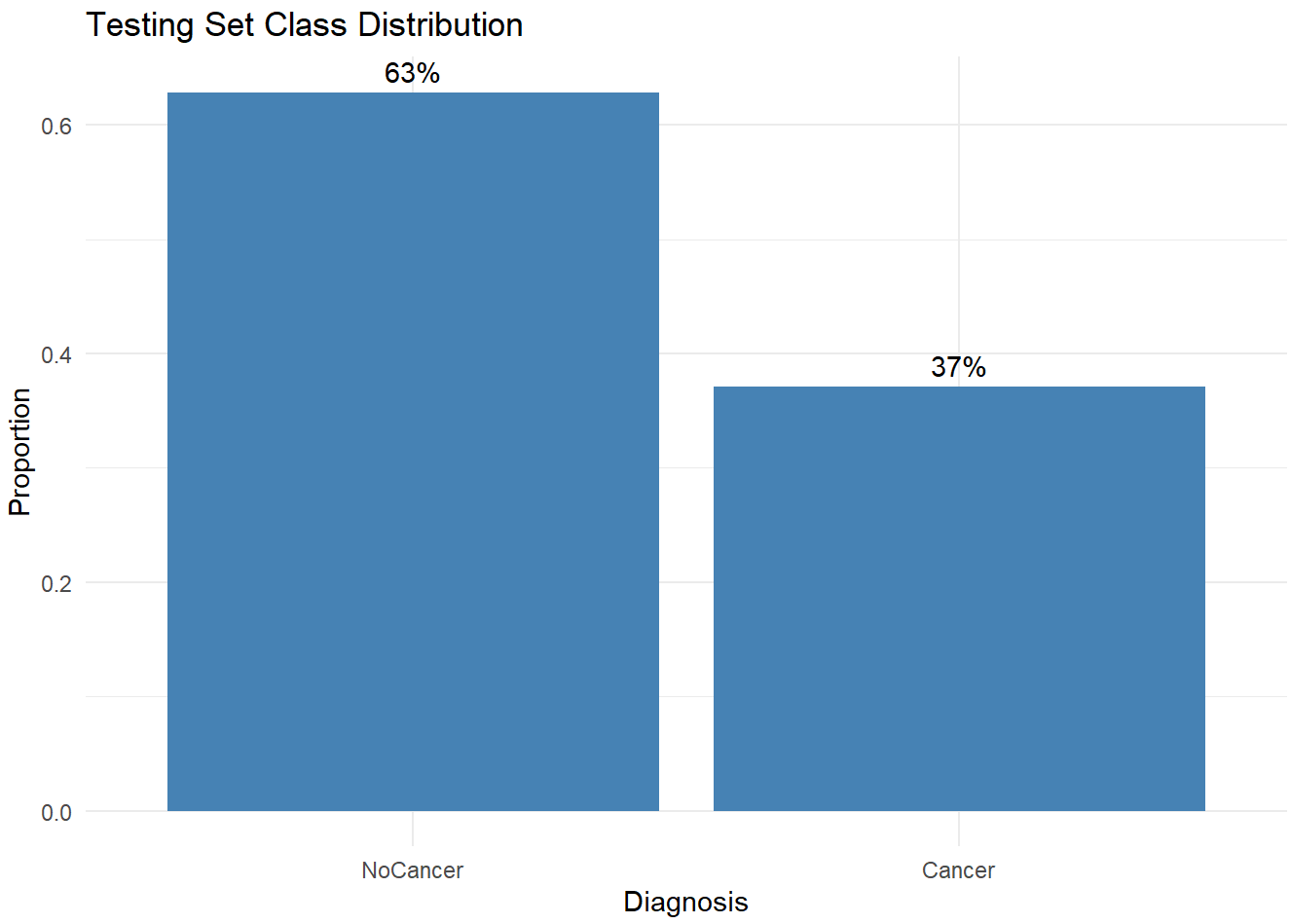
```
library(ggplot2)

ggplot(train_data, aes(x = Diagnosis)) +
  geom_bar(aes(y = (..count..)/sum(..count..)), fill = "steelblue") +
```

```
  geom_text(aes(y = (..count..)/sum(..count..), label = scales::percent((..count..)/sum(..count..
            stat = "count", vjust = -0.5) +
  ylab("Proportion") +
  ggtitle("Training Set Class Distribution") +
  theme_minimal()
```

```
Warning: The dot-dot notation (`..count..`) was deprecated in ggplot2 3.4.0.
ℹ Please use `after_stat(count)` instead.
