Machine Learning Applications and Methods

Numeric Prediction
Generalized Linear Models
Regression Trees

Different Approaches => Different Models

- What to Optimize
  - Minimize Prediction Error
  - Minimize Classification Errors
  - Maximize Probabilities
- How to Find Parameters
  - Search space of solutions
  - Constraints and Assumptions
- What kinds of functions to use
  - E.g. linear vs non-linear
  - E.g. divide input into pieces

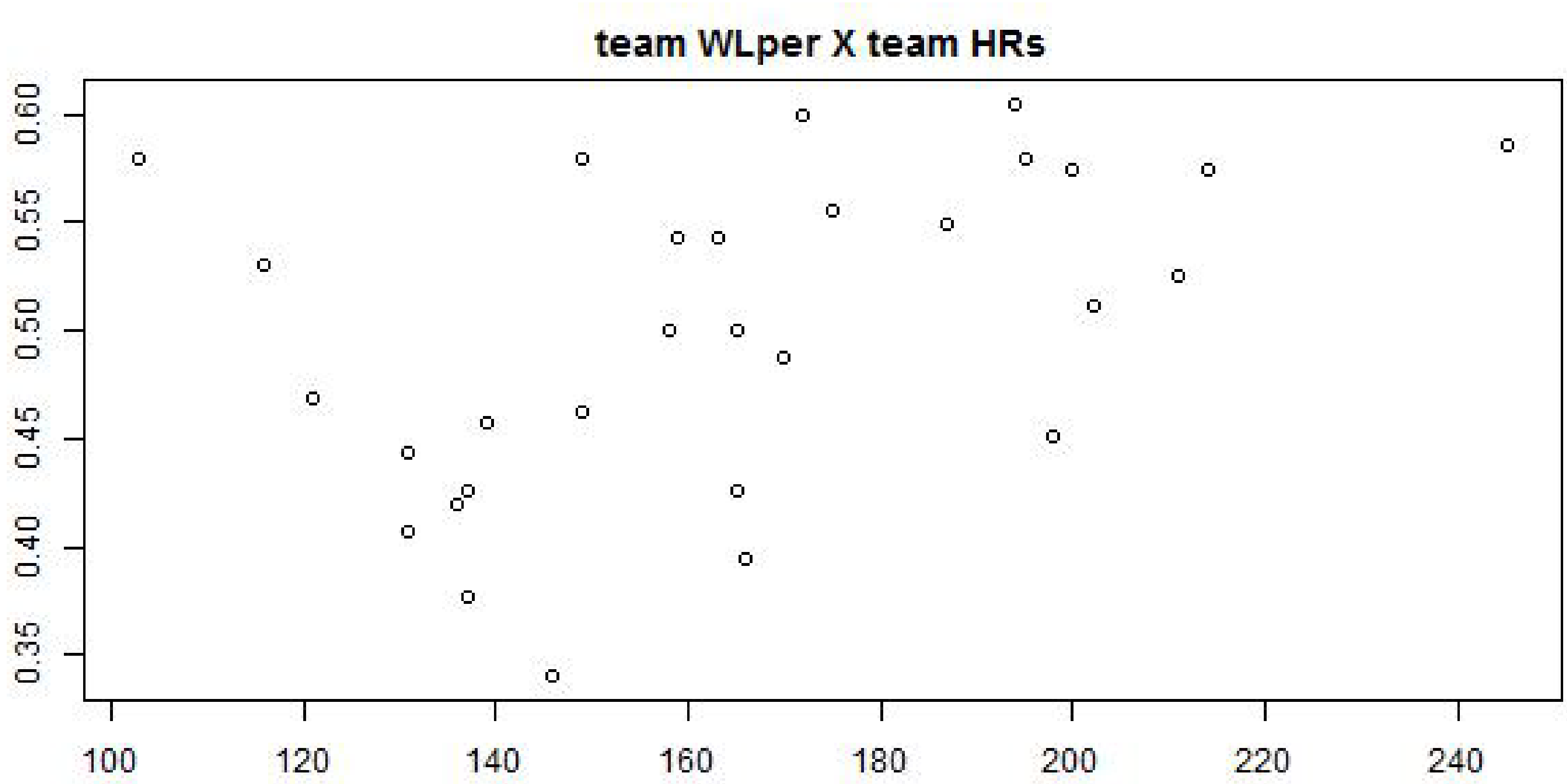
Varieties of Regression

- Linear Model: $Y = X * B$

  where Y=outcomes , X=data matrix
- Solve for B directly by algebraic manipulation
- Solve for B directly by setting derivatives to 0
- Solve for B iteratively by derivatives and small changes (that decrease error)
- Solve for B but reweight by variance in X
- Solve for B but constrain size

