Data Mining

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Contemporary Regression Models

- **Linear Methods for Regression**
- **Bias-Variance Tradeoff**
- **Logistic Methods for Regression**
- **Assessing Logistic Regression**

Linear Regression

Carl Friedrich Gauss
(1777–1855)

Linear Regression

A linear regression model assumes that the regression function $E(Y|X)$ is linear in the input variables $X_1, X_2, ..., X_p$. Linear models are:

- Simple and often provide an interpretable model
- Sometimes outperform nonlinear models with low signal-to-noise or sparse data
- Can be applied to transformations of the inputs - basis-function methods
- Many nonlinear models are direct generalizations of linear methods

Linear Regression

Let $X^T = (X_1, X_2, ..., X_p)$ be the input vectors for which we want to predict output Y. The linear regression model has the form:

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j \tag{1}$$

where $\beta_j's$ are unknown parameter coefficients and X_j are input vectors.

Linear Regression

Input vectors, X_j, can be:

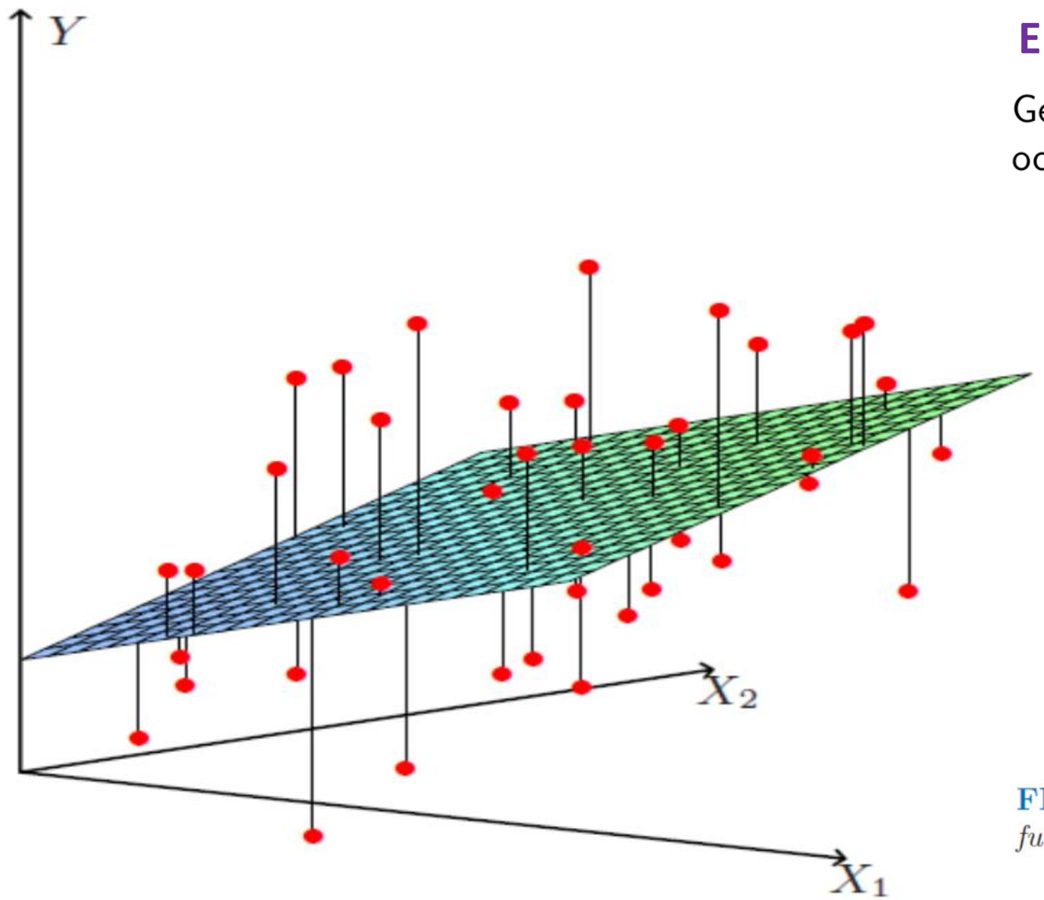
- Quantitative or transformations of quantitative inputs
- Basis expansion that leads to a polynomial representation
- Numeric or dummy coding: level-dependent constants
- Interactions between the input variables

Linear Regression

Regression methods estimates the model parameters $\beta's$ with the training data to minimize the residual sum of squares, $\boldsymbol{RSS(\beta)}$.

$$\begin{aligned} RSS(\beta) &= \sum_{i=1}^{N}(y_i - f(x_i))^2 \\ &= \sum_{i=1}^{N}(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 \end{aligned} \tag{2}$$

Regression: Least-Squared Method



Elements of Statistical Learning (pg.45)

Geometry of least-square fitting in the $\mathbb{R}^{p+1}$-dimensional space occupied by the pairs (X, Y).

