# Data Mining

CS57300 Purdue University

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- Regression
- Posteriors
- Working with Data

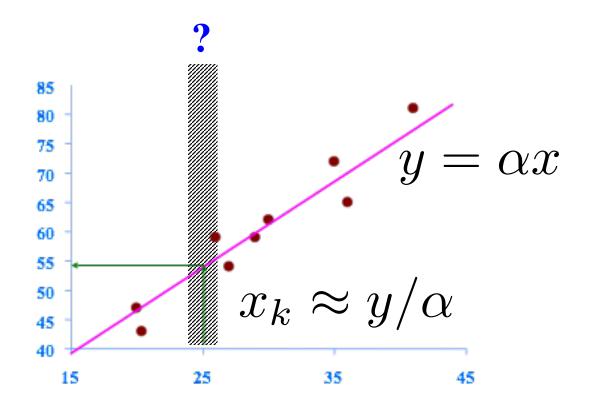
Linear Regression: Review

# Linear Regression (use A)

 Interpolation (something is missing)

• 
$$(x_1, ..., x_t)$$

• 
$$(y_1, ..., y_t)$$



## Auto-regression: Predicting Next Value After t Steps Linear Regression (use B)

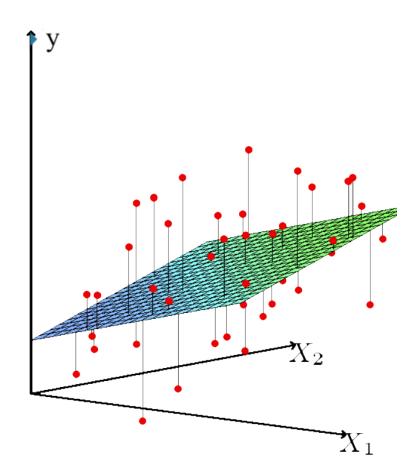


$$x_{t+1} = \sum_{i=t-w}^{t} a_i x_i + \epsilon_{\text{noise}}$$

Similar problem to linear regression: express unknowns as a linear function of knowns

# Predictions from High-Dimensional Historical Data

$$\mathbf{y}_{[t \times 1]} = \mathbf{X}_{[t \times w]} \mathbf{a}_{[w \times 1]}$$



- Over-constrained problem
  - a is the vector of the regression coefficients
  - X has the *t* values of the *w* independent variables. These independent variables can mix user characteristics with a window of past observations
  - y has the t values of the dependent variable

### Looking Into Multiplication

may want to add social media variables







time

$$\begin{bmatrix} X_{11}, X_{12}, \dots, X_{1w} \\ X_{21}, X_{22}, \dots, X_{2w} \\ \vdots \\ X_{t1}, X_{t2}, \dots, X_{tw} \end{bmatrix} \times \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_w \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_t \end{bmatrix}$$

$$\times \left[ \begin{array}{c} a_1 \\ a_2 \\ \vdots \\ a_w \end{array} \right] = \left[ \begin{array}{c} y_1 \\ y_2 \\ \vdots \\ y_t \end{array} \right]$$

#### How to Estimate *a*?

• 
$$\mathbf{a} = (\mathbf{X}^{\mathrm{T}} \cdot \mathbf{X})^{-1} \cdot (\mathbf{X}^{\mathrm{T}} \cdot \mathbf{y})$$

 $\mathbf{X}^+ = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T$  is the Moore–Penrose pseudoinverse

Or: 
$$\mathbf{a} = \mathbf{X}^+ \mathbf{y}$$

 $\boldsymbol{a}$  is the vector that minimizes the Root Mean Squared Error (RMSE) of  $(y-X\cdot\boldsymbol{a}^T)$ 

### Details: Least Squares Optimization

Least squares cost function:

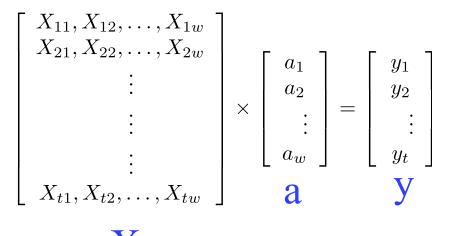
$$C = \frac{1}{2} \sum_{i=1}^{t} (\mathbf{y}_i - \mathbf{x}_i^T \mathbf{a})^2 = \frac{1}{2} (y - \mathbf{X}a)^T (y - \mathbf{X}a)$$