…

Data Example: Home Runs and W-L

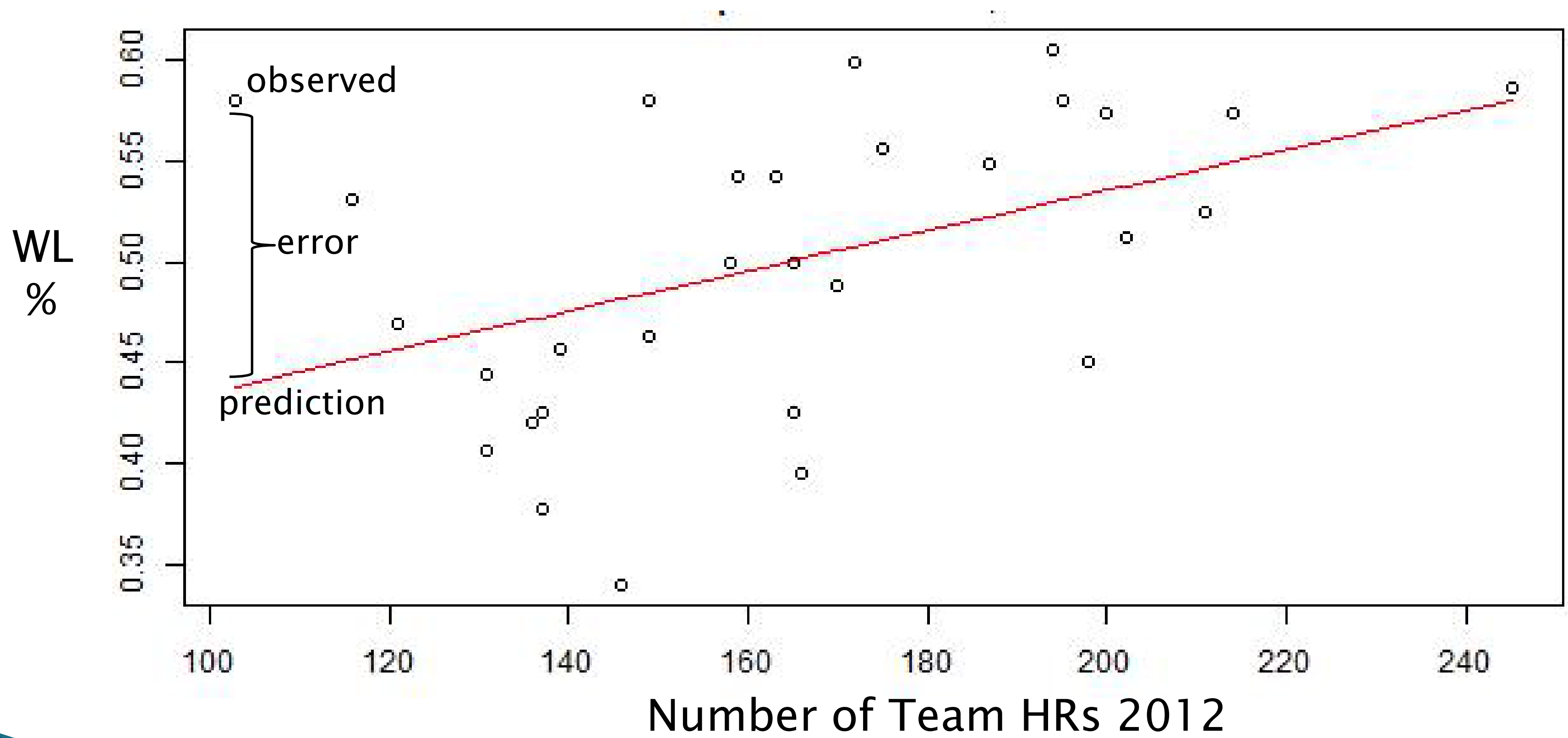


W-L %

Number of Team HRs 2012

Linear Regression Model

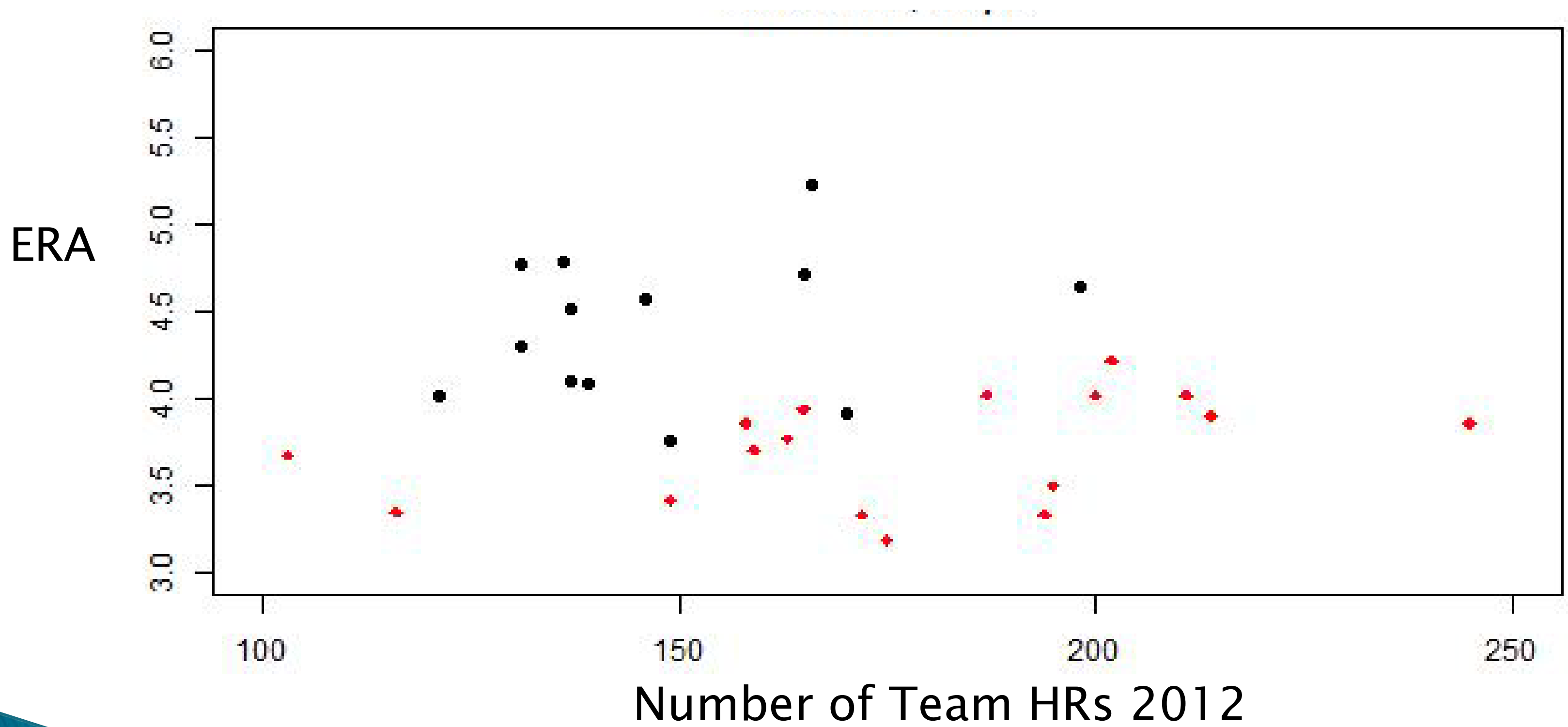
Q: What is the relationship between HRs and Winning %



A Linear Model for Classification

- target is 1 (WL%>=.5) and -1 (WL%<.5)

Q: Can you classify winning records based on HRs and ER

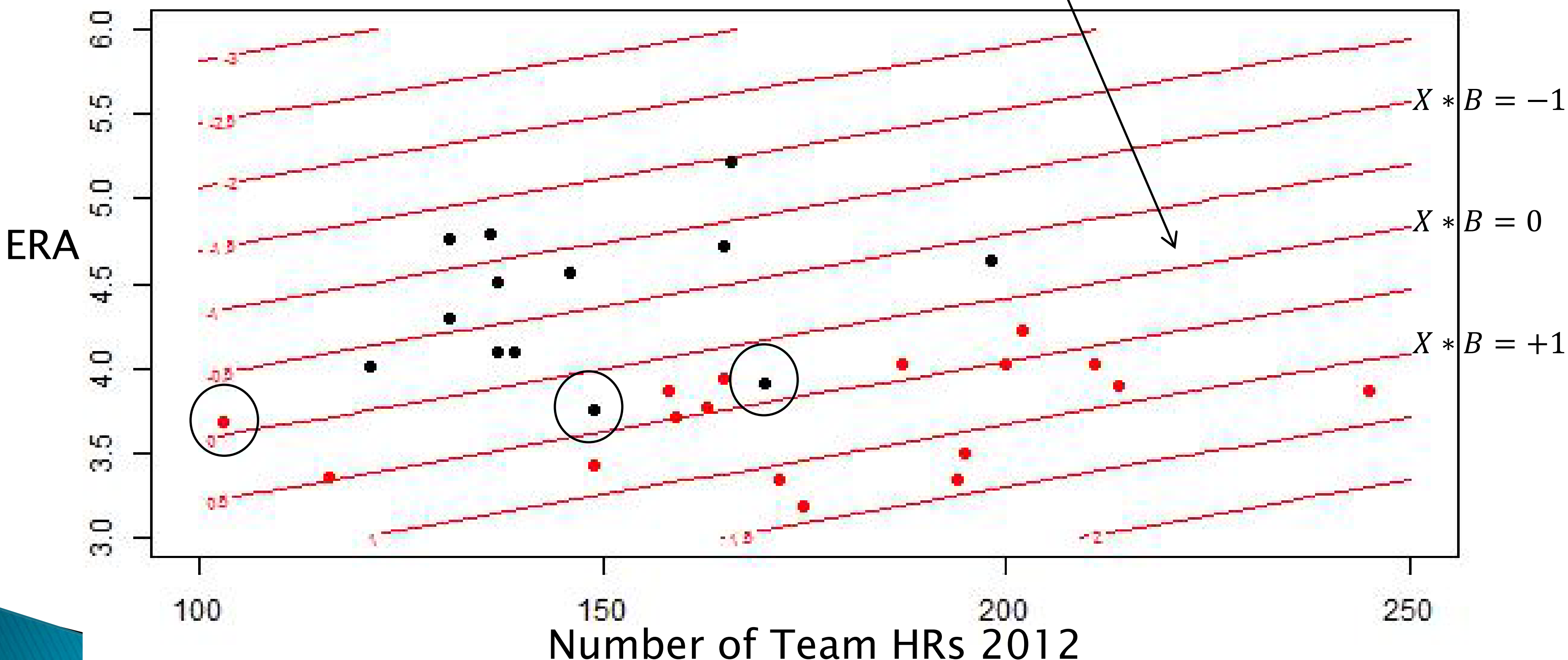


Linear Model for Classification (cont')

: misclassifications

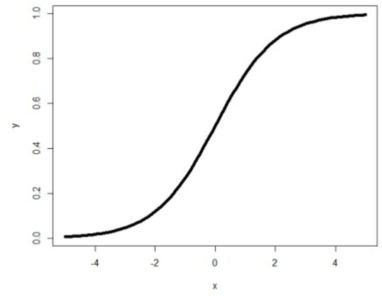
$X * B = 0$ gives decision threshold

(i.e. the combination of HR,ERA where W–L prediction is 5



Linear to Logistic Regression

- Squash X*B to 0,1 range using Logistic Function:



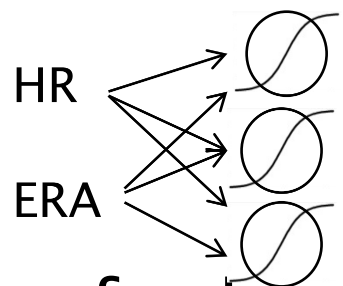
- Directly Model P(Y|X)

    e.g. Probability(Y=Winning given HR,ERA values)

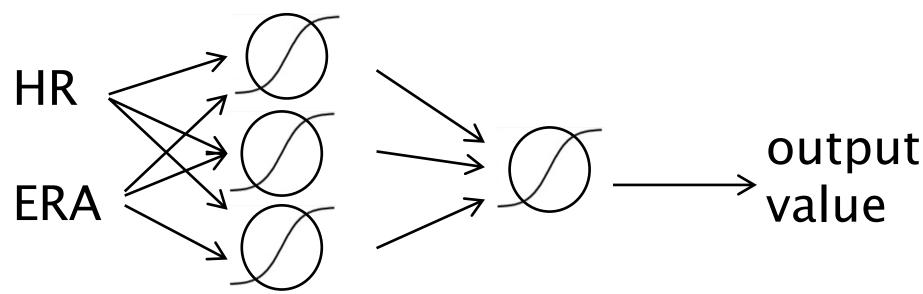
- Solve with maximization methods

Logistic Regression to Neural Networks

- Use several squash functions (hidden layer)



- Take further combinations (output layer)



- More powerful but more complex
  - many parameters, many options, needs more training