FIGURE 3.1. *Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of X that minimizes the sum of squared residuals from Y.*

Interpreting Linear Regression

AVE_ave_provider_charge ~ AVE_ave_medicare_payment + AVE_num_service

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	2	3.85E+11	1.92E+11	1148.9	<.0001
Error	3334	5.58E+11	167376011		
Corrected Total	3336	9.43E+11			

Root MSE	12937	R-Square	0.408
Dependent Mean	24721	Adj R-Sq	0.4076
Coeff Var	52.33355		

Parameter Estimates							
Variable	Label	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|	Variance Inflation
Intercept	Intercept	1	-1219.43	598.38	-2.04	0.0416	0
AVE_ave_medicare_payment	Average Medicare Payment	1	3.83	0.08	47.88	<.0001	1.02
AVE_num_service	Number of Services	1	-5.84	1.17	-4.96	<.0001	1.02

AVE_ave_provider_charge ~ AVE_ave_medicare_payment + AVE_num_service

SSM = $\sum(\hat{y}_i - \bar{y})^2$

SSE = $\sum(y_i - \hat{y}_i)^2$

SST = SSM + SSE

F = MSM/MSE, scaled ratio of the model variance to the error/residual variance.

Interpreted here as “rejecting the null hypothesis that all regression parameters equal 0,” i.e. the regression model is valid.

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R^2 = SSM/SST, always interpreted as “the proportion of variance in the response variable explained by the model.”

R^2 adjusted for more than one variable.

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VIF > 10 is considered an indicator of possible multicollinearity problems.

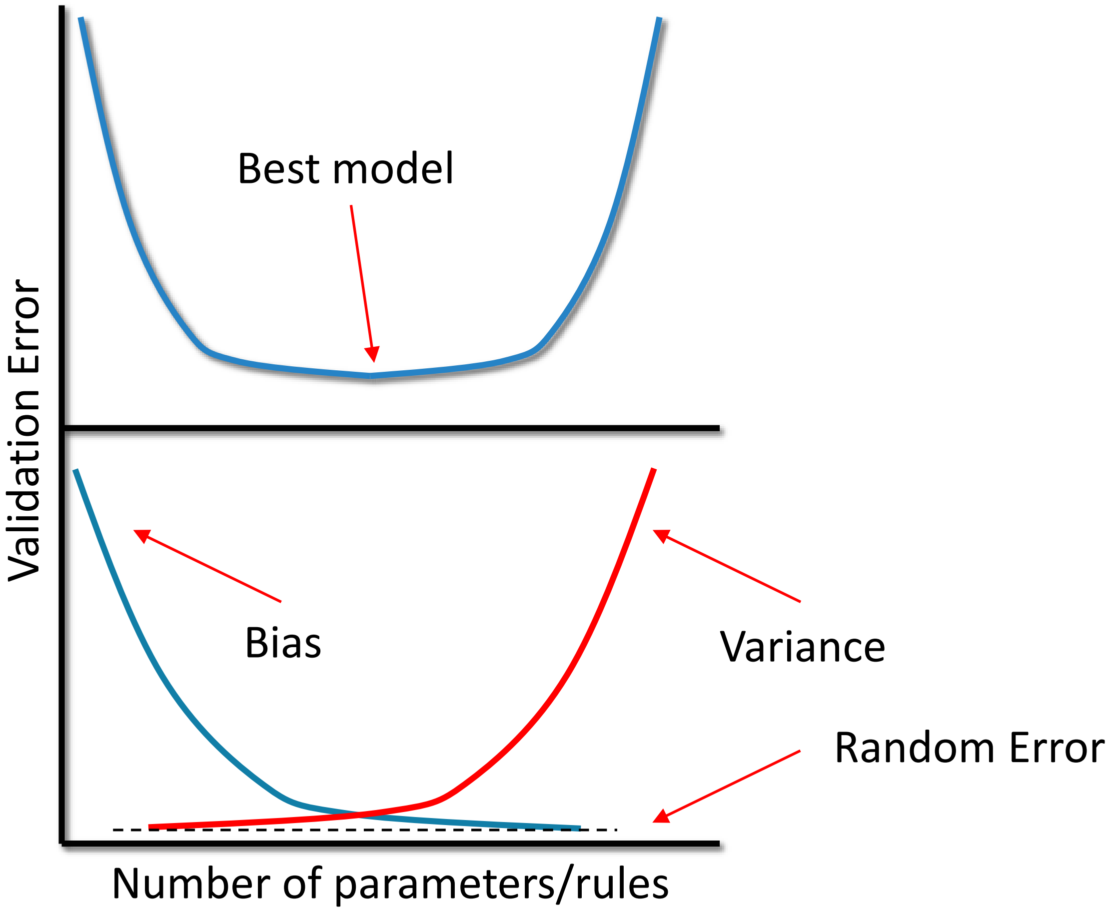
Estimated parameter for the input, here interpreted as “holding all other inputs constant, for a one unit increase in average Medicare payment, average provider charge will increase by 3.83 units on average.”