Find a that minimizes cost C

$$\frac{\partial C}{\partial \mathbf{a}} = \frac{1}{2} \frac{\partial}{\partial \mathbf{a}} (\mathbf{y} - \mathbf{X}\mathbf{a})^T (\mathbf{y} - \mathbf{X}\mathbf{a})$$
$$= -(\mathbf{y} - \mathbf{X}\mathbf{a})^T \mathbf{X}$$

· Optimal value at:

timal value at: 
$$\frac{\partial C}{\partial \mathbf{a}} = 0 \implies \mathbf{X}^T \mathbf{y} = \mathbf{X}^T \mathbf{X} \mathbf{a} \implies \mathbf{a} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$



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Or: 
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**a** is the vector that minimizes the Root Mean Squared Error (RMSE) of  $(y - X \cdot a^T)$ 

#### Problems:

Matrix X grows over time & needs matrix inversion

- O(t·w²) computation
- O(t·w) storage

#### Recursive Least Squares

At time t we know  $\mathbf{X}_t = (x_1, \dots, x_t), \quad \mathbf{y}_t = (y_1, \dots, y_t)$ Least squares is solving

$$\underset{\mathbf{a}^{\star}}{\operatorname{argmax}} \|\mathbf{a}^{T}\mathbf{X}_{t} - \mathbf{y}_{t}\|^{2}$$

which gives

$$\mathbf{a}^{\star} = \mathbf{X}^{+}\mathbf{y}$$

where  $\mathbf{X}^+ = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T$ 

Let

$$\mathbf{\Phi}_t = \mathbf{X}_t^T \mathbf{X}_t \qquad \theta_t = \mathbf{X}_t^T y_t$$

Then  $\Phi_{t+1}^{-1}$  is

$$\mathbf{\Phi}_{t+1}^{-1} = (\mathbf{\Phi}_t + \mathbf{x}_{t+1} \mathbf{x}_{t+1}^T)^{-1} = \mathbf{\Phi}_t^{-1} - \frac{\mathbf{\Phi}_t^{-1} \mathbf{x}_{t+1} \mathbf{x}_{t+1}^T \mathbf{\Phi}_t^{-1}}{1 + \mathbf{x}_{t+1}^T \mathbf{\Phi}_t^{-1} \mathbf{x}_{t+1}}$$

# Recursive Least Squares Algorithm

$$\mathbf{\Phi}_{t+1}^{-1} = \mathbf{\Phi}_{t}^{-1} - \frac{\mathbf{\Phi}_{t}^{-1} \mathbf{x}_{t+1}^{T} \mathbf{x}_{t+1}^{T} \mathbf{\Phi}_{t}^{-1}}{1 + \mathbf{x}_{t+1}^{T} \mathbf{\Phi}_{t}^{-1} \mathbf{x}(t+1)}$$

$$\theta_{t+1} = \theta_{t} + \mathbf{x}_{t+1}^{T} \mathbf{y}_{t+1}$$

$$\mathbf{a}_{t+1} = \mathbf{\Phi}_{t+1}^{-1} \theta_{t+1}$$

## Exponentially Weighted Recursive Least Squares Algorithm

for 
$$\lambda > 1$$

$$\mathbf{\Phi}_{t+1}^{-1} = \frac{1}{\lambda} \mathbf{\Phi}_{t}^{-1} - \frac{1}{\lambda^{2}} \frac{\mathbf{\Phi}_{t}^{-1} \mathbf{x}_{t+1}^{T} \mathbf{x}_{t+1}^{T} \mathbf{\Phi}_{t}^{-1}}{1 + \mathbf{x}_{t+1}^{T} \mathbf{\Phi}_{t}^{-1} \mathbf{x}(t+1)}$$
$$\theta_{t+1} = \lambda \theta_{t} + \mathbf{x}_{t+1}^{T} \mathbf{y}_{t+1}$$
$$\mathbf{a}_{t+1} = \mathbf{\Phi}_{t+1}^{-1} \theta_{t+1}$$

### Comparison

#### Original Least Squares

- Needs large matrix (growing in size) O(t×w)
- Costly matrix operation O(t×w²)