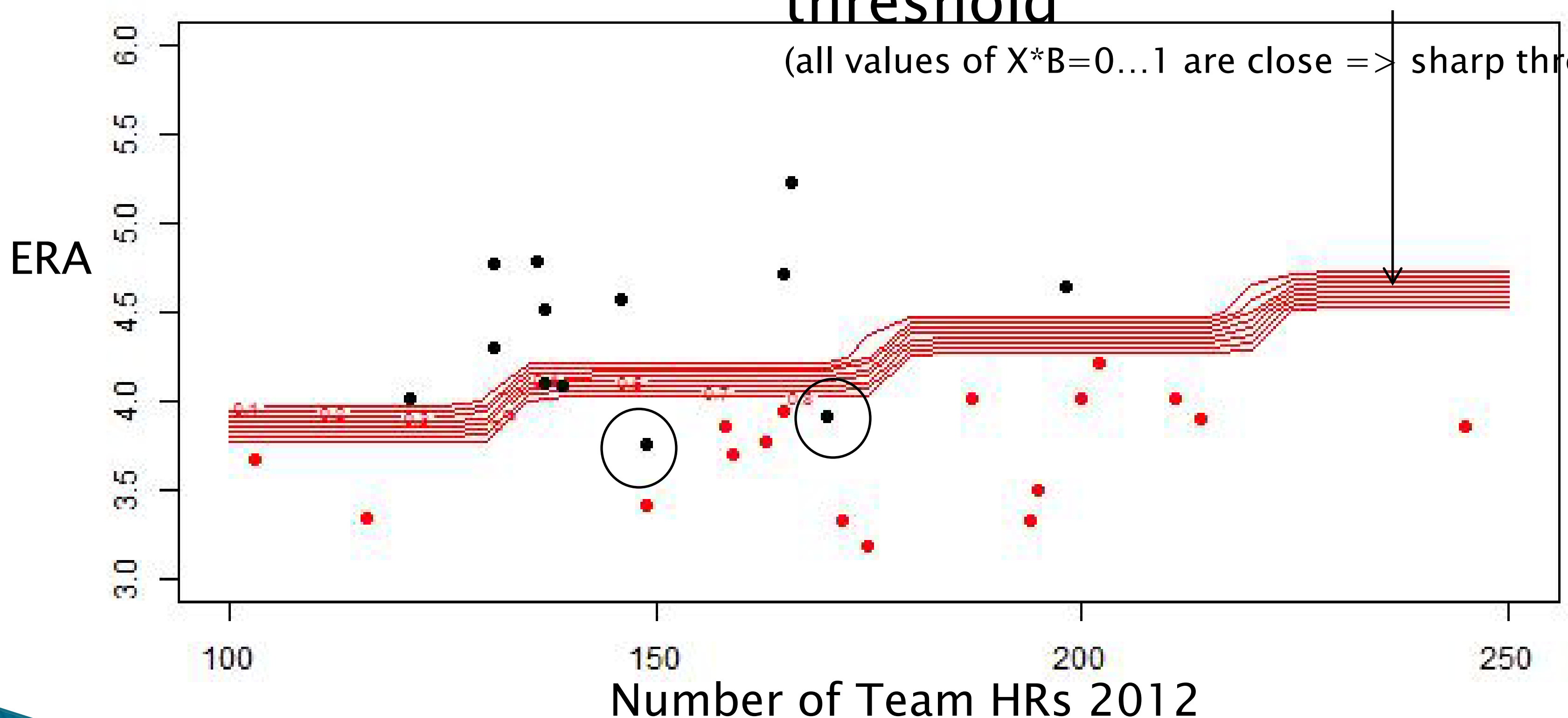
Neural Network classification

(R nnet() with 8 hidden units, 100 training iterations)

: misclassifications

$X * B = .5$ gives decision threshold

(all values of X*B=0…1 are close => sharp threshold)



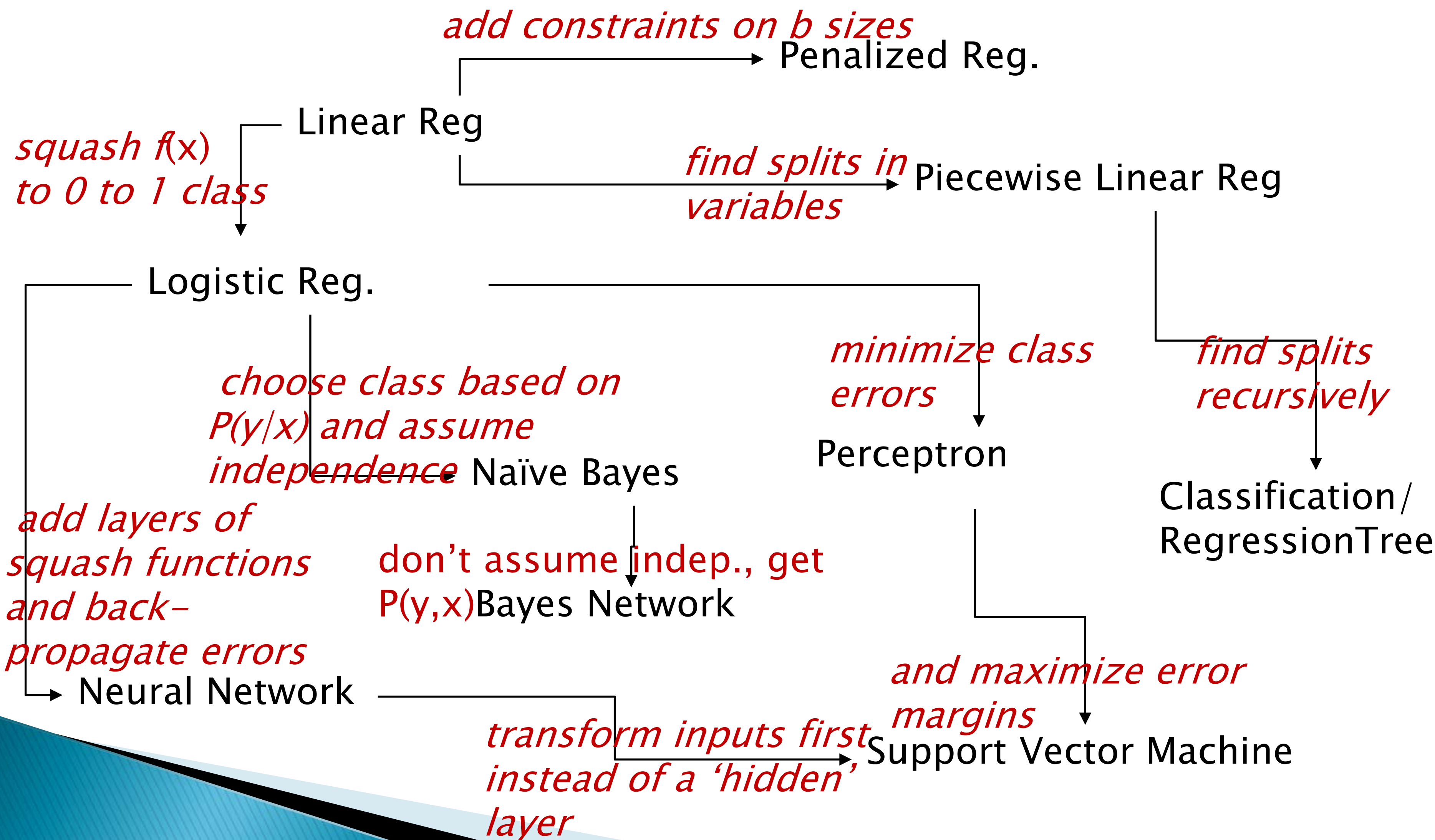
Other NonLinear Options:

- **Polynomial and multiplicative variable interaction**
  - add new variables: HR*HR, HR/ERA, etc..

- Divide and conquer:
  - Condition model on cut points (“knots”)
    - e.g. HR<140, HR>140
  - Splines or Trees (smooth or not smooth predictions around cuts)

Model Space Map

(one view on some parts)



The Big Picture of Models

	Function	Target	Error	Parameter Estimation
Linear Reg.	linear	numeric	squared residual	Solve for least sq.
Logistic Reg.	nonlinear	prob. of class	misclass.	max likelihood
Neural net.	nonlinear	Numeric or Class	squared resid. X-entropy	Gradient descent
Trees (classification and regression)	piecewise	Numeric or Class	squared resid. Or misclass.	Greedy search and prune
Support vector	linear or nonlinear	Class	margin of misclass	Constrained optimization
PCA,PLS	Dim. reduction	Data reproduce	squared resid.	solve
kNearest Nbr	Local means	Numeric or class	squared resid. or misclass	Xvalidation on k
…				

The Big Picture of Models

	Function	Target	Error	Parameter Estimation
Splines	Polynomial, interactions	numeric	squared error	Solve w/ contraints
Bayesian	Use Prob. Dens.Fnctns	prob. of data and parameters	(un)expected values	Expectation max., Monte Carlo Markov Chain
Ridge Regression	linear	numeric	squared resid.	Solve w/penalty
Matrix Factor	linear	Data reproduction	squared resid. w/ penalty	iterate
Lasso	linear	numeric	absolute resid	Iterate in steps
Perceptron	linear	Class separation	Min classification errors	iterate
Linear Discriminant	linear	Class separation	Min variances	Matrix solution
…				

Other Model Areas

- Time Series
  - i.e. linear regression with time steps
- Network Analysis/Graphs
  - i.e. model links and properties over whole graph
- Many techniques combine
  - e.g. Bayesian SVM, Bayesian network
  - e.g. Elastic Net (Lin. Reg. w/abs. & squared error)
- Nonlinear Kernel transformations
  - Kernel PCA, Kernal PLS, Kernel Ridge regression
- Penalty can be added
  - e.g. minimum norm in neural nets

Different Considerations => Different Model Choices

- Data and Problem Issues to Consider:
  - Dimension reduction to Factors?
  - Sparsity (in data or response)?
  - Multiresponse (prediction)/Multiclass (classification)?
  - Number of Observations vs. Variables?
  - Interpretability vs Model Complexity?
  - Bias vs Variance trade-offs (good vs stable estimates)
  - Scale

App Recommendations

- Usually no absolute choice and no silver bullets
  (otherwise we wouldn't be here)
- Start with simple methods
- Consider trade off as you go more complex
- Find similar application examples
  (what works in this domain)
- Find paradigmatic examples for models
  (what works for this model)
  - **Goals and Expectations!**

Numeric Predictions

Numeric Predictions

- Numeric prediction is interpreted as prediction of a continuous class
  - Like classification learning but with numeric "class"
- Counterparts exist for all schemes
  - Decision trees, rule learners, SVMs, etc.
- Almost all classification schemes can be applied to regression problems using discretization
  - Discretize the class into intervals
  - Predict weighted average of interval midpoints
  - Weight according to class probabilities
- Learning is supervised
  - Scheme is being provided with target value

Numeric Prediction

- Example: modified version of weather data

Outlook	Temperature	Humidity	Windy	Play (time minutes)
Sunny	85	85	False	5
Sunny	80	90	True	0
.	.	.	.	.