```

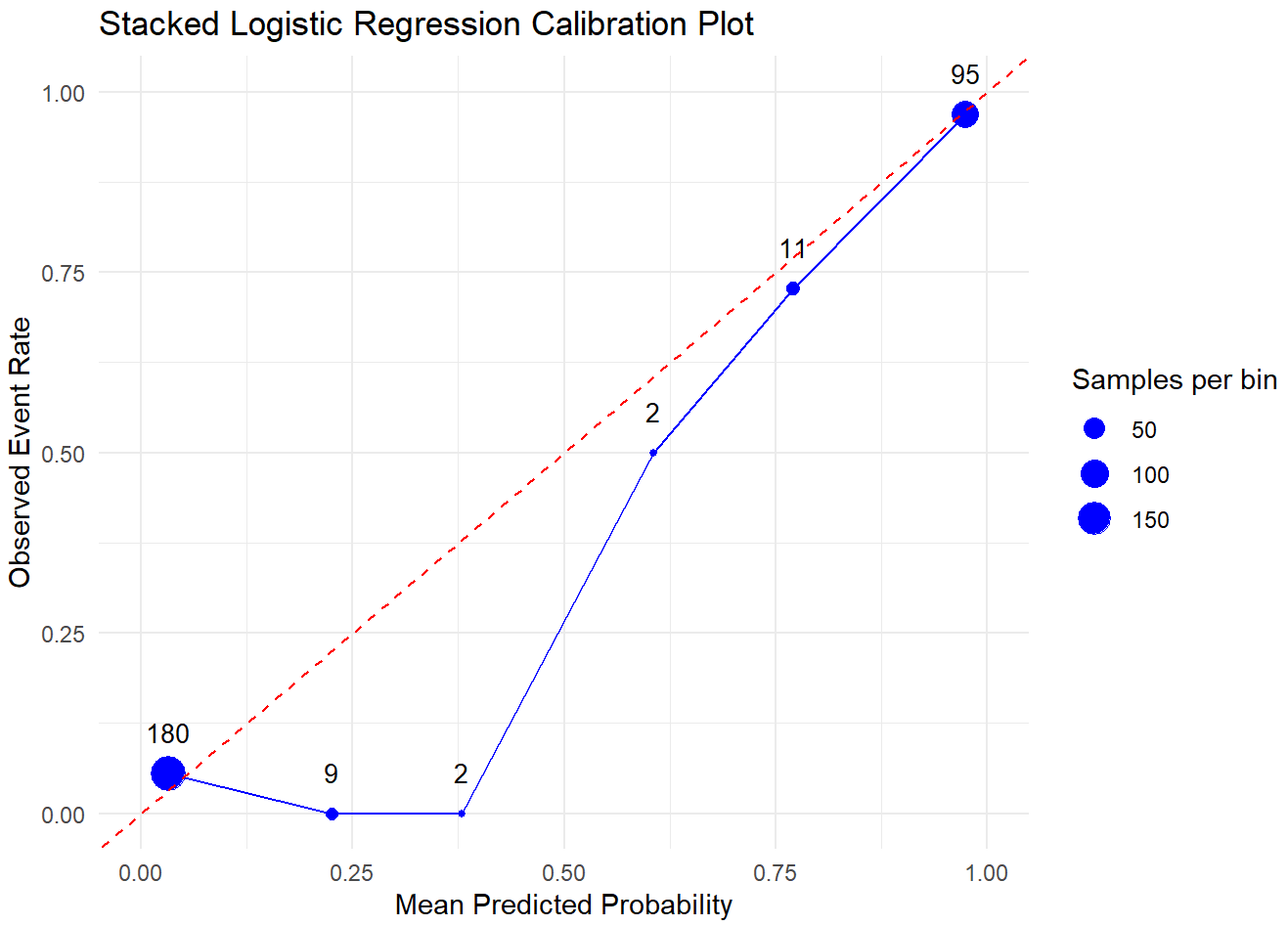



```
ggplot(test_data, aes(x = Diagnosis)) +
  geom_bar(aes(y = (..count..)/sum(..count..)), fill = "steelblue") +
  geom_text(aes(y = (..count..)/sum(..count..), label = scales::percent((..count..)/sum(..count..
            stat = "count", vjust = -0.5) +
  ylab("Proportion") +
  ggtitle("Testing Set Class Distribution") +
  theme_minimal()
```




```r
# 3. (iii) Calibration Plot
# 创建数据框
df_calib <- data.frame(
  prob = final_probs_vector,
  true = y_true
)

# 2. 将预测概率分组
n_bins <- 6
df_calib$bin <- cut(df_calib$prob, breaks = seq(0,1,length.out = n_bins+1), include.lowest = TRUE

calib_summary <- df_calib %>%
  group_by(bin) %>%
  summarise(
    mean_pred = mean(prob),
    obs_rate  = mean(true),
    n         = n()
  )

# 3. 绘制校准曲线
ggplot(calib_summary, aes(x = mean_pred, y = obs_rate)) +
  geom_point(aes(size = n), color = "blue") +             # 每个 bin 点大小按样本数
  geom_line(color = "blue") +
```

```
  # 3. 添加文本标签：显示每个点的样本量 n
  # vjust/hjust 用于微调文本位置，使其不与点重叠
  geom_text(aes(label = n), vjust = -1.5, hjust = 0.5, size = 3.5, color = "black") +
  geom_abline(slope = 1, intercept = 0, linetype = "dashed", color = "red") +
  xlim(0, 1) + ylim(0, 1) +
  xlab("Mean Predicted Probability") +
  ylab("Observed Event Rate") +
  ggtitle("Stacked Logistic Regression Calibration Plot") +
  theme_minimal() +
  scale_size_continuous(name = "Samples per bin")
```




```
# 4. Calculate Brier Score
brier_score <- mean((final_probs_vector - y_true)^2)
cat("Brier Score:", round(brier_score, 4), "\n")
```

```
Brier Score: 0.0525
```

```
# (iv) Evaluate feature importance / Explainability（模型可解释性）
# rf 特征重要性
rf_imp <- varImp(rf_full)$importance
rf_imp %>% arrange(desc(Overall))
```

```
                   Overall
CancerHistoryYes  100.00000
BMI                83.93317
AlcoholIntake      80.48403
GeneticRiskHigh    79.50337
PhysicalActivity   75.92005
Age                74.19066
GenderFemale       42.45197
SmokingYes         26.34592