Standard error of the coefficient – should be much smaller than the coefficient. (Std. deviation for the coefficient.)

t-test for the coefficient, here interpreted as “rejecting the null hypothesis that this coefficient is equal to 0,” i.e. this variable is “significant.”

Cross-Validation & Parameter Tuning

The Bias / Variance Trade-off



Total Error = Bias + Variance + Random

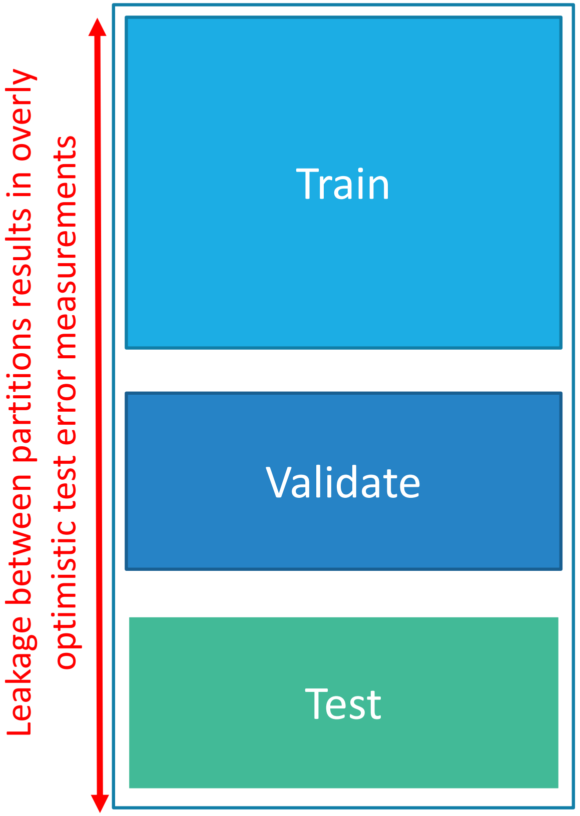
Error = $(\hat{f}(x) - f(x))^2$

Bias = $E[\hat{f}(x)] - f(x)$ or the error that arises from a model's inability to replicate the fundamental phenomena represented by a data set.

Variance = $(\hat{f}(x) - E[\hat{f}(x)])^2$ or the error that arises from a model's ability to produce differing predictions from the values in a new data set.

Bias/Variance Trade-off in Practice: Honest assessment

Available labeled data



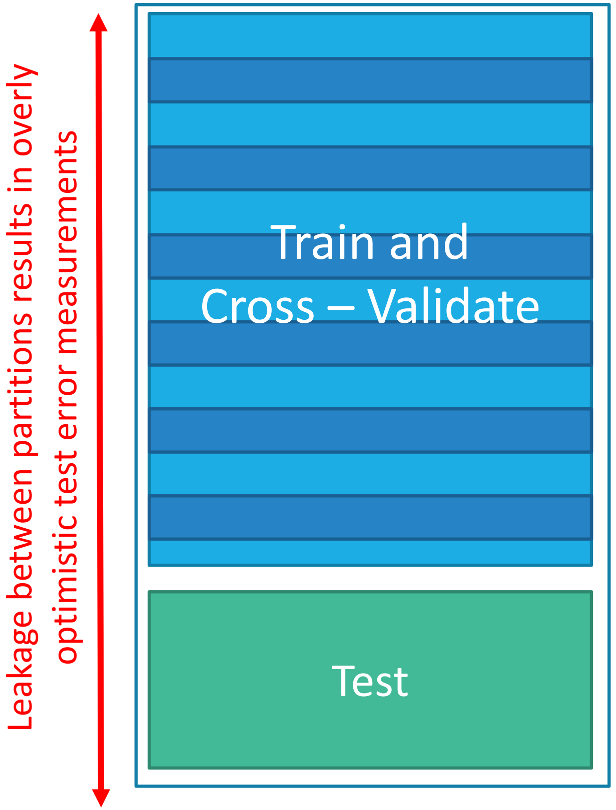
Estimate parameters or rules

Model selection

Final ***honest*** assessment

Best suited for big data or linear models using traditional forward, backward, or stepwise selection.

Available labeled data



- Estimate parameters or rules
- Model selection and hyper-parameter tuning

Final ***honest*** assessment

Nearly always a more generalizable approach, but computationally intensive. Best suited for complex models with many hyper-parameters and small to medium sized data.