CPU Performance Data

	Cycle Time (ns)	Main Memory (Kb)		Cache (Kb)	Channels		Perfor mance
	MYCT	MMIN	MMAX	CACH	CHMIN	CHMAZ	PRP
1	125	256	6000	256	16	128	198
2	29	8000	32000	32	8	32	269
.							
208	480	512	8000	32	0	0	67
209	480	1000	4000	0	0	0	45

Classifiers for Numeric Prediction

- Schemes for numeric prediction include: linear regression, model tree generators, locally weighted regression, instance-based learners, decision tables, multi-layer perceptron

- Classifiers available in WEKA for Numeric prediction
  - LinearRegression: (functions) linear regression
    - The simplest is linear regression
  - m5.M5Prime: model trees
    - M5Prime is a rational reconstruction of Quinlan's M5 model tree inducer
  - IBk: k-nearest neighbor learner
  - LWR: Locally Weighted Regression
    - LWR is an implementation of a more sophisticated learning scheme for numeric prediction, using locally weighted regression
  - RegressionByDiscretization: uses categorical classifiers

Numeric Prediction in Python

- Available methods in
  - Statsmodels
  - Scikit-learn
  - NumPy

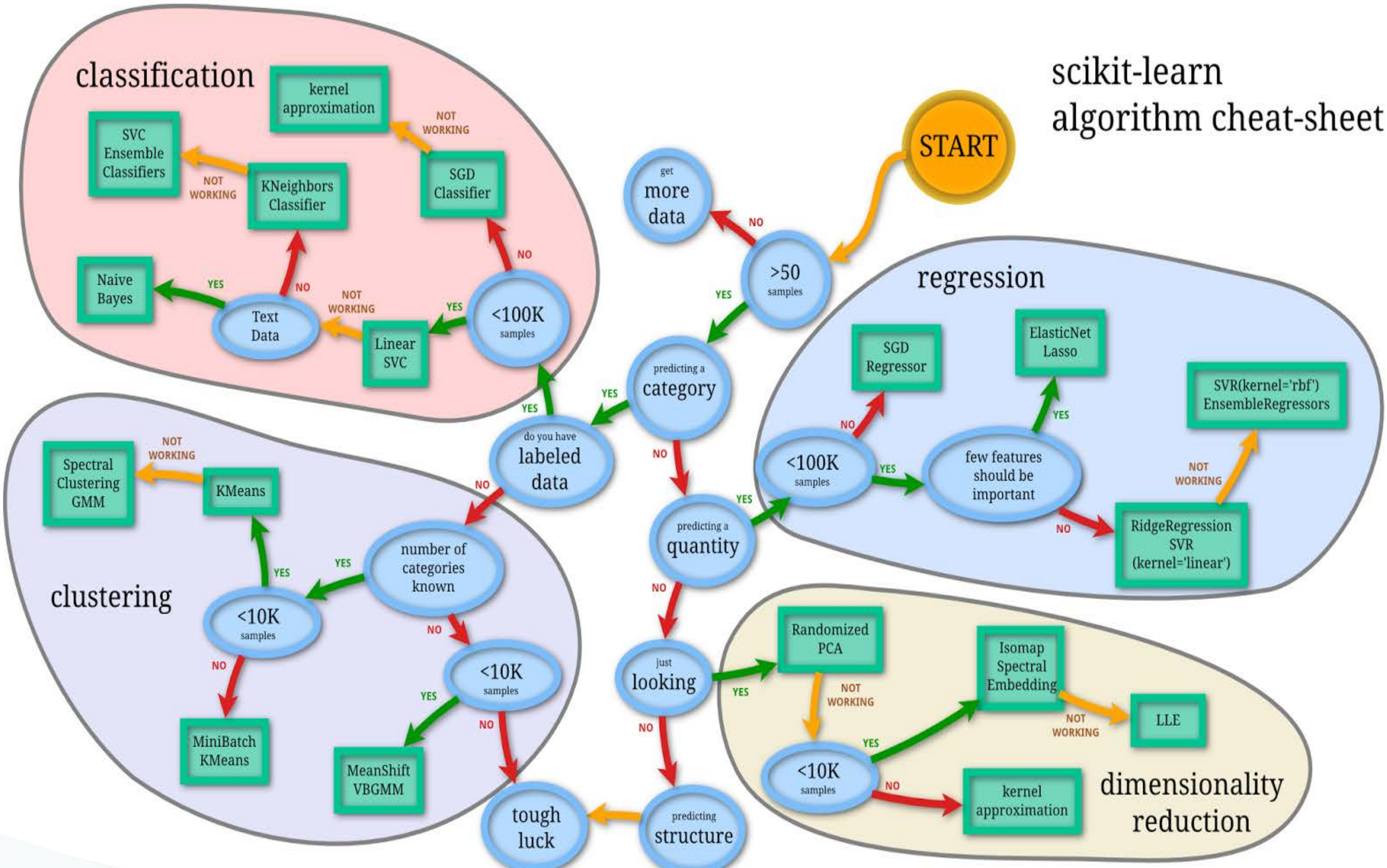
Statsmodel

- Linear regression models:
  - Generalized least squares (including weighted least squares and least squares with autoregressive errors),
  - ordinary least squares.
  - glm: Generalized linear models with support for all of the one-parameter exponential family distributions.
  - discrete: regression with discrete dependent variables, including Logit, Probit, MNLogit, Poisson, based on maximum likelihood estimators
  - rlm: Robust linear models with support for several M-estimators.
  - tsa: models for time series analysis - univariate time series analysis:
  - AR, ARIMA - vector autoregressive models,
  - VAR and structural VAR - descriptive statistics and process models for time series analysis nonparametric : (Univariate) kernel density estimators

Scikit
Generalized Linear Models

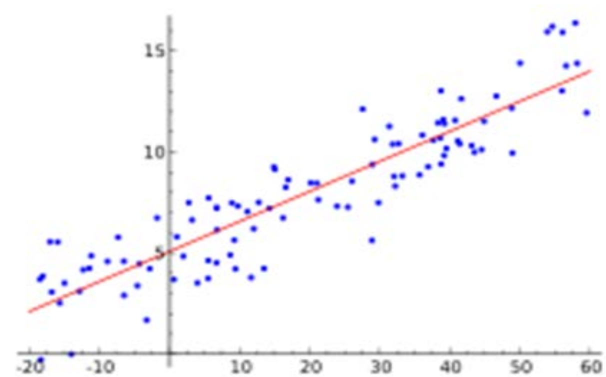
http://scikit-learn.org/stable/modules/linear_model.html

- Ordinary Least Square
- Ridge Regression
- Lasso
- Elastic Net
- Least Angel Regression
- Bayesian Regression
- Logistic Regression
- Stochastic Gradient Decent


scikit-learn
algorithm cheat-sheet
START
>50 samples
get more data
predicting a category
do you have labeled data
predicting a quantity
just looking
predicting structure
tough luck
classification
<100K samples
SGD Classifier
kernel approximation
Linear SVC
Text Data
Naive Bayes
KNeighbors Classifier
SVC Ensemble Classifiers
clustering
number of categories known
<10K samples
KMeans
Spectral Clustering GMM
MiniBatch KMeans
<10K samples
MeanShift VBGMM
regression
<100K samples
SGD Regressor
few features should be important
ElasticNet Lasso
RidgeRegression SVR (kernel='linear')
SVR(kernel='rbf') EnsembleRegressors
dimensionality reduction
Randomized PCA
<10K samples
Isomap Spectral Embedding
LLE
kernel approximation
YES
NO
NOT WORKING

Linear Regression: Description

- Linear regression is a prediction technique used when the class and all attributes are numeric
- One of the easiest technique to use
- Bound by "linearity"
  - If data exhibits a linear dependency, the best-fitting straight line will be found, where best is interpreted as the least mean-squared difference.