GeneticRiskMedium   0.00000
```

```r
# GBM 特征重要性
gbm_imp <- summary(gbm_full$finalModel, n.trees = gbm_full$bestTune$n.trees, plotit = FALSE)
print(gbm_imp)
```

```
                              var     rel.inf
CancerHistoryYes   CancerHistoryYes 20.90859506
GeneticRiskHigh     GeneticRiskHigh 17.85936796
AlcoholIntake         AlcoholIntake 11.10167064
GenderFemale           GenderFemale 10.90965907
BMI                             BMI 10.68898422
PhysicalActivity   PhysicalActivity 10.60143407
Age                             Age 10.51628965
SmokingYes               SmokingYes  7.33820859
GeneticRiskMedium GeneticRiskMedium  0.07579074
```

```r
coef(stack_lr, s = "lambda.min")  # 查看各 base model 概率的权重
```

```
3 x 1 sparse Matrix of class "dgCMatrix"
            lambda.min
(Intercept) -5.1876271
rf_prob      0.6420093
gbm_prob    10.9185016
```

```r
library(dplyr)
library(tidyr)

rf_data <- data.frame(
  Feature = c("CancerHistoryYes", "BMI", "AlcoholIntake", "GeneticRiskHigh", "PhysicalActivity",
              "Age", "GenderFemale", "SmokingYes", "GeneticRiskMedium"),
  RF_Importance = c(100.00, 83.93, 80.48, 79.50, 75.92, 74.19, 42.45, 26.35, 0.00)
)

# --- 模拟您提供的 GBM 数据 ---
gbm_data <- data.frame(
  Feature = c("CancerHistoryYes", "GeneticRiskHigh", "AlcoholIntake", "GenderFemale", "BMI",
              "PhysicalActivity", "Age", "SmokingYes", "GeneticRiskMedium"),
  GBM_Importance = c(20.91, 17.86, 11.10, 10.91, 10.69, 10.60, 10.52, 7.34, 0.08)
)
```

```r
# --- 统一格式和合并 ---
combined_imp <- full_join(rf_data, gbm_data, by = "Feature") %>%
  # 简化/统一特征名称
  mutate(
    Feature_Clean = case_when(
      grepl("CancerHistory", Feature) ~ "Cancer History (Yes)",
      grepl("GeneticRiskHigh", Feature) ~ "Genetic Risk (High)",
      grepl("GenderFemale", Feature) ~ "Gender (Female)",
      grepl("SmokingYes", Feature) ~ "Smoking (Yes)",
      grepl("GeneticRiskMedium", Feature) ~ "Genetic Risk (Medium)",
      TRUE ~ Feature # 保留其他变量原名
    )
  ) %>%
