Regression



Adrian Barbu

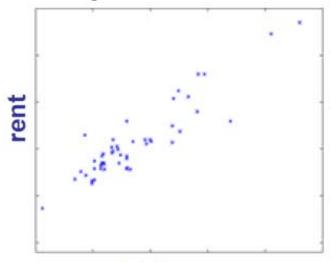
Apartment Rent Modeling

- Want to predict the rent amount
- We are given:
 - The living area (sq ft) of the apartment
 - Number of bedrooms
 - Distance from campus
- Learning=Target function approximation
- Training set:

Living Area	# Bedrooms	Dist from campus	Rent
655	1	2.5	700
550	1	2.1	600
820	2	1.8	1000
830	2	1.1	1200

Test set

675	1	1.5	?
800	2	2.2	?



Living area

Problem Setup

- Features (aka predictors or attributes)
 - Area, #Bedrooms, dist from campus, ...
 - Obtain a feature vector $\mathbf{x} = (x_1, ..., x_p)$
- Target
 - Rent amount y
- Training Set $\{(\mathbf{x}_i, y_i), i = 1, ..., N\}$
- Learn a function $y = f(\mathbf{x})$ that best interpolates

$$\{(\mathbf{x}_i, y_i), i = 1, ..., N\}$$

Linear Regression

Assume f is linear in the predictors

$$f(\mathbf{x}) = f_{\beta}(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

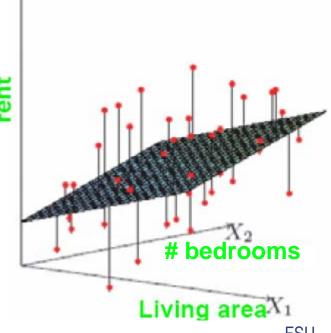
A measure (cost) of how well it interpolates the training data

$$L(\beta) = \sum_{i=1}^{N} (y_i - f_{\beta}(\mathbf{x}_i))^2 + \lambda \|\beta\|^2$$

Write

$$X = \begin{pmatrix} 1 & \mathbf{x}_1 \\ \dots & \\ 1 & \mathbf{x}_N \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1p} \\ \dots & \ddots & \\ 1 & x_{N1} & \dots & x_{Np} \end{pmatrix} \mathbf{E}$$

$$Y = \begin{pmatrix} y_1 \\ \dots \\ y_N \end{pmatrix}$$



Linear Regression

- $\blacksquare \quad \text{Then } f(X) = X\beta$
- Can write the cost in matrix form

$$L(\beta) = (Y - X\beta)^{T} (Y - X\beta) + \lambda \beta^{T} \beta$$

- \blacksquare Quadratic function in β , one global minimum
- Set partial derivatives to zero
- By matrix calculus (or tedious computation) obtain the normal equations

$$X^T X \beta + \lambda \beta = X^T Y$$

Obtain

$$\beta = (X^T X + \lambda I_p)^{-1} X^T Y$$

Linear Regression

Analytical solution

$$\beta = (X^T X + \lambda I_p)^{-1} X^T Y$$

Pros and cons:

- Pros: Easy to implement, obtain result in one step
- Cons: memory problems, stability is X^TX is almost singular
- Gradient descent

$$\beta^{t+1} = \beta^t + \eta(X^T Y - X^T X \beta^t - \lambda \beta^t)$$

Pros and cons:

- Pros: Obtain a result even if X^TX is singular
- Cons: iterative, need to wait to converge

Cross-validation

- A more reliable estimate of prediction accuracy
- K-fold cross-validation:
 - Divide all data into K subsets randomly
 - Repeat for j=1 to K:
 - Train an all data except subset j
 - Evaluate prediction accuracy on subset j, obtain ε_i
 - Final prediction accuracy is the average of all $\epsilon_{\rm i}$

$$\epsilon = \frac{1}{K} \sum_{j=1}^{K} \epsilon_j$$

- Usually K=4-10 or even more
- In some cases K=N (the number of samples)
 - Leave one out cross-validation