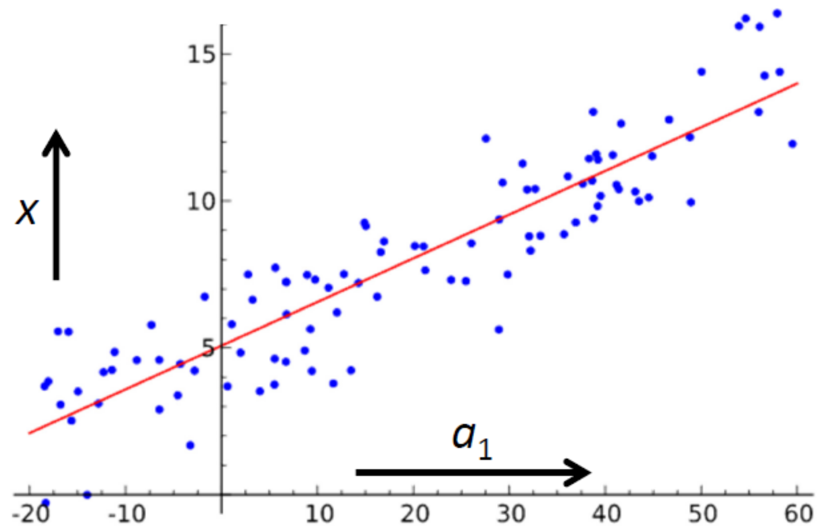


Linear Models: Linear Regression

- In linear regression the class is expressed as a liner combination of the attributes, each of which has a specific weight:

$$A = \boldsymbol{w_0} + \boldsymbol{w_1 a_1} + \boldsymbol{w_2 a_2} + \cdots + \boldsymbol{w_k a_k}$$

$j=0$

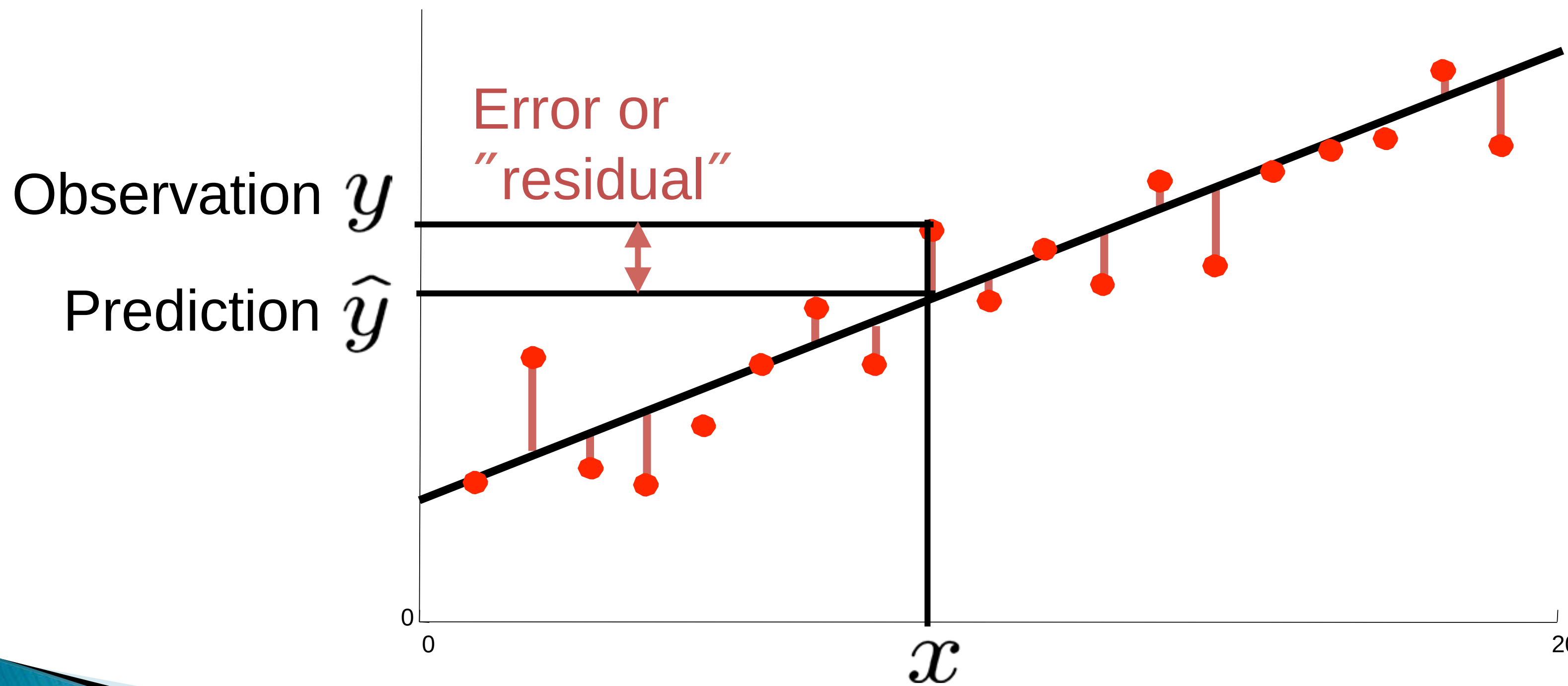


Linear Models: Linear Regression

- The goal in linear regression is to choose the weights that will minimize the sum of the squares of the difference between the predicted class value and the actual class values in the dataset.
- The weights are calculated from the training data
- Squared error:
  - $\sum_{i=1}^{n}(x^{(i)} - \sum_{j=0}^{k} w_j \, a_i{}^{(i)})^2$

Ordinary Least Squares (OLS)

$$\text{total error} = \sum_i (y_i - \hat{y}_i)^2 = \sum_i \left(y_i - \sum_k w_k f_k(x_i) \right)^2$$



Linear Regression for House Data

House Size	Lot Size	Bedrooms	Granite	Upgraded Bathrooms	Selling price
3529	9191	6	0	0	205,000
3247	10061	5	1	1	224,900
4032	10150	5	0	0	197,900
2397	14156	4	1	0	189900
2200	9600	4	0	1	195000
3536	19994	6	1	1	325000
2983	9365	5	0	1	23000
3198	9669	5	1	1	?????

Linear regression for the Housing data

- Selling Price =

  −26.6882 * House Size +

  7.0551 * Lot Size +

  43166.0767 * Bedrooms +

  42292.0901 * Upgraded Bathroom +

  − 21661.1208

Linear regression for the Housing data

- Selling Price =

  −26.6882 * 1871+

  7.0551 * 5884 +

  43166.0767 * 4+

  42292.0901 * 1+

  − 21661.1208

Selling price = $184,873.86

Zillow = $448,545.00

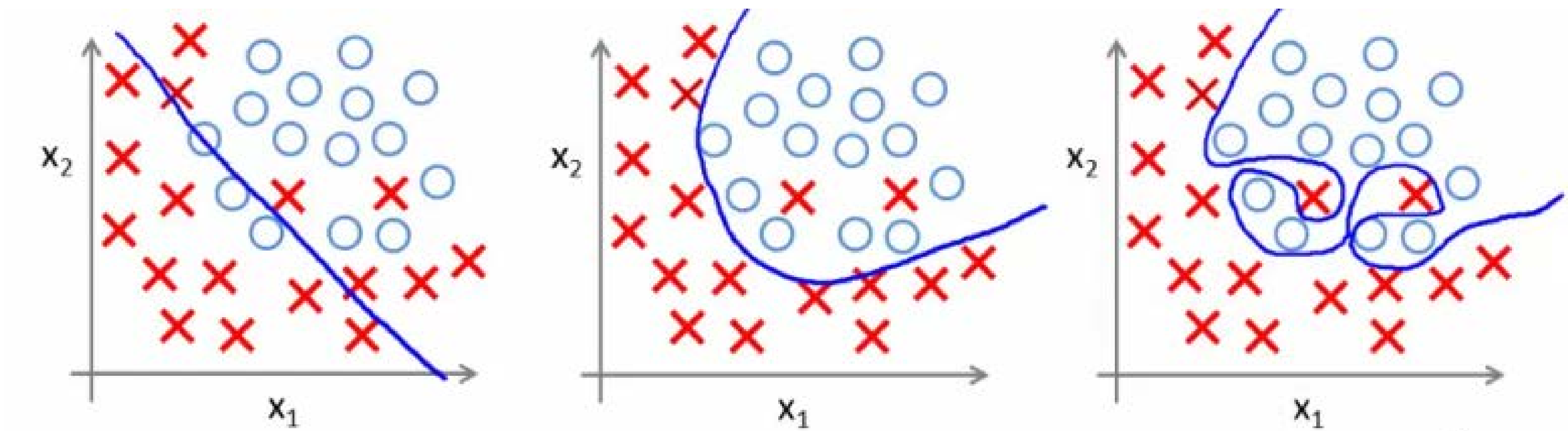
Regression Analysis Assumptions

- The sample is representative of the population for the inference prediction
- The error is a random variable with a mean of zero conditional on the explanatory variables
- The independent variables are measured with no error
- The predictors are linearly independent, i.e. it is not possible to express any predictor as a linear combination of the others
- The errors are uncorrelated, that is, the variance-covariance matrix of the errors is diagonal and each non-zero element is the variance of the error

Ordinary Least Squares (OLS) Weaknesses

- Coefficient estimates for OLS rely on the independence of the model terms
- When terms are correlated and the columns of the design matrix have an approximate linear dependence – estimate becomes highly sensitive to random errors – producing a large variance
- *Multicollinearity* problem