  select(Feature_Clean, RF_Importance, GBM_Importance) %>%
  arrange(desc(RF_Importance)) # 以 RF 重要性作为主排序

# 打印最终结果
print(combined_imp)
```

```
          Feature_Clean RF_Importance GBM_Importance
1  Cancer History (Yes)        100.00          20.91
2                   BMI         83.93          10.69
3         AlcoholIntake         80.48          11.10
4   Genetic Risk (High)         79.50          17.86
5      PhysicalActivity         75.92          10.60
6                   Age         74.19          10.52
7       Gender (Female)         42.45          10.91
8         Smoking (Yes)         26.35           7.34
9 Genetic Risk (Medium)          0.00           0.08
```

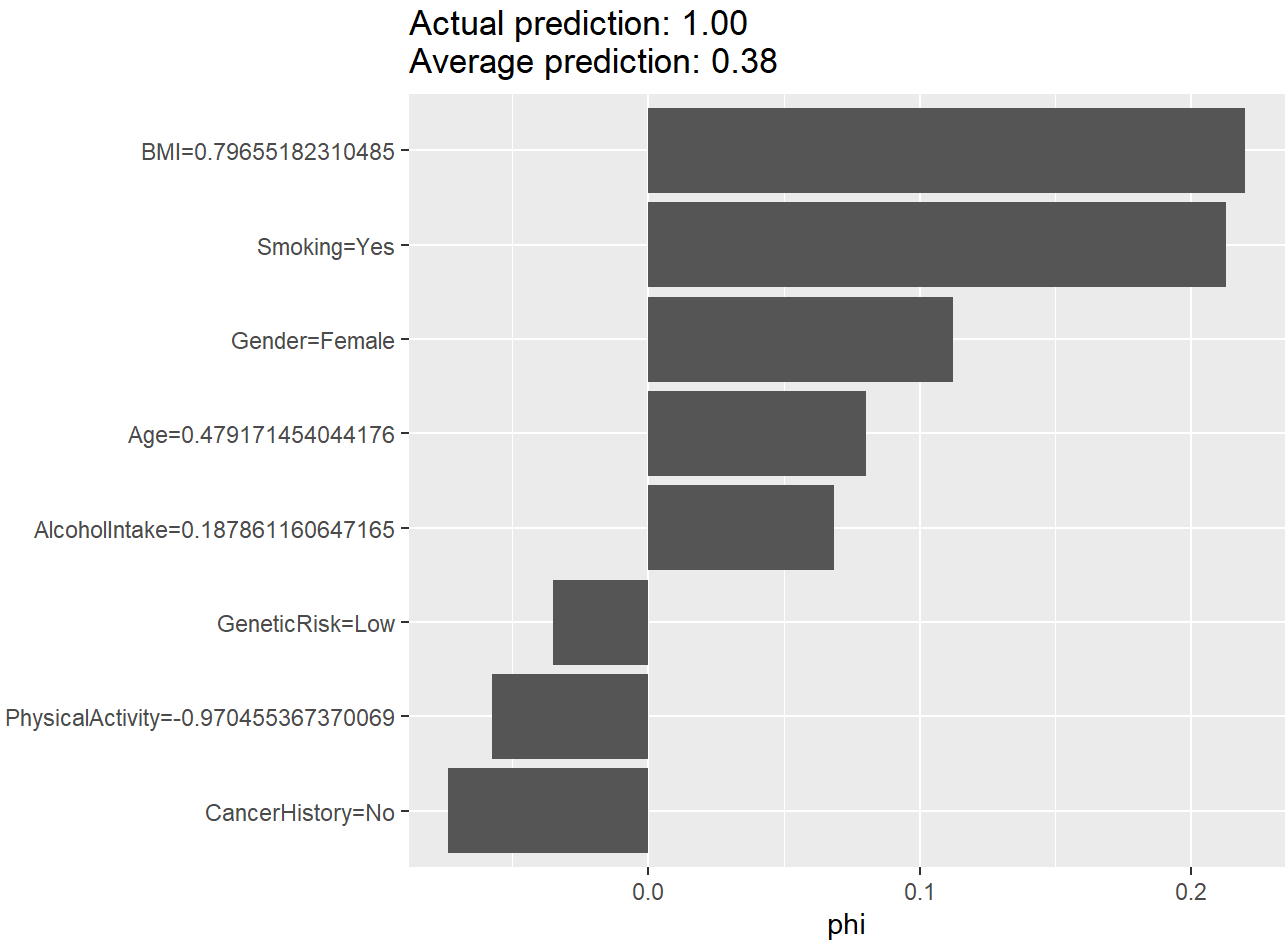
```r
# 定义一个函数，用于计算 Stacked 模型的最终概率
stacked_predict_prob <- function(object, newdata) {
  # 1. Base Learner Predictions
  rf_test_prob <- predict(rf_full, newdata = newdata, type = "prob")[, "Cancer"]
  gbm_test_prob <- predict(gbm_full, newdata = newdata, type = "prob")[, "Cancer"]
# ⚠️ Sanity Check 1: 检查 Base Learner 预测长度是否匹配输入
  if (length(rf_test_prob) != nrow(newdata) || length(gbm_test_prob) != nrow(newdata)) {
  warning("Sanity Check Failed: Base Learner prediction length does not match input data rows. Ch
  NA/missing rows due to new factor levels.")
  # 理想情况下，应该停止执行
  # stop("Inconsistent prediction length detected.")
}
  # 2. Create Stacked Feature Matrix (Level 1)
  if (any(is.na(rf_test_prob)) || any(is.na(gbm_test_prob))) {
  warning("Sanity Check Failed: Base Learner probabilities contain NA values.")
}
  stacked_test <- as.matrix(data.frame(
    rf_prob  = rf_test_prob,
    gbm_prob = gbm_test_prob
```

```
  ))

  # 3. Final Prediction using Meta Learner
  final_probs <- predict(stack_lr, newx = stacked_test, s = "lambda.min", type = "response")
  # ⚠️ Sanity Check 2: 检查最终概率是否有效
  if (any(final_probs < 0) || any(final_probs > 1) || any(is.na(final_probs))) {
  warning("Sanity Check Failed: Final probabilities contain values outside [0, 1] or contain NA."