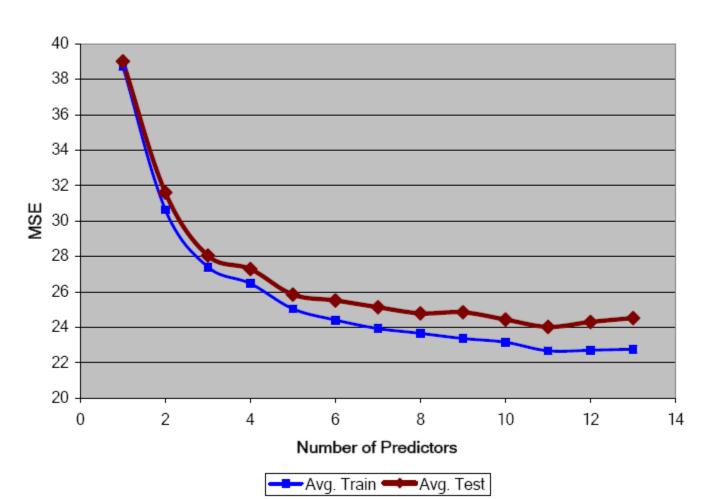
Example: Boston Housing Data

- 506 observations
- 13 predictors:
 - 1. crime per capita crime rate by town
 - zoned proportion of residential land zoned for lots over 25,000 sq.ft.
 - industry proportion of non-retail business acres per town
 - 4. chas Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
 - 5. nox nitric oxides concentration (parts per 10 million) 3.
 - 6. rooms average number of rooms per dwelling
 - age proportion of owner-occupied units built prior to 1940
 - 8. dist weighted distances to five Boston employment centres
 - 9. hwy index of accessibility to radial highways
 - tax full-value property-tax rate per \$10,000
 - 11. pteacher pupil-teacher ratio by town
 - bk 1000(Bk 0:63)2 where Bk is the proportion of blacks by town
 - 13. Istat % lower status of the population
- Output: house value

Boston Housing Data

- Optimal number of predictors: 11
- 2-fold cross-validation

Average Training MSE and Testing MSE vs. Number of Predictors



Avoiding Overfitting

- Variable selection
 - Prefer fewer variables (Occam's razor)
- Two types of model (variable) selection methods:
 - Testing-based procedures
 - Forward selection
 - Backward elimination
 - Stepwise regression
 - Criterion-based procedures
 - Akaike Information Criterion, Bayes Information Criterion
 - Adjusted R²
 - Mallow C_p statistic

P-value

Fit the model

$$\beta = (X^T X)^{-1} X^T Y$$

Standardize the i-th coefficient

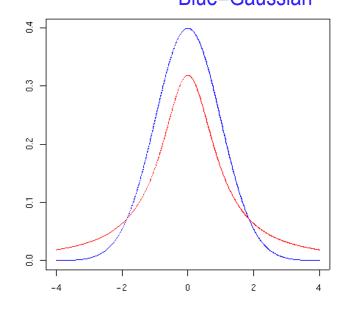
$$t_i = \hat{\beta}_i / se(\hat{\beta}_i) = \hat{\beta}_i / \sqrt{(X^T X)_{i+1,i+1}^{-1}} \hat{\sigma}$$

- Under the null hypothesis β_i =0:
 - t_i should follow a t-distribution (red)
- p-value = probability that for a random value ρ from the t-distribution

$$|\rho| \ge |t_i|$$

■ Small p-value means β_i is significant





Testing-Based Variable Selection

Backward Elimination

- 1. Fit a model with all variables
- 2. Remove least significant variable with p-value at least 0.05
- 3. Refit the model and repeat step 2 while possible

Forward Selection

- Start with a constant model
- 2. Compute the p-value for each variable when added to the model
- 3. Add the most significant variable with p-value less than 0.05
- 4. Repeat steps 2-3 as long as possible

Stepwise Regression

- A combination of Forward Selection and Backward Elimination
- Has many variants

Criterion-Based Variable Selection

- Test all combinations of variables
- Tradeoff accuracy (RSS) with model complexity (p)
- Select best tradeoff according to a criterion:
 - Akaike Information Criterion

$$AIC = -2N\log(RSS/N) + 2p$$

Bayes Information Criterion

$$BIC = -2N\log(RSS/N) + p\log N$$

Adjusted R²

$$R_a^2 = 1 - \frac{RSS/(N-p)}{\sum_{i=1}^n (y_i - \bar{y})^2/(N-1)}$$

Mallow C_p statistic

$$C_p = \frac{RSS_p}{\hat{\sigma}^2} + 2p - N$$

Advantages and Disadvantages

- Testing-based procedures:
 - Fast
 - Greedy, suboptimal
 - Might not solve the right problem
- Criterion-based procedures
 - Exhaustive, more powerful
 - Slow, can only deal with as many as 15-20 variables
- Sensitive to Outliers