Overfitting



$h_\theta(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$

(g = sigmoid function)

$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 \\ + \theta_3 x_1^2 + \theta_4 x_2^2 \\ + \theta_5 x_1 x_2)$$

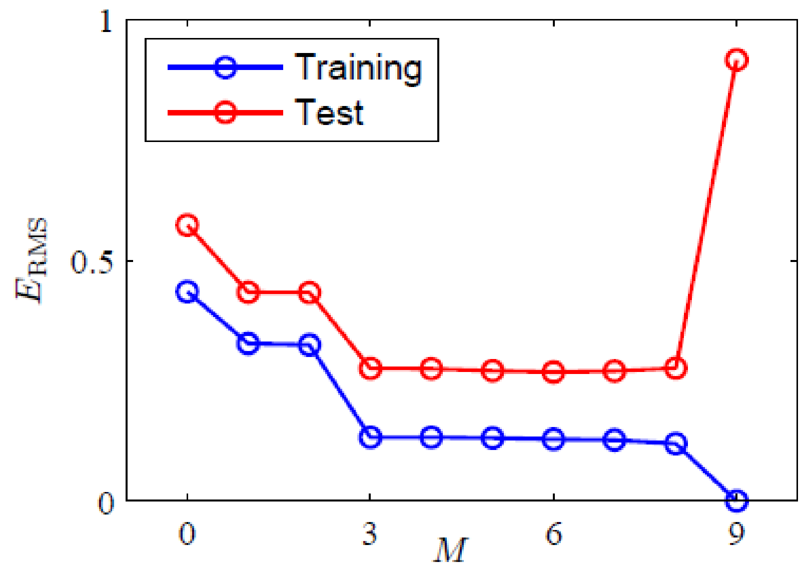
$$g(\theta_0 + \theta_1 x_1 + \theta_2 x_1^2 \\ + \theta_3 x_1^2 x_2 + \theta_4 x_1^2 x_2^2 \\ + \theta_5 x_1^2 x_2^3 + \theta_6 x_1^3 x_2 + \ldots$$

UNDERFITTING
(high bias)

OVERFITTING
(high variance)

Overfitting Example

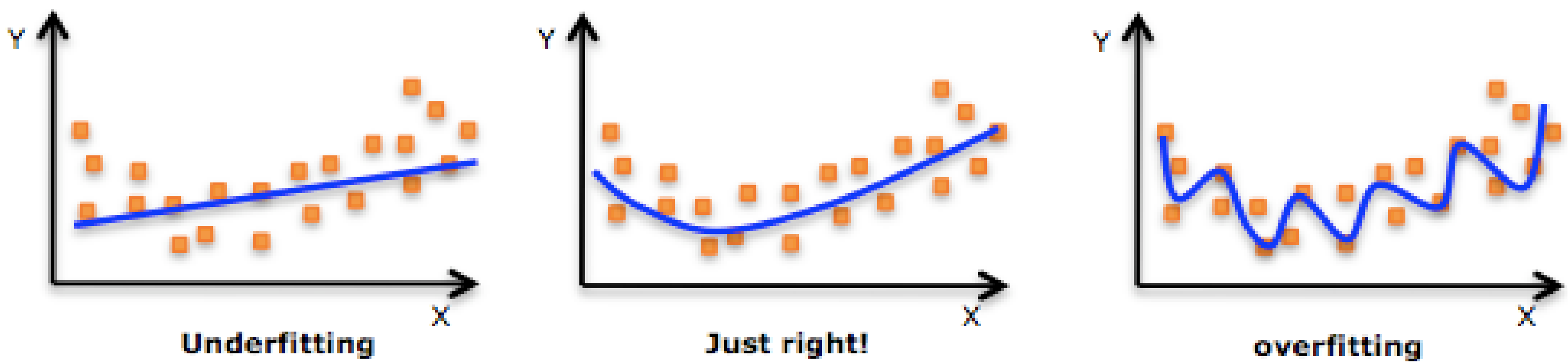
Example from Bishop, Figure 1.5



For any given N, some h of sufficient complexity fits the data but may have very bad generalization error!!

Regularization

Tuning or selecting the preferred level of model complexity so your models are better at predicting (generalizing)



Regularization Concept

- Non-negative loss function
  L(actual value, predicted value)
- Fit your model in a such way that its predictions minimize mean of loss function, calculated only on training data

$$\text{Model} = \text{argmin} \sum L(\text{actual}, \text{predicted}(\text{Model}))$$

- Explain patterns but also explains random noise
- Degradation of generalization ability

$$\text{Model} = \text{argmin} \sum L(\text{actual}, \text{predicted}(\text{Model})) + \lambda R(\text{Model})$$

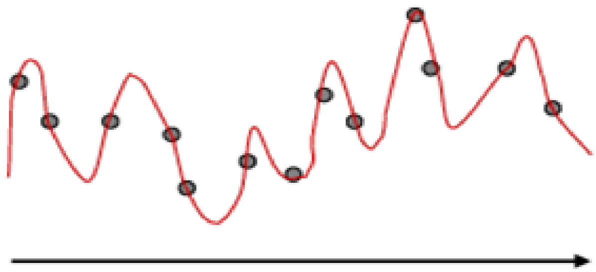
Regularization

– The minimization

$$\min_f |Y_i - f(X_i)|^2$$

may be attained with zero errors.

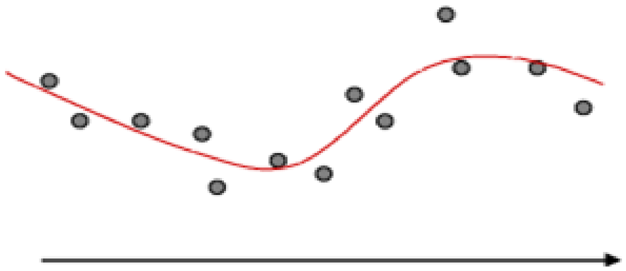
But the function may not be unique.



– Regularization

$$\min_{f \in H} \sum_{i=1}^{n} |Y_i - f(X_i)|^2 + \lambda \|f\|_H^2$$

- Regularization with smoothness penalty is preferred for uniqueness and smoothness.



Ridge Regression

- Technique for analyzing multiple regression data that suffer from multicollinearity
- Addresses some of the problems of OLS by imposing a penalty on the size of coefficients
- The ridge coefficients minimize a penalized residual sum of squares

$$\min_{w} {\|Xw - y\|_2}^2 + \alpha {\|w\|_2}^2$$

- Complexity parameter that controls the amount of shrinkage: the larger the value of , the greater the amount of shrinkage and thus the coefficients become more robust to collinearity

Lasso

- Least absolute shrinkage and selection operator
- Linear model that estimates sparse coefficients
- Tendency to prefer solutions with fewer parameter values
- Reducing the number of variables upon which the given solution is dependent

$$\min_{w} \frac{1}{2n_{samples}} ||Xw - y||_2^2 + \alpha ||w||_1$$

Elastic Net

- Overcomes the limitations of Lasso
- Large *p*, small *n*" case – high-dimensional data with few examples or group of highly correlated variables
- Adds a quadratic part to the penalty $\|\beta\|^2$

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}}(\|y - X\beta\|^2 + \lambda_2\|\beta\|^2 + \lambda_1\|\beta\|_1).$$

- includes the LASSO and ridge regression

Logistic Regression

- Analyze relationships between a dichotomous dependent variable and metric or dichotomous independent variables
- The log odds of the outcome is modeled as a linear combination of the predictor variables
- Combines the independent variables to estimate the probability that a particular event will occur, i.e. a subject will be a member of one of the groups defined by the dichotomous dependent variable
- Classification using Regression

What Logistic Regression Predicts

- The variate or value produced by logistic regression is a probability value between 0.0–1.0
- Probability for group membership in the modeled category is above/below some cut point (the default is 0.50) determines the group
- For any given case, logistic regression computes the probability that a case with a particular set of values for the independent variable is a member of the modeled category

Logistic Regression

- Models relationship between set of variables X_i
  - dichotomous (yes/no, smoker/nonsmoker)
  - categorical (social class, race)
  - continuous (age, weight, gestational age)