  # stop("Invalid probability detected.")
}

  # 返回概率向量
  return(as.numeric(final_probs))
}
```

```
library(iml)
```

```
Warning: package 'iml' was built under R version 4.4.3
```

```
# --- 1. 创建 Stacked 模型的解释器对象 ---
# 传入一个占位符模型 (rf_full) 作为 model，但关键是传递自定义预测函数
predictor_stacked <- Predictor$new(
  # model = rf_full, # 占位符
  data = train_data[,-which(names(train_data)=="Diagnosis")],
  y = train_data$Diagnosis,
  predict.function = stacked_predict_prob, # 关键：指定 Stacked 预测函数
  class = "Cancer" # 明确指定要解释的类别
)

# --- 2. 选取要解释的样本 (测试集第 50 个样本) ---
x_interest_test_sample <- test_data[50, -which(names(test_data)=="Diagnosis")]

# --- 3. 计算 Stacked 模型的 SHAP 值 ---
shapley_stacked <- Shapley$new(
  predictor = predictor_stacked,
  x.interest = x_interest_test_sample
)

# --- 4. 绘图 ---
shapley_stacked$plot()
```




```r
# Sanity check
# 1. 创建一个测试数据框 (例如，使用训练集的前 10 行)
test_data_sample <- train_data[1:10, -which(names(train_data) == "Diagnosis")]

# 2. 运行你的 Stacked 预测函数
test_probs <- stacked_predict_prob(object = rf_full, newdata = test_data_sample)

# 3. 严格检查最大值
max_prob <- max(test_probs, na.rm = TRUE)
min_prob <- min(test_probs, na.rm = TRUE)