Nonlinear Basis Functions

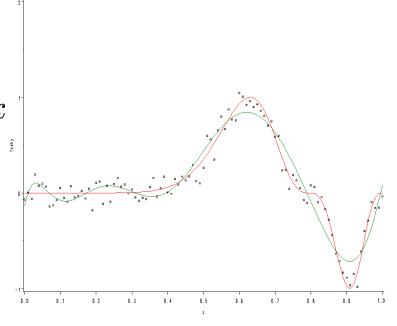
- Can transform the features through any functions we want
- Apply LR to the transformed features (basis functions)

$$y = \beta_0 + \beta_1 \phi_1(\mathbf{x}) + \dots + \beta_k \phi_k(\mathbf{x}) = \beta^T \phi(\mathbf{x})$$

E.g. polynomial regression

$$\phi = (1, x, x^2, ..., x^k)$$

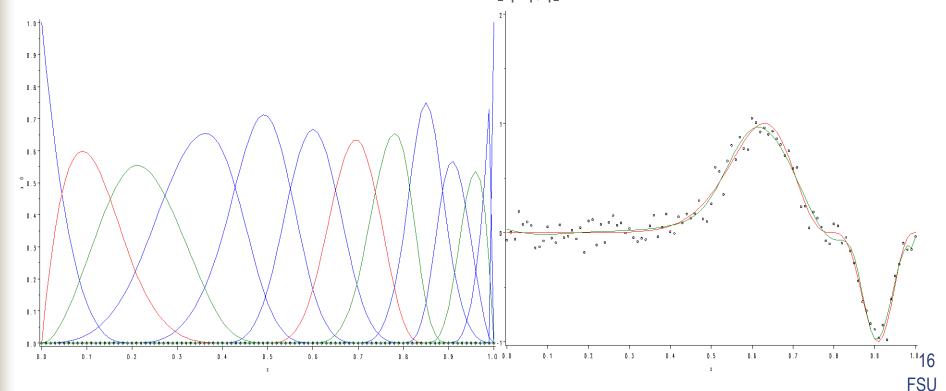
$$y = \beta_0 + \beta_1 x + ... + \beta_k x^k$$



Spline Basis Functions

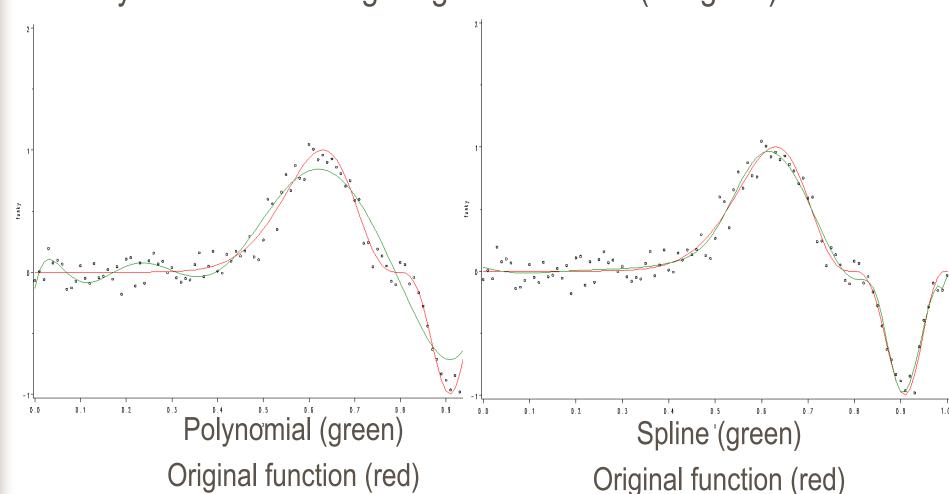
Basis functions

- A set of interval points $t_0, t_1, ..., t_k$ called knots
- Degree 3 polynomial on each interval [t_i,t_{i+1}]
- C¹ continuity
- Basis function i is zero outside [t_i,t_{i+4}]



Spline vs Polynomial Basis Functions

- Splines are local and more flexible
- Polynomials have long range interactions (not good)