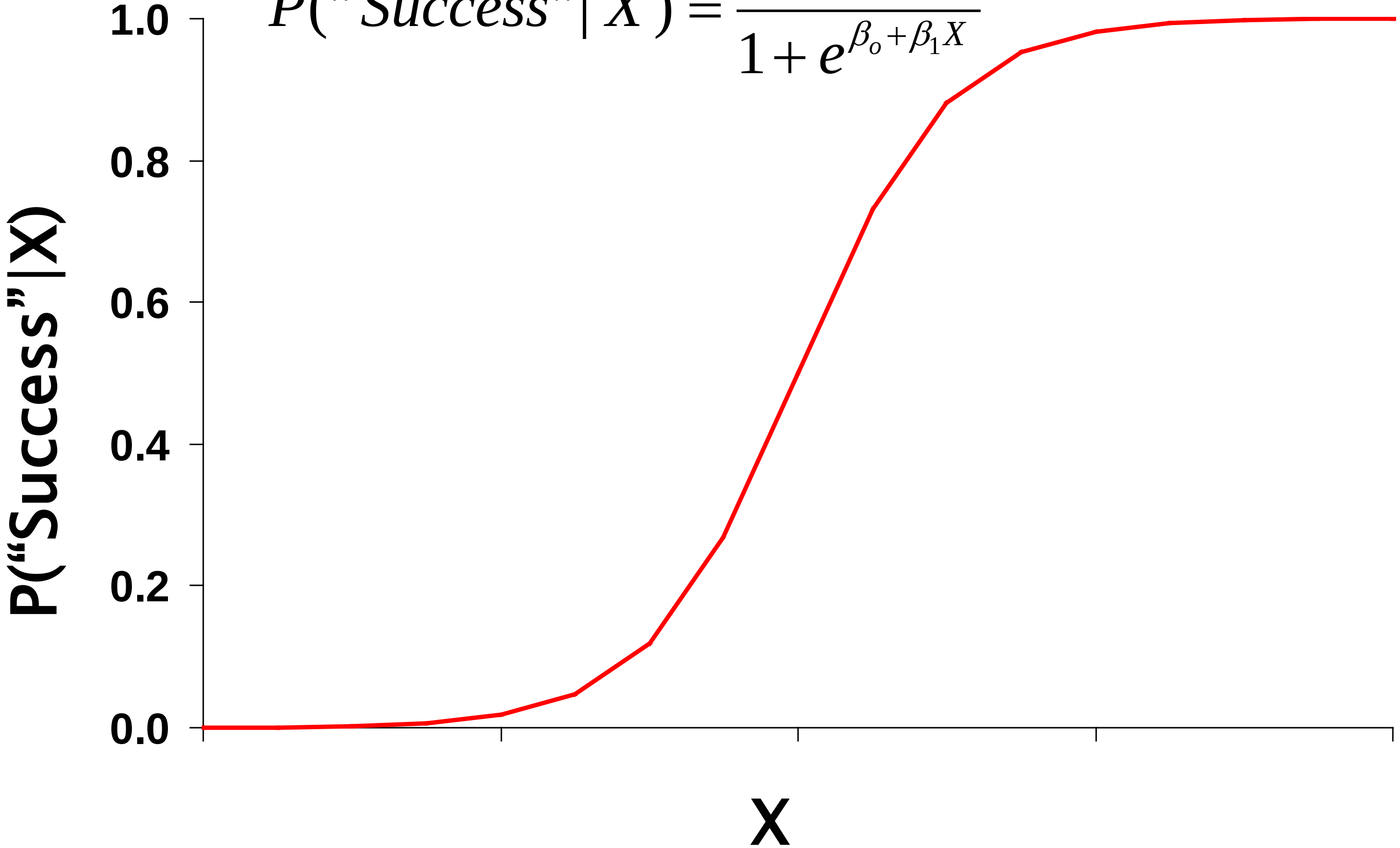
and

  - dichotomous categorical response variable Y

    e.g. Success/Failure, Remission/No Remission Survived/Died, CHD/No CHD, Low Birth Weight/Normal Birth Weight

Logistic Function

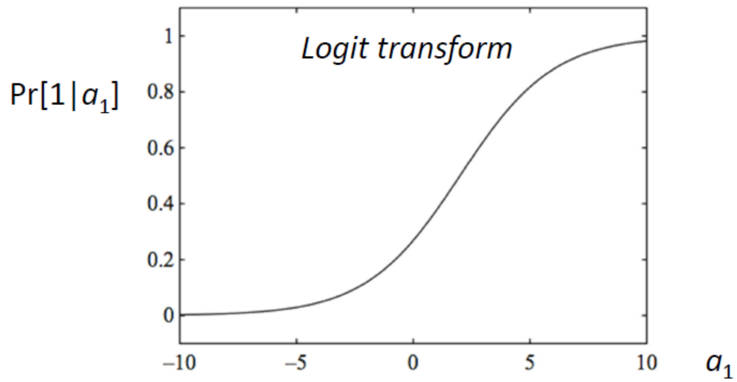
$$P(\text{"}Success\text{"} \mid X) = \frac{e^{\beta_o + \beta_1 X}}{1 + e^{\beta_o + \beta_1 X}}$$



Logit Transform

- Linear regression calculate a linear function and threshold
- Logistic Regression estimate class probabilities directly

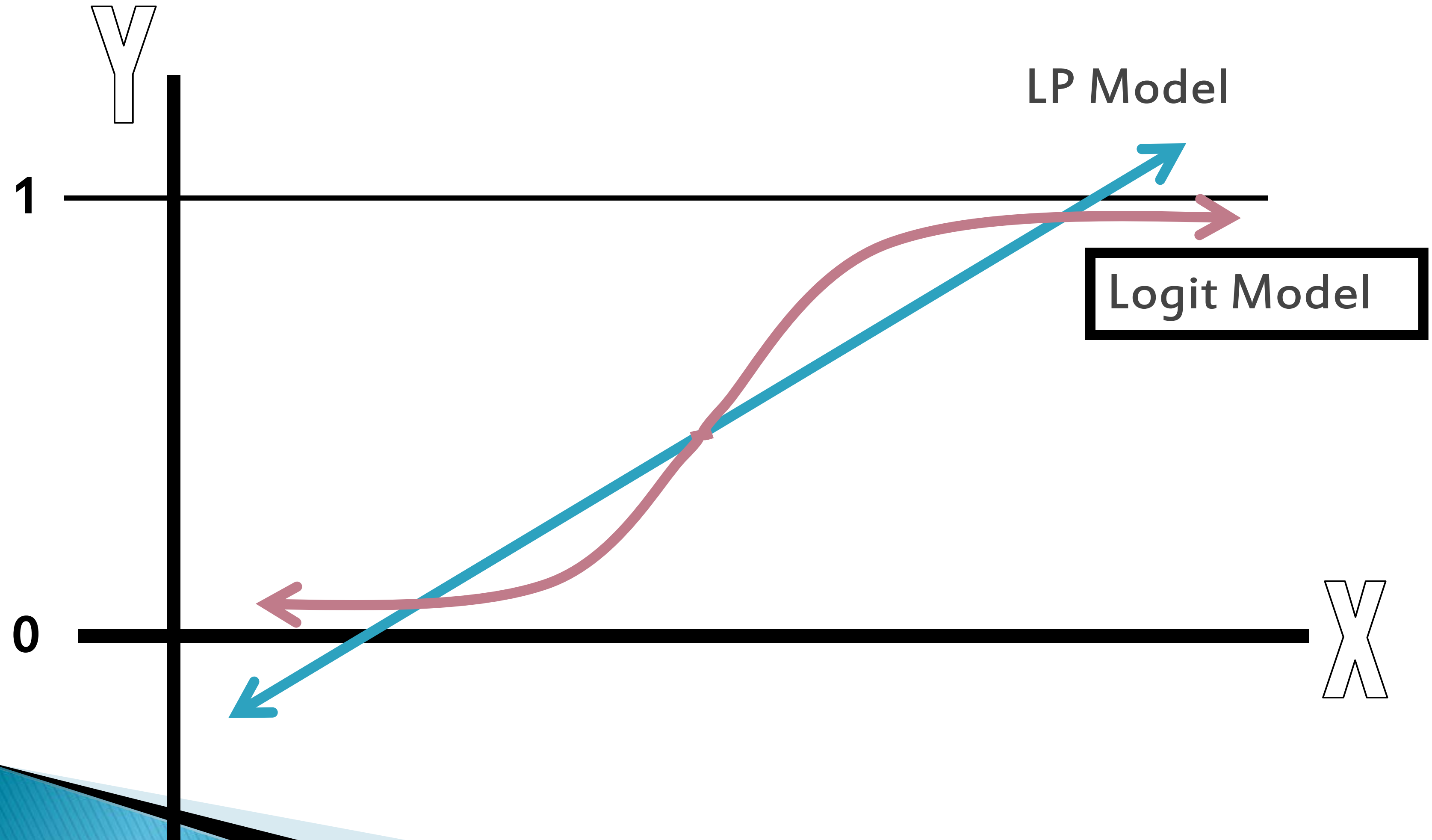
$$\Pr[1 \mid a_1, a_2, \dots, a_k] = 1/(1+\exp(-w_0 - w_1 a_1 - \dots - w_k a_k))$$



- Choose the weights to maximize the log-likelihood

$$\sum_{i=1}^{n} (1 - x^{(i)}) \log(1 - \Pr[1 \mid a_1^{(1)}, a_2^{(2)}, \dots, a_k^{(k)}]) + x^{(i)} \log(\Pr[1 \mid a_1^{(1)}, a_2^{(2)}, \dots, a_k^{(k)}])$$

Comparing LP and Logit Models



When To Use Logistic Regression

- In logistic regression the response (Y) is a dichotomous categorical variable
- Uses logit transform to predict probabilities directly (similar to Naïve Bayes)
- Used widely in many fields, including the medical and social sciences
- Predict whether an American voter will vote Democratic or Republican