print(paste("Maximum calculated probability:", max_prob))
```

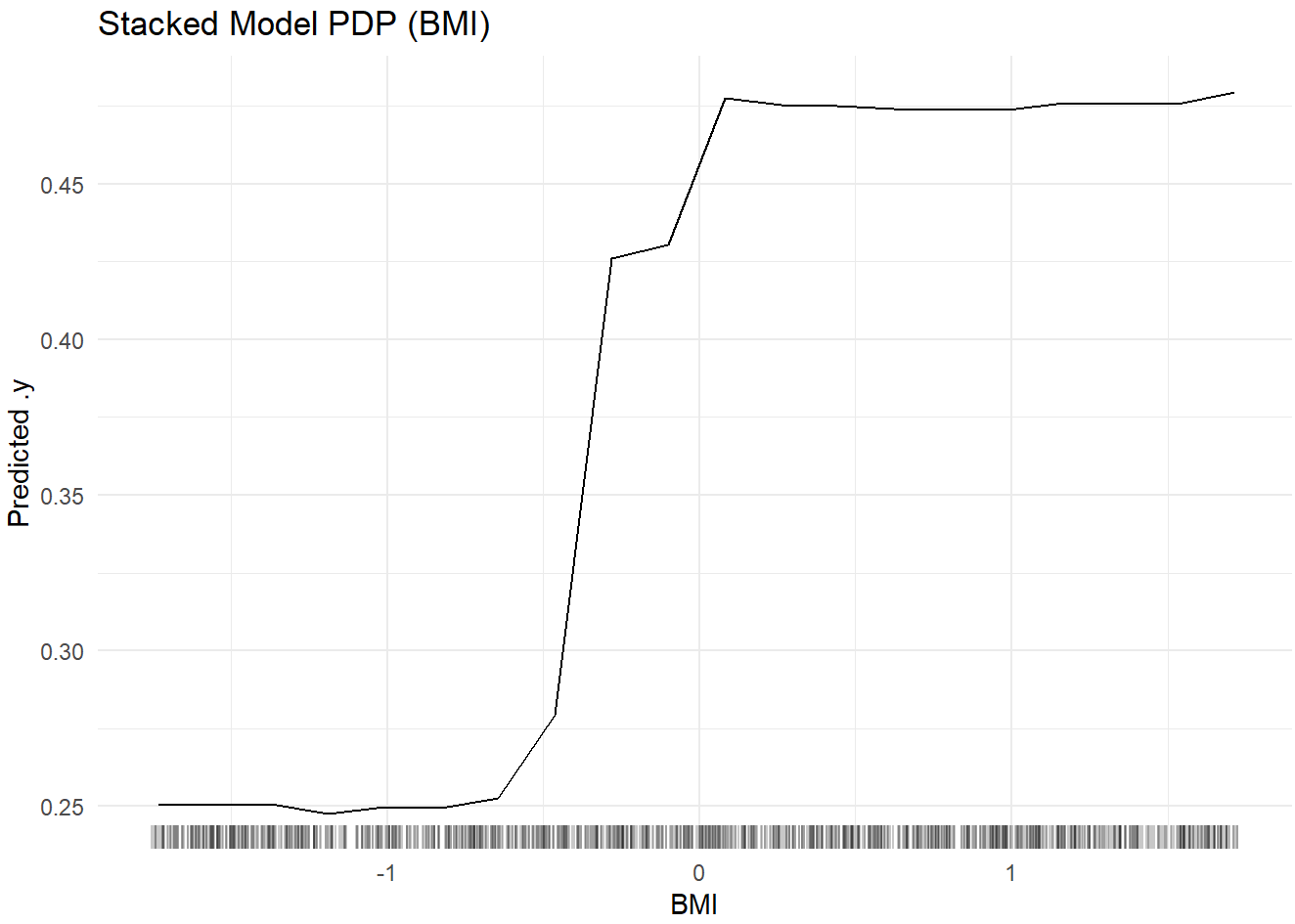
```
[1] "Maximum calculated probability: 0.997020085345288"
```

```r
print(paste("Minimum calculated probability:", min_prob))
```

```
[1] "Minimum calculated probability: 0.00626285133180356"
```

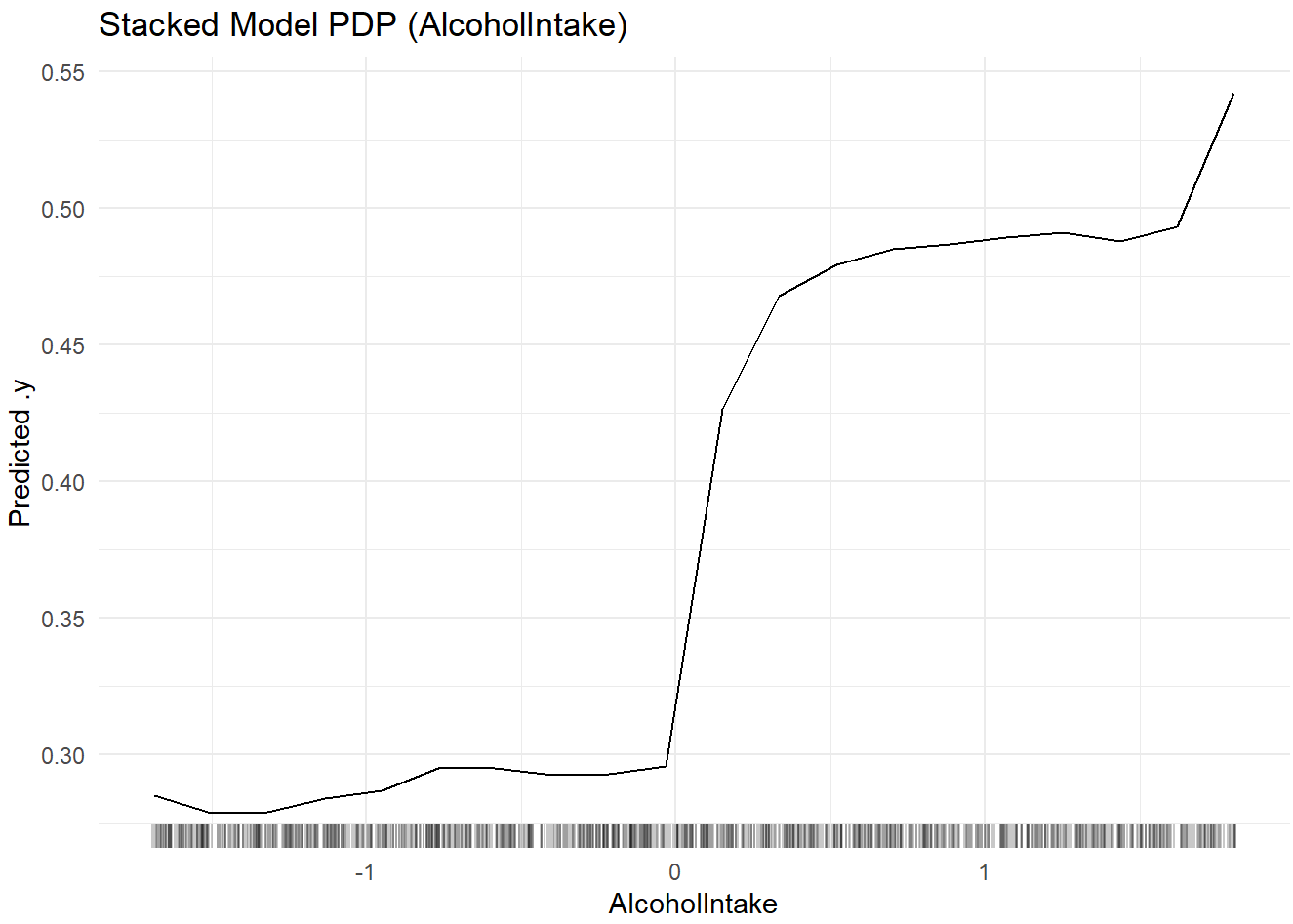
```r
library(iml)
library(ggplot2)
# Validated that our stacked logistic regression has learned non-linear relationship
```

```r
# --- 1. 使用 iml::FeatureEffect 计算 PDP 数据 ---
# method = "pdp" 是偏依赖图
effect_bmi <- FeatureEffect$new(
    predictor = predictor_stacked,
    feature = "BMI",
    method = "pdp"
)

# --- 2. 绘制 PDP 图 ---
# iml 的 plot() 方法会自动处理 PDP 的标签和尺度
# 确保 y 轴在 0 到 1 之间
plot_pdp_bmi <- effect_bmi$plot() +
    labs(title = "Stacked Model PDP (BMI)",
         y = "Predicted Cancer Probability (0-1)") +
    theme_minimal()

print(plot_pdp_bmi)
```




```r
# AlcholIntake plot
effect_alch <- FeatureEffect$new(
    predictor = predictor_stacked,
    feature = "AlcoholIntake",
    method = "pdp"
```

```r
)

plot_pdp_alch <- effect_alch$plot() +
    labs(title = "Stacked Model PDP (AlcoholIntake)",