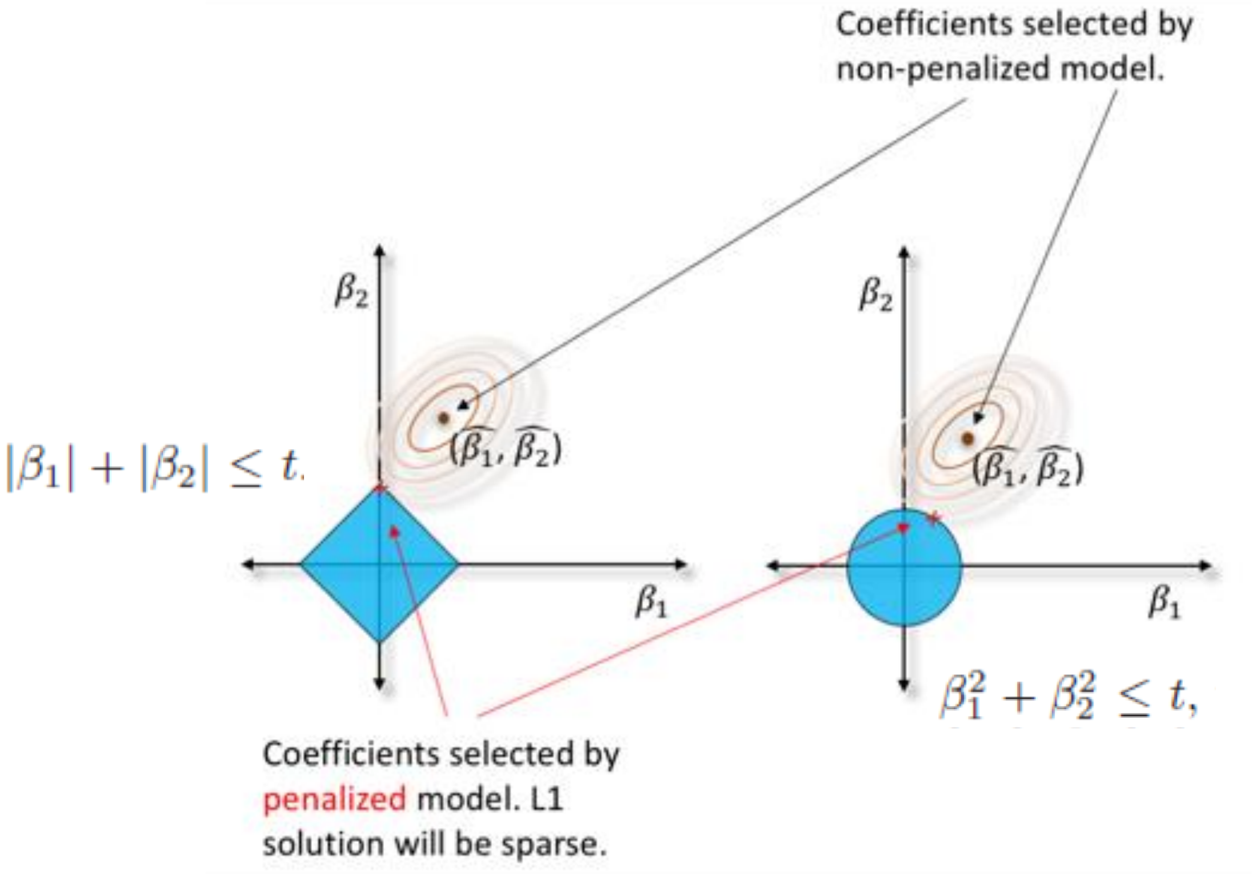
OLS Linear Regression Assumptions

Requirements	If broken …
Linear relationship between inputs and targets; normality of y and errors	Inappropriate application/unreliable results; use a machine learning technique; use GLM
N > **p**	Underspecified/unreliable results; use LASSO or Elastic Net penalized regression
No strong multicollinearity	Ill-conditioned/unstable/unreliable results; Use Ridge(L2/Tikhonov)/Elastic Net penalized regression
No influential outliers	Biased predictions, parameters, and statistical tests; use robust methods, i.e. IRLS, Huber loss, investigate/remove outliers
Constant variance/no heteroskedasticity	Lessened predictive accuracy, invalidates statistical tests; use GLM in some cases
Limited correlation between input rows (no autocorrelation)	Invalidates statistical tests; use time-series methods or machine learning technique

Elastic Net - Modern Approach

Hui Zou and Trevor Hastie
Regularization and variable selection via the elastic net,
Journal of the Royal Statistical Society, 2005

Shrinkage/Regularization Method



Anatomy of Elastic Net: L1 & L2 Penalty

λ - Controls magnitude of penalties. Variable selection conducted by refitting model many times while varying λ. Decreasing λ allows more variables in the model.

L1/LASSO penalty – for variable selection.