Generalized Models in Scikit

- http://scikit-learn.org/stable/modules/linear_model.html

Linear regression equation for the CPU data

- PRP =

  – 56.1

  + 0.049 MYCT

  + 0.015 MMIN

  + 0.006 MMAX

  + 0.630 CACH

  – 0.270 CHMIN

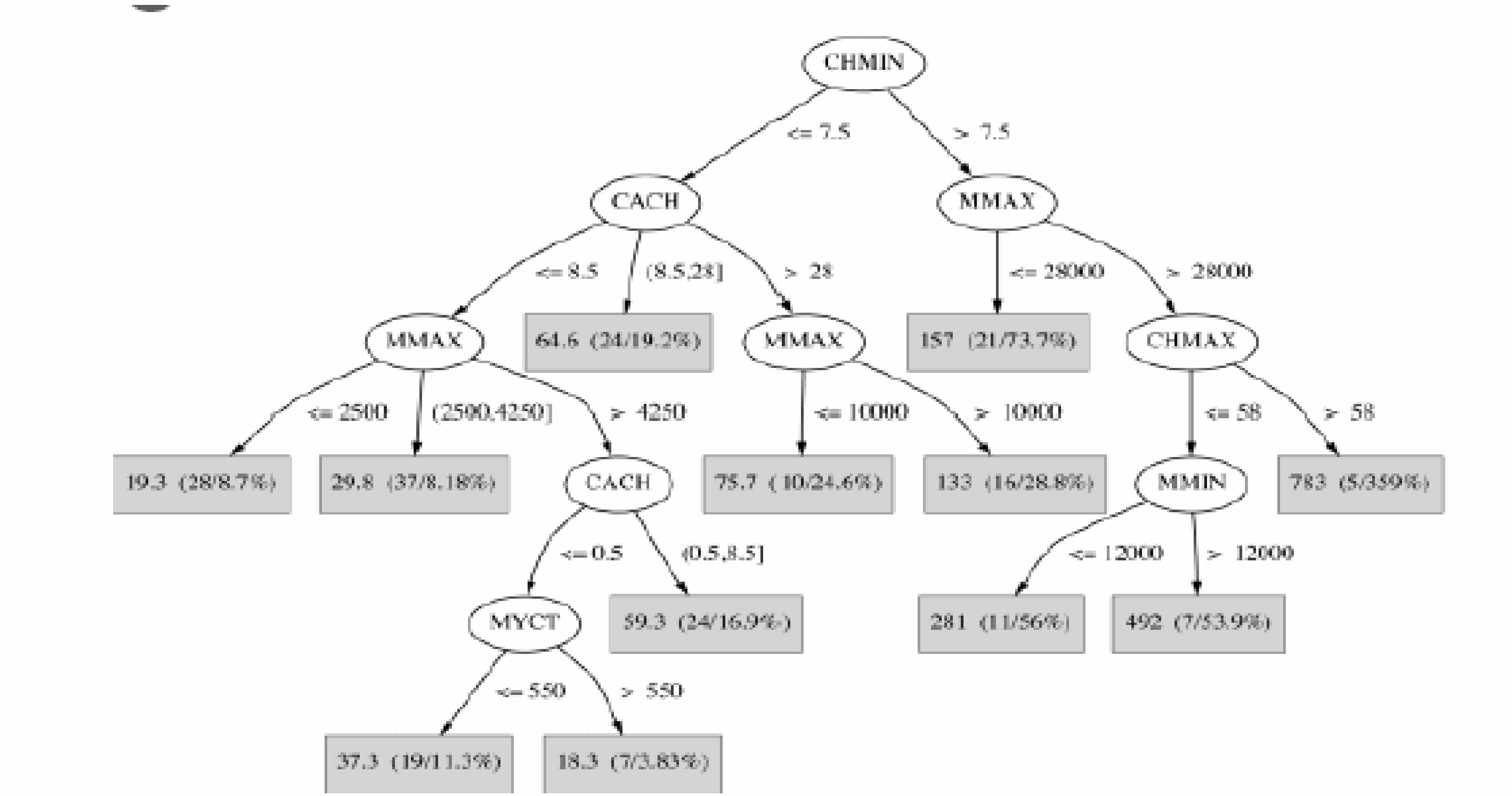
  + 1.46 CHMAX

	Cycle Time (ns)	Main Memory (Kb)		Cache (Kb)	Channels		Performance
	MYCT	MMIN	MMAX	CACH	CHMIN	CHMAX	PRP

Non-linear Regression: Regression and Model trees

- Similar to decision trees
- Modifications
  - Splitting criterion to minimize intra-subset variation
  - Termination criterion reached when standard deviation becomes insignificant
  - Pruning criterion based on numeric error measure
  - Leaf predicts average class values of instances
- Easy to interpret
- Python:
  http://scikitlearn.org/0.11/modules/tree.html#classification

Regression tree for the CPU data

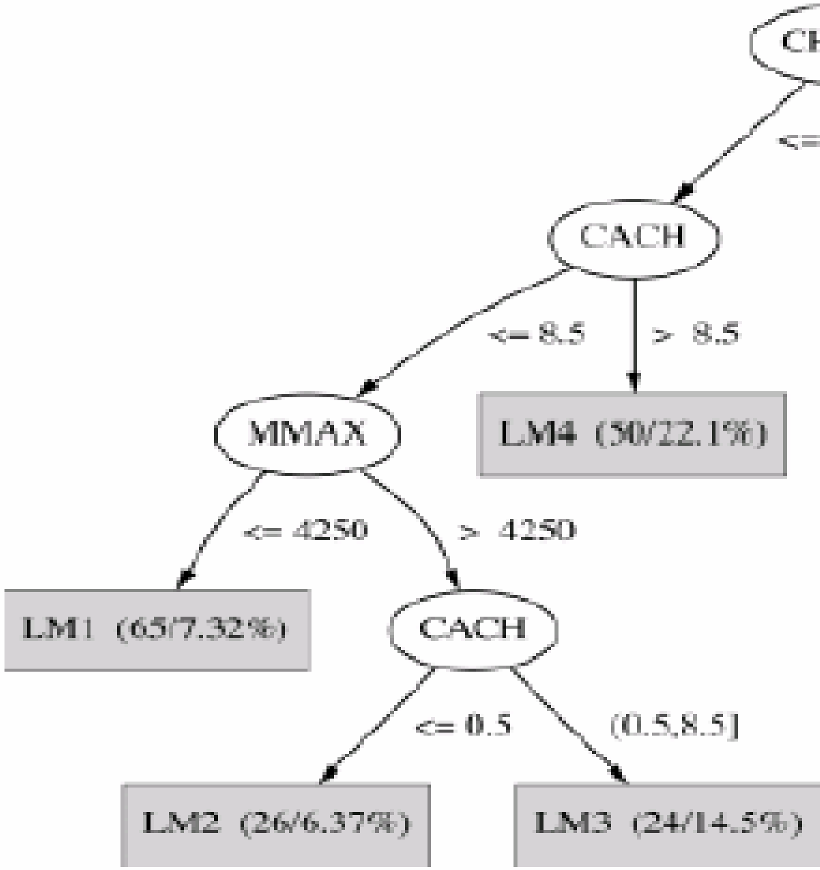


From Witten, Frank, Third Edition

Model trees

- Build a regression tree
- Each leaf -> linear regression function
- Smoothing: factor in ancestor's predictions
  - Smoothing formula: (function) $p' = (np+kq)/(n+k)$
  - Same effect can be achieved by incorporating ancestor models into the leaves
- Need linear regression function at each node
- At each node, use only a subset of attributes
  - Those occurring in subtree (+maybe those occurring in path to the root)
- Fast: tree usually uses only a small subset of the attributes

Model tree for CPU data set



LM1 PRP = 8.29 + 0.004 MMAX + 2.77 CHMIN
LM2 PRP = 20.3 + 0.004 MMIN – 3.99 CHMIN + 0.946 CHMAX
LM3 PRP = 38.1 + 0.012 MMIN
LM4 PRP = 19.5 + 0.002 MMAX + 0.698 CACH + 0.969 CHMAX
LM5 PRP = 285 – 1.46 MYCT + 1.02 CACH – 9.39 CHMIN
LM6 PRP = –65.8 + 0.03 MMIN – 2.94 CHMIN + 4.98 CHMAX

Model Trees: Building the tree (Splitting)

- Splitting: standard deviation reduction
- $SDR = sd(T) - \Sigma i \; |Ti/T| \times sd(Ti)$ (function)
- Termination:
  - Small Standard Deviation (example < 5% of its value on full training set
  - Too few instances remain (e.g. < 4)

Model Trees: Building a Tree (Pruning)

- Heuristic estimate of absolute error of LR models:
- Function (n+v)/(n−v) * average_absolute_error
- Greedily remove terms from LR models to minimize estimated error
- Heavy pruning: single model may replace whole subtree
- Proceed bottom up: compare error of LR model at internal node to error of subtree

Evaluating Numeric Prediction

- Same strategies: independent test set, cross validation, significance tests, etc.
- Difference: error measures
- Most popular measure: mean squared error
- Easy to manipulate mathematically

Summary

- Regression: the process of computing an expression that predicts a numeric quantity
- Linear Regression: simple method for numeric prediction of for linear data
- Regression Tree: “decision tree” where each leaf predicts a numeric quantity
  - Predicted value is average value of training instances that reach the leaf
- Model Tree : “regression tree” with linear regression models at the leaf nodes
  - Linear patches approximate continuous function
    - Linear regression model that predicts the class value of instances that reach the leaf