Robust Regression

- Quadratic Cost Function → sensitive to outliers
- One solution: M-estimation
 - Minimize

$$Cost(\beta) = \sum_{i=1}^{N} \rho(y_i - \mathbf{x}_i \beta)$$

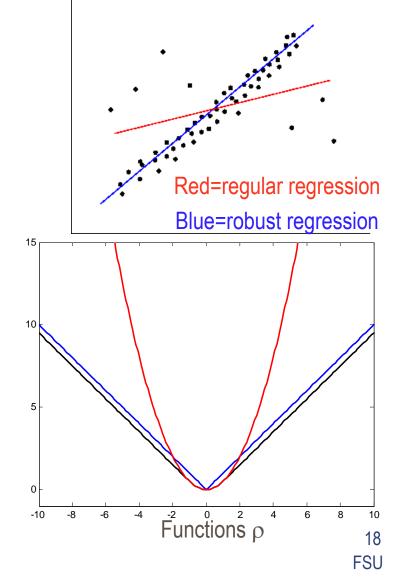
- Regular regression has $\rho(x) = x^2$
- Least Absolute Deviation (LAD)

$$\rho(x) = |x|$$

Huber

$$\rho(x) = \begin{cases} x^2/2 & \text{if } |x| < c \\ c|x| - c^2/2 & \text{otherwise} \end{cases}$$

 ρ gives smaller weight to large errors



M-Estimation

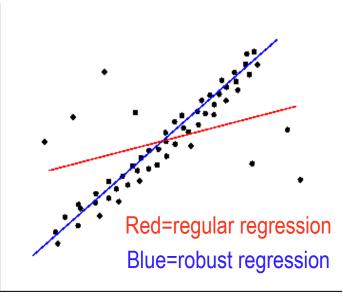
- M-estimation=Convex optimization
- One algorithm:
- Initialize β
- 2. Compute weights

$$w_i = \rho'(y_i - \mathbf{x}_i\beta)/(y_i - \mathbf{x}_i\beta)$$

3. Reestimate β by weighted regression

$$Cost_W(\beta) = \sum_{i=1}^{N} w_i (y_i - \mathbf{x}_i \beta)^2$$

4. Repeat 2-3 until convergence



Robust Regression

- Another solution: Least Trimmed Squares
 - Robust cost function

$$Cost(\beta) = \sum_{i=1}^{q} \hat{\epsilon}_{(i)}^2$$

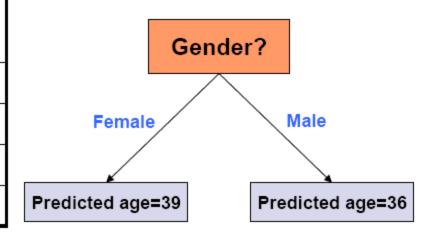
where $\hat{\epsilon}_{(i)}$ are the sorted residuals $\hat{\epsilon}_i = y_i - \mathbf{x}_i \beta$ (in increasing order) and q is about N/2

- Largest errors do not influence the cost (hence robustness)
- Minimization is tricky since Cost is not convex
 - Use a random method such as MCMC
- Slower but more powerful than M-estimation

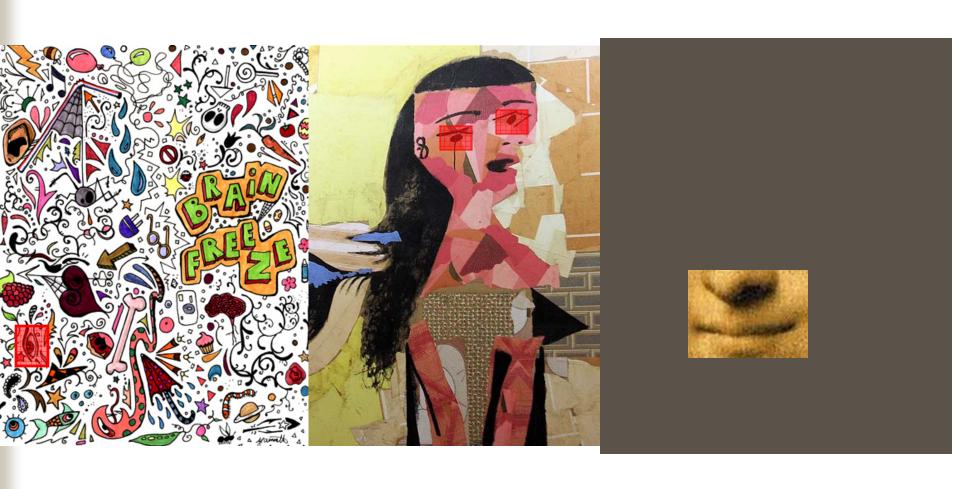
Regression Tree

Decision tree for regression

Gender	Rich?	Num. Children	# travel per yr.	Age
F	No	2	5	38
M	No	0	2	25
М	Yes	1	0	72
:	:	:	:	:



Object Detection and Context

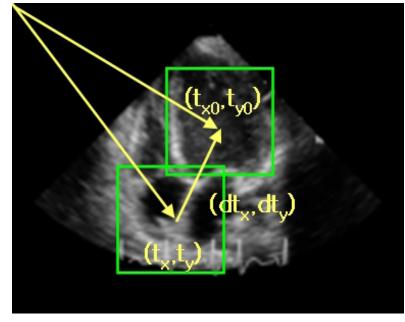


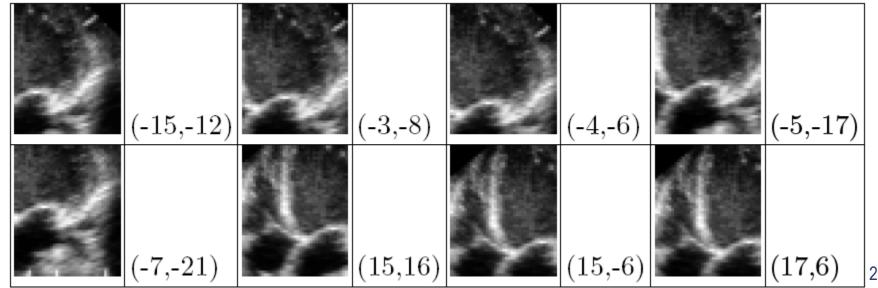
Application: Image Based Regression

Given a location, want the relative position of the LV Center

Training

- Each coordinate is trained independently
- Training data: 13,500 pairs image + relative location





Regression Details

- 10,000 predictors (Haar features)
- Only 200 are selected to be used
- Train a regressor for each coordinate independently
- Use a linear combination of locally constant regressors
 - Select best one
 - Select next one that minimizes the residual error
 - And so on

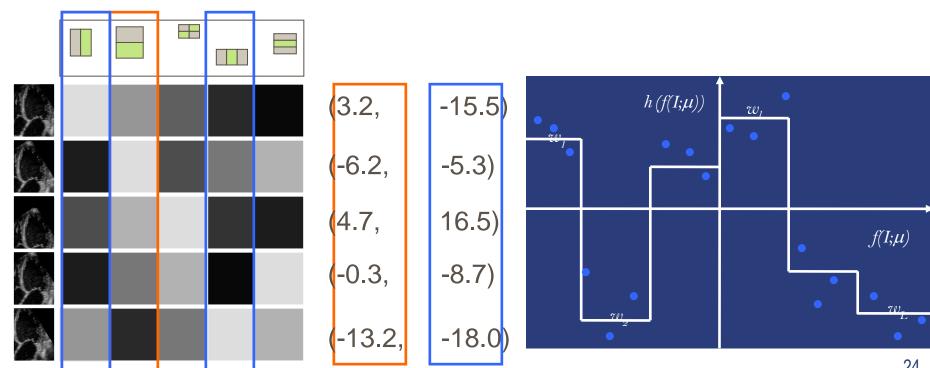
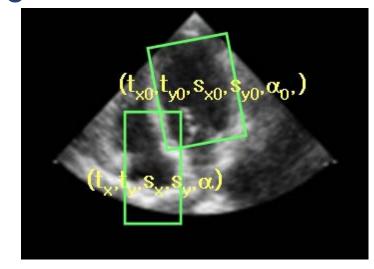
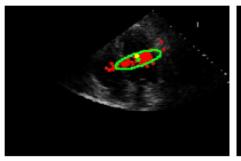


Image Based Regression

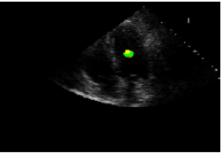
- 5 LV parameters:
 - Position (t_x, t_y)
 - Scale (s_x, s_y)
 - Rotation angle α
- Start from 200 random locations



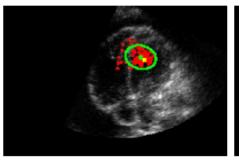
- Use a detector based on Boosting to filter the final result
- S. Zhou and D. Comaniciu. Shape Regression Machine. Information Processing in Medical Imaging (IPMI), 2007



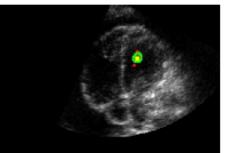
Top 100 locations



After detector



Top 100 locations



After detector

Conclusions

- Regression = learning target functions with continuous output
- Issues with regression:
 - Overfitting → variable selection
 - Outliers → robust regression
 - Linear vs. non-linear → polynomial, splines, locally constant

- Applications:
 - Apartment rent, house prices
 - Diabetes, prostate, BMI, age
 - Relative location of LV