L2/Ridge/Tinkhonov Penalty – helps address multicollinearity.

$$\tilde{\beta} = \min_{\beta} \left\{ \boxed{\sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} * \beta_j \right)^2} + \boxed{\lambda} \sum_{j=1}^{p} \left(\boxed{\alpha} * \boxed{\beta_j^2} + (1 - \boxed{\alpha}) * \boxed{|\beta_j|} \right) \right\}$$

Least squares minimization – finds β's for linear relationship.

α - tunes balance between L1 and L2 penalties.

Elastic Net – Iteratively Reweighted Least Squares

Iteratively Reweighted Least Square complements fitting methods in the presence of the outliers by:

- Initially giving all observations equal weight then…
  - Train the model to estimate the β's and find a linear relationship/equation

$$\tilde{\beta} = \min_{\beta}\left\{\sum_{i=1}^{N}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} * \beta_j\right)^2\right\}$$

"Inner Loop"

  - Calculate the residuals given these β's/ linear equation
  - Re-weight observations that cause high residuals to have a lower impact in the train model
  - Re-train to find new β's/linear equation
  - Continue calculating residuals, re-weighting observations, and re-training until β's become stable and weighted residuals are small…

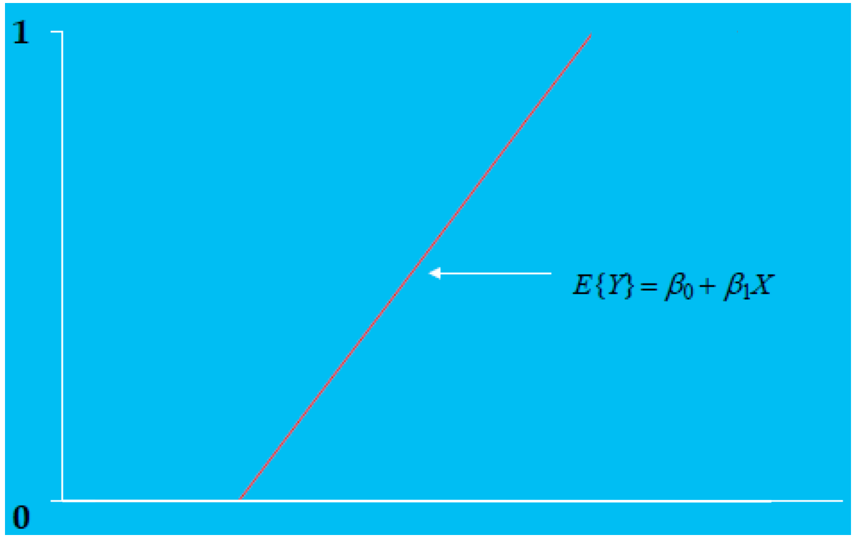
"Outer Loop"

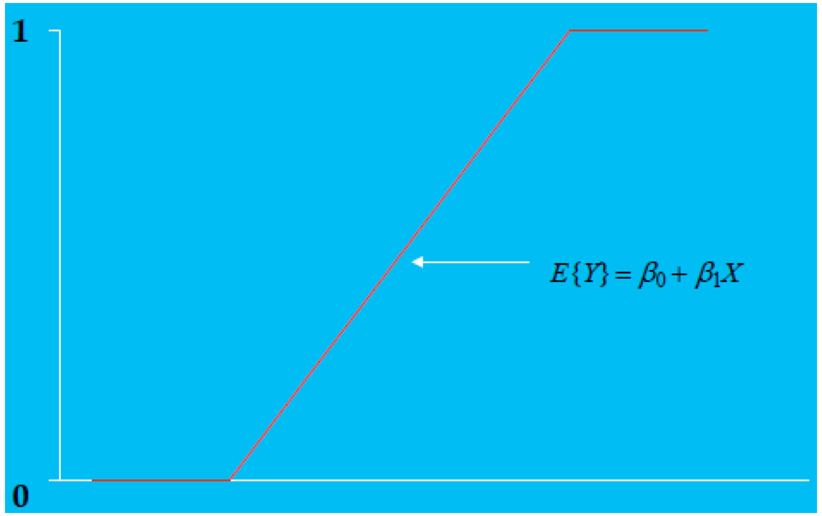
Logistic Regression

Issues with Linear Regression

Best-Fit Linear Regression or Truncated Linear Regression:

- Boundary Problems
- Non-normal Error Terms
- Non-constant error variance





Non-Linear Logistic Model

- Solve the boundary constraint problems and also permit more plausible model that would model the relationship between the target and model parameters
- The model is constructed based on:
  - Ability to predict the probability of target occurrence based on various model parameter inputs
  - determine if there are any model parameters which are particularly salient to predict the model target

Linear Regression Prediction Formula

input measurement

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \cdot x_1 + \hat{w}_2 \cdot x_2$$

prediction estimate

intercept estimate *parameter estimate*

Choose intercept and parameter estimates to *minimize*.