         y = "Predicted Cancer Probability (0-1)") +
    theme_minimal()

print(plot_pdp_alch)
```



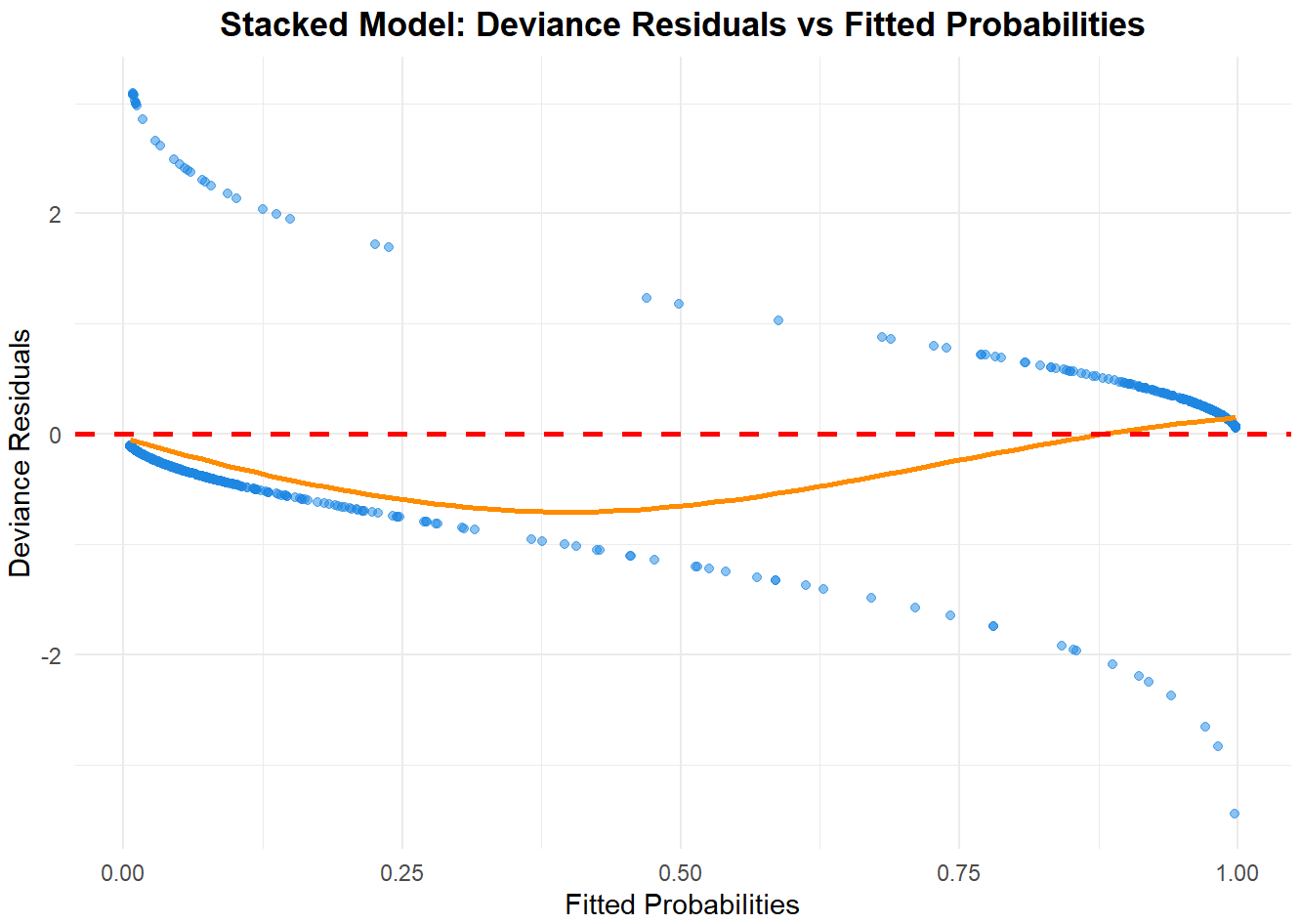

```r
# (v) Deviance and QQ-plot as diagnosis
# --- 1. 准备训练集预测概率 ---
X_train_stack <- as.matrix(data.frame(
  rf_prob  = predict(rf_full, newdata = train_data, type = "prob")[, "Cancer"],
  gbm_prob = predict(gbm_full, newdata = train_data, type = "prob")[, "Cancer"]
))
y_train <- ifelse(train_data$Diagnosis == "Cancer", 1, 0)

train_pred_prob <- as.vector(predict(stack_lr, newx = X_train_stack, s = "lambda.min", type = "re
# --- 2. 计算残差 ---
# Deviance residuals
dev_resid <- ifelse(y_train == 1,
                    sqrt(-2 * log(train_pred_prob)),
                    -sqrt(-2 * log(1 - train_pred_prob)))
```

```r
# Standardized residuals
std_resid <- scale(dev_resid)

# --- 2. 偏差残差 vs 拟合值图 (Residuals vs Fitted) ---
# 检查残差是否随机分布在 0 附近
residual_data <- data.frame(Fitted = train_pred_prob, DevianceResid = dev_resid)

plot_resid_fitted <- ggplot(residual_data, aes(x = Fitted, y = DevianceResid)) +
  geom_point(alpha = 0.5, color = "#1E88E5") + # 蓝色散点
  geom_smooth(method = "loess", color = "darkorange", se = FALSE, linetype = "solid") + # 添加平滑