#### Recursive LS

- Need much smaller, fixed size matrix O(w×w)
- Fast, incremental computation
   O(1 x w²)
- no matrix inversion



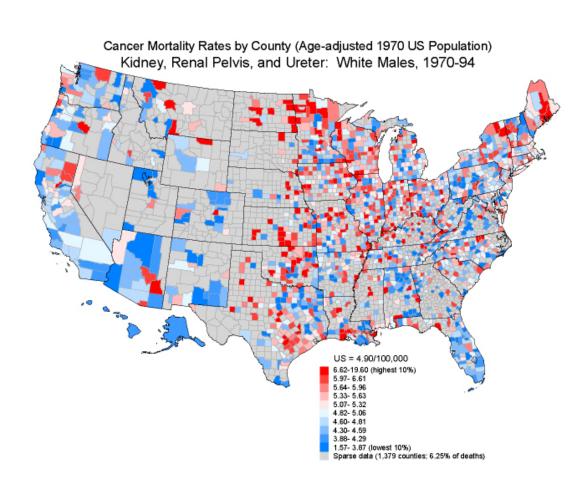
#### Posteriors

### Finding (Real) Patterns in Data

Data shows: rural counties have the highest average mortality rates. But rural counties also have small populations

Cancer Mortality Rates by County (Ag Kidney, Renal Pelvis, and Ureto populations

- Why rural counties have the highest rates of cancer?
  - A: Small sample variance
  - Solution?
  - P[ cancer rate | data]



#### Posteriors (e.g. Representing Fractions)

- Consider creating a model that predicts if a soccer striker will score a goal in a game
- Data includes no. shots on goals and no. goals during the player's career
- Problems with absolute values:
  - number of goals (older players have larger values than young players)
  - no. shots on goals
     (does not reflect rate of shot → goal conversion)
- Feature: % shots on goal resulting in goal
  - Alice (Novice): 1 out of 1  $\rightarrow$  100%
  - Bob (Senior): 300 out of 1000 → 30%
- Solution? (same problem as in the previous slide (cancer rate). The solution is also Bayesian.

#### Reaching (Real) Conclusions with Data

- Whatever conclusion using "cold data", there are always assumptions
- Example: Simpson's Paradox (a.k.a. Yule–Simpson effect)
  - At Berkeley, women applicants overall have lower acceptance rate than men
  - But if you look at every department women are accepted at the same rate as men
  - How? What was our wrong assumption?
    - $O_i$  is a random variable that denotes candidate i gets an offer from Berkeley.
    - $O_{i,j}$  is a random variable that denotes candidate i gets an offer from department j at Berkeley.
    - $A_{i,j}$  is a random variable that denotes candidate i has applied to department j.

$$P[O_i] = \sum_{j} P[O_{i,j}] = \sum_{j} P[O_{i,j}|A_{i,j}]P[A_{i,j}]$$

Working with Data

#### Data Issues

- How to represent the data plays a huge role in the question we can ask and the answers we get
  - It influences similarity metrics
  - It influences the data models we can use
- Data biases (last class)
- Missing data also plays a huge role
- And the problem of outliers in the data
  - Outlier chicken-and-egg problem:
    - Outliers may skew decisions
    - But defining what constitutes an outlier requires deciding a model that describes the "normal" data
    - Deciding such a model requires fitting the data, which may fit the outliers

#### Missing values

- Reasons for missing values
  - Information is not collected (e.g., people decline to give their age)
  - Attributes may not be applicable to all cases (e.g., annual income is not applicable to children)
- Ways to handle missing values
  - Eliminate entities with missing values
  - Estimate attributes with missing values
  - Ignore the missing values during analysis
  - Replace with all possible values (weighted by their probabilities)
  - Impute missing values

Tan, Steinbach, Kumar. Introduction to Data Mining

# Duplicate Data

- Data set may include data entities that are duplicates, or almost duplicates of one another
  - Major issue when merging data from heterogeneous sources
  - Example: same person with multiple email addresses
- Sometimes "duplication" happens (different users, same features).
  - Issues with some models.
- Data cleaning
  - Finding and dealing with duplicate entities
  - Finding and correcting measurement error
  - Dealing with missing values