squared error function

$$\sum_{\text{training data}} (y_i - \hat{y}_i)^2$$

Logistic Regression: Log of Odds

Logistic Regression Prediction Formula

$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_0 + \hat{w}_1 \cdot x_1 + \hat{w}_2 \cdot x_2 \quad \textit{logit scores}$$

RECALL: Odds=probability/(1-probability) AND Probability=Odds/(1+Odds)

Logit Link Function

$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_0 + \hat{w}_1 \cdot x_1 + \hat{w}_2 \cdot x_2 = \operatorname{logit}(\hat{p})$$

$$\hat{p} = \frac{1}{1 + e^{-\operatorname{logit}(\hat{p})}}$$

To obtain prediction estimates, the logit equation is solved for $\hat{p}$.

From: *Advanced Analytics with SAS Enterprise Miner*

Interpreting Logistic Regression

Probability to Log Odds:

For categorical

- p = event rate for that level
- odds = p/(1-p)
- odds ratio = $odds_{level}/odds_{reference\ level}$
- log odds ratio = ln(odds ratio)

Log odds ratio against reference level = 1.2
Odds ratio against reference level = $e^{1.2}$ = 3.32
Probability/event rate in training data = 3.32/(1 + 3.32) = 0.76
"Holding all other variables constant, a person being male changes the odds of the event occurring by a factor of 3.32 over the reference level on average."

$$\hat{y} = \text{“log odds”} = \log(p/(1-p)) = 1.7 - \boxed{0.54} * age + \boxed{1.2} * male$$

For interval:

- p = change in event rate for one unit increase; this is ***not*** constant
- odds = $odds_{level}$ - $odds_{level+1}$, this ***is*** constant
- Log odds = ln(odds)

Log odds = -0.54
Odds = $e^{-0.54}$ = 0.58
"Holding all other variables constant, for a one unit increase in age, the odds of the event occurring change by a factor of 0.58 on average."

Confusion Matrix

		True condition	
	Total population	Condition positive	Condition negative
Predicted condition	Predicted condition positive	**True positive**, Power	**False positive**, Type I error
	Predicted condition negative	**False negative**, Type II error	**True negative**

From: https://en.wikipedia.org/wiki/Confusion_matrix

Confusion Matrix

		True condition				
	Total population	Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) $= \frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	
Predicted condition	Predicted condition positive	**True positive**, Power	**False positive**, Type I error	Positive predictive value (PPV), Precision $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Predicted condition positive}}$	False discovery rate (FDR) $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$	
	Predicted condition negative	**False negative**, Type II error	**True negative**	False omission rate (FOR) $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Predicted condition negative}}$	Negative predictive value (NPV) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$	
		True positive rate (TPR), Recall, Sensitivity, probability of detection $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) $= \frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR+}}{\text{LR–}}$	F_1 score $= \frac{2}{\frac{1}{\text{Recall}} + \frac{1}{\text{Precision}}}$
		False negative rate (FNR), Miss rate $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR–) $= \frac{\text{FNR}}{\text{TNR}}$		

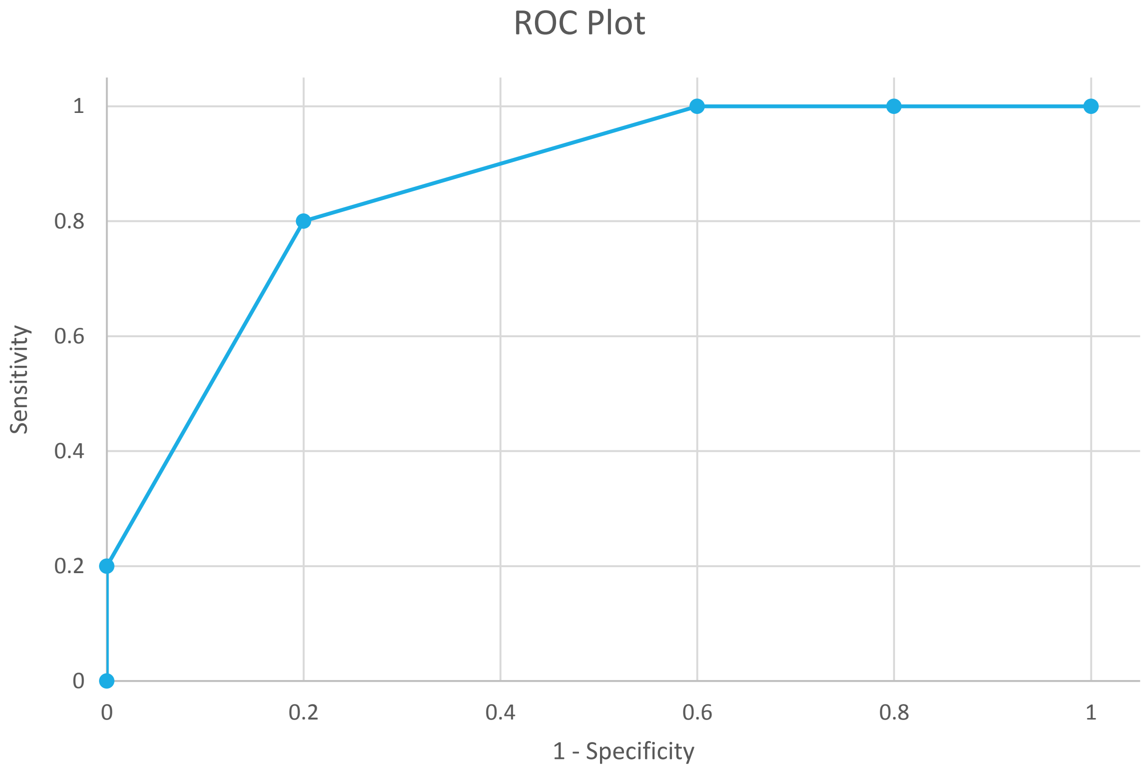
From: https://en.wikipedia.org/wiki/Confusion_matrix