  geom_hline(yintercept = 0, color = "red", linetype = "dashed", size = 1) +
  labs(title = "Stacked Model: Deviance Residuals vs Fitted Probabilities",
       x = "Fitted Probabilities",
       y = "Deviance Residuals") +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5, face = "bold"))
```

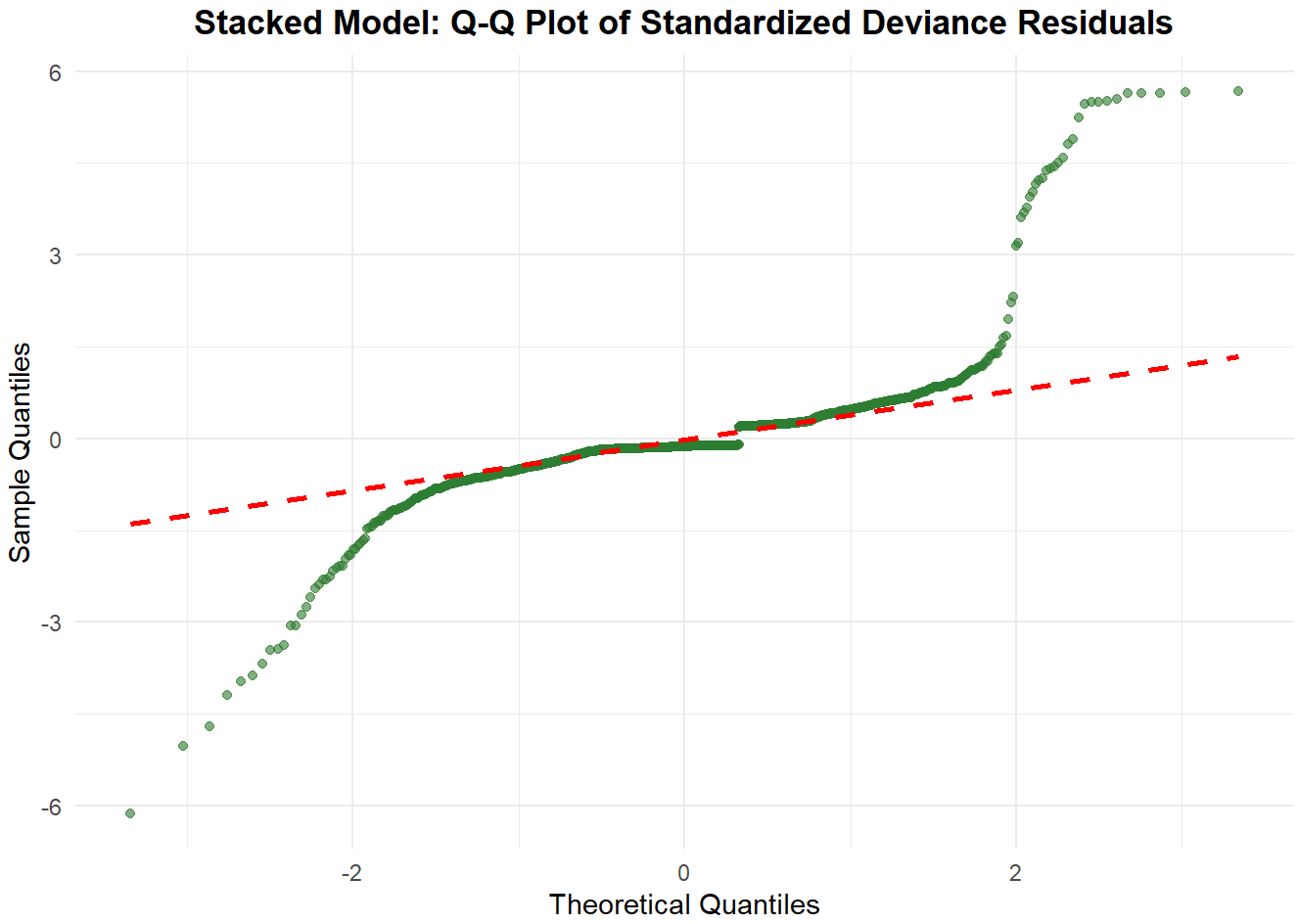
```
Warning: Using `size` aesthetic for lines was deprecated in ggplot2 3.4.0.
ℹ Please use `linewidth` instead.
```

```r
print(plot_resid_fitted)
```

```
`geom_smooth()` using formula = 'y ~ x'
```




```r
# --- 3. 标准化残差 Q-Q Plot ---
# 检查偏差残差是否近似正态分布
qq_data <- data.frame(StdResid = std_resid)

plot_qq <- ggplot(qq_data, aes(sample = StdResid)) +
  stat_qq(alpha = 0.6, color = "#2E7D32") + # 绿色散点
  stat_qq_line(color = "red", linetype = "dashed", size = 1) +
  labs(title = "Stacked Model: Q-Q Plot of Standardized Deviance Residuals",
       x = "Theoretical Quantiles",
       y = "Sample Quantiles") +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5, face = "bold"))

print(plot_qq)
```


Stacked Model: Q-Q Plot of Standardized Deviance Residuals
Sample Quantiles
Theoretical Quantiles
6
3
0
-3
-6
-2
0
2