Confusion Matrix & Classification Table

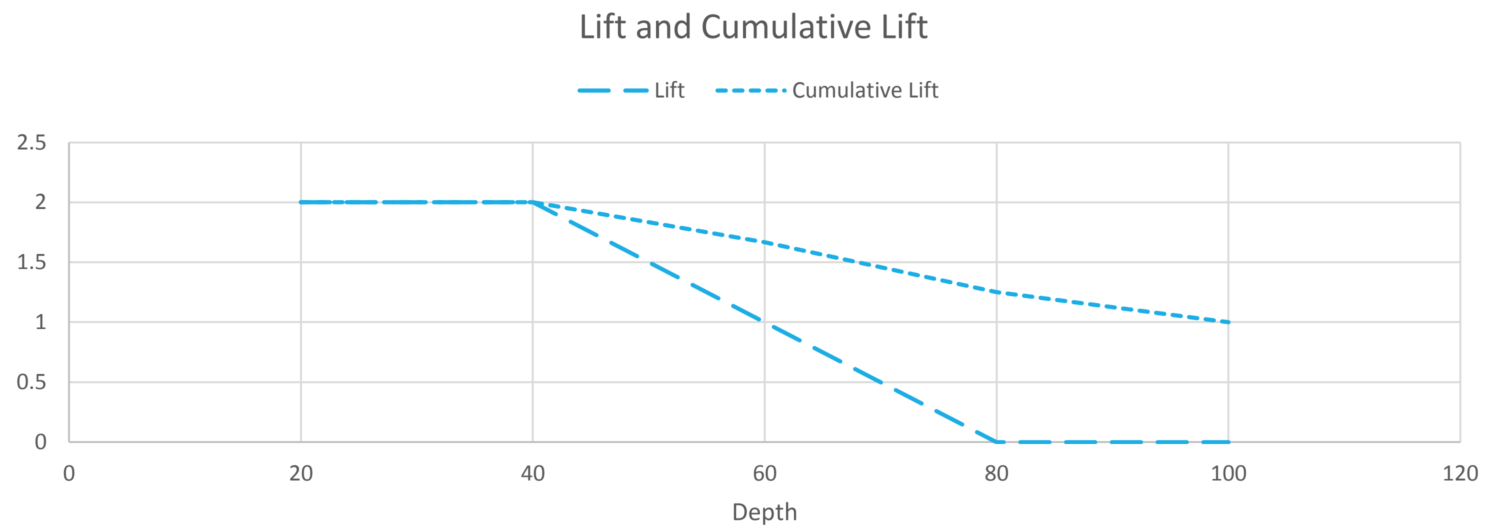
Actual	Predicted
1	0.85
1	0.75
1	0.7
1	0.65
0	0.65
1	0.55
0	0.55
0	0.45
0	0.3
0	0.1

Cutoff	TP	FP	FN	TN	1 - Spec.	Sens.
0	5	5	0	0	1	1
0.2	5	4	0	1	0.8	1
0.4	5	3	0	2	0.6	1
0.6	4	1	1	4	0.2	0.8
0.8	1	0	4	5	0	0.2
1	0	0	5	5	0	0

ROC Curve Example

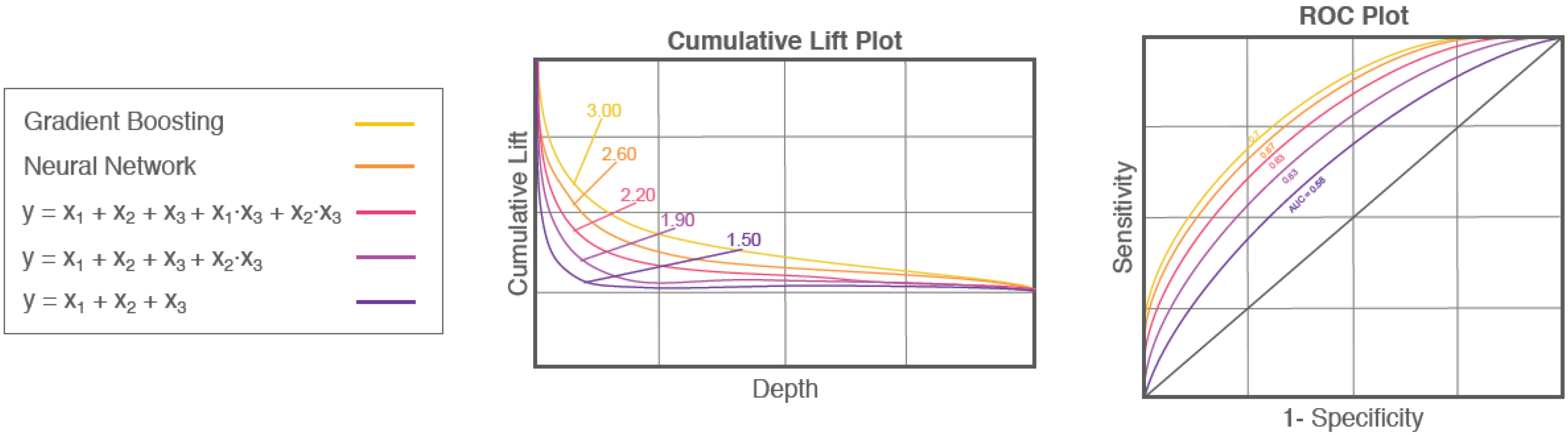


LIFT PLOT

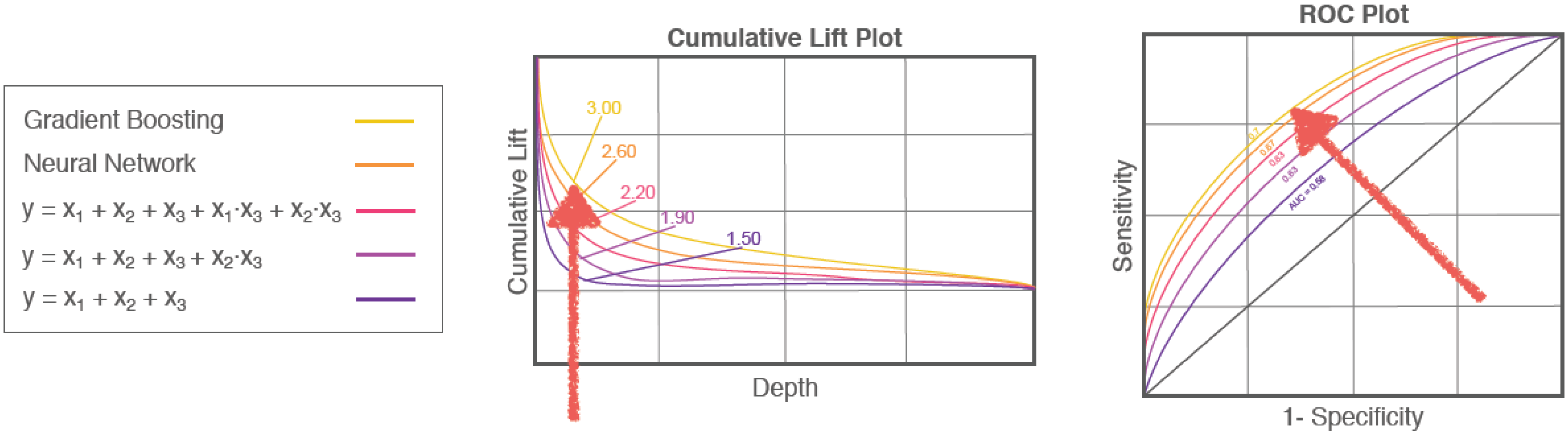


Lift and Cumulative Lift
Lift
Cumulative Lift
2.5
2
1.5
1
0.5
0
0
20
40
60
80
100
120
Depth

Interpreting Assessment Measures



- Area under the ROC curve (AUC) is bounded between 0 and 1. Values below and including 0.5 indicate serious problems with the model. Values above 0.5, as they approach 1, indicate a better model.
- AUC is interpreted as "The expectation that a uniformly drawn random positive is ranked before a uniformly drawn random negative."



- Lift is typically measured at a certain percentile, say the 10th
- Higher lift indicates a better model
- Lift is interpreted as: "In the 10th percentile of highest predicted probabilities, this model predicted 3 times more events correctly than in a random selection of 10% of the data."