NAVAL
POSTGRADUATE
SCHOOL

OS4118
Statistical and Machine Learning

Introduction

Prof. Sam Buttrey

Fall AY 2020

Who Am I?

- Prof. Sam Buttrey, buttrey@nps.edu
- A.B., Princeton, Statistics; M.A., Ph.D., U. California-Berkeley, Statistics
- Naval Postgraduate School, Department of Operations Research, 1996-Present
- Interests: Data Analysis, Data Mining, Big Data Analytics and Computing, Classification, Modeling and Applications
- I have taught this course once before…
  - …with a slightly different set-up…
  - …apologies in advance

Admin Notes

- Course via Sakai & Collaborate
- I love email! buttrey@nps.edu
- Telephone: 831-656-3035
- **Travel**: I will miss 6 Nov and 13 Nov classes. My current plan:
  - Pre-record the lecture of 6 Nov
  - Guest lecturer 13 Nov; she will take emails during my absence
  - Sorry for the hassle here

Admin Notes 2

- Exercises: one per week, graded
- Grades: I'll record grades for the exercises on Sakai, but the final grade is mine
- R: I plan to demonstrate stuff in (regular) R; I'm willing to use RStudio too. We may have to turn to AWS – we'll discuss.
- CS approach vs Statistics approach

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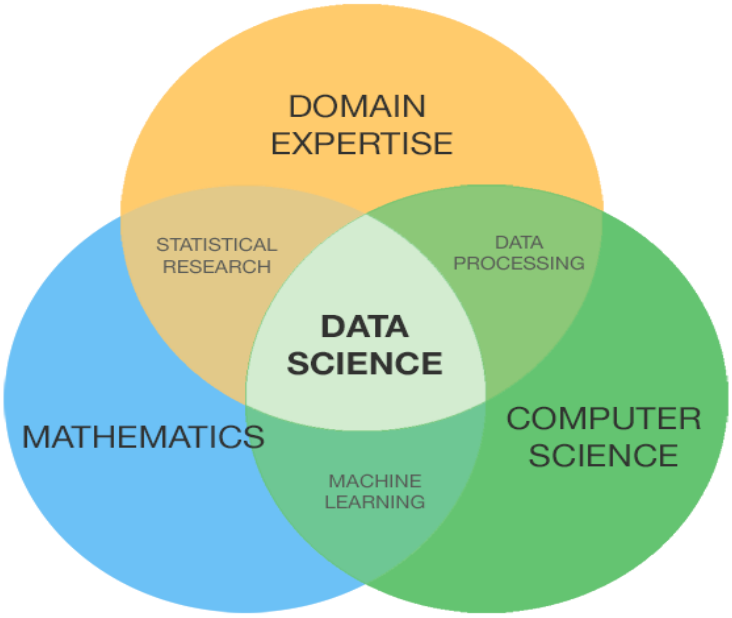
Data Science vis-à-vis Statistics

Math and Statistics Competencies

- Statistical modeling
- Machine learning
- Bayesian inference
- Optimization
- Simulation
- Network science
- Model development



Source: Palmer, Shelly. Data Science for the C-Suite. New York: Digital Living Press, 2015. Print.

Domain Expertise Competencies

- Specific functional area
- Curious about data
- Influence with leaders
- Problem solver
- Make narratives w/data
- Visual design and communication
- Creative, innovative, and collaborative

Computer Science Competencies

- Scripting (Python)
- Statistical computing (R)
- Databases (No/SQL)
- Distributed storage (Hadoop Distributed FS)
- Distributed processing (MapReduce)
- Cloud computing (AWS)

Data pipelines (Pig/Hive)

Data Science is a team sport!

So Far (1)

- Great problems of statistics/analytics:
- **Regression**: we have a series of $(y_i, \boldsymbol{X}_i)$ observations, where the y_i are **numeric**
  - Typically meaning "continuous"
- Goal: predict E $(y \mid \boldsymbol{X}_0)$ for some $\boldsymbol{X}_0$ – or predict some other attribute of $y \mid \boldsymbol{X}_0$
- Tools: linear regression, regularization, regression trees/ensembles…
- Issues: categorical predictors; transformations; interactions;

Issues in Regression

- Ongoing issues
  - Incorporating **categorical** predictors
  - Incorporating **transformations** of *y*, or of one or more X's, or both
  - **Interactions**, where the relationship between *y* and *Xp* depends on the value of *Xq* (and higher-order interactions)
  - **Missing value** handling (both at the time we build the model and at prediction time)
  - Resisting the effect of **outliers**, anomalies, points of high influence

Extending the Regression Model

- Extensions: **integer** data
  - There is a version of GLM that allows the distribution of $y \mid \boldsymbol{X}$ to be Poisson
  - Negative binomial also sometimes used
  - Often there is over-dispersion or weirdly frequent zero counts ("zero-inflated Poisson")
  - **Log-linear models** for counts in tables
- **Repeated measures**
  - Common in experiments on humans
  - Introduces correlation structure for measurements made on the same person

Extending Regression (cont'd)

- **Random effects**
  - When, e.g.. the experimental units are a sample from a population of units – e.g. people – and we're interested in the distribution of effects across the whole population
- Multivariate ANOVA, for a vector-valued *y*
- Non-linear regression, common in chemical and biological applications
- Lots of extensions to these models!

So Far (2)

- **Classification**: we have a series of $(y_i, \boldsymbol{X}_i)$ observations, where the y_i are **categorical**
  - Often binary
- Goal: predict Pr $(y = 1 \mid \boldsymbol{X}_0)$ for some $\boldsymbol{X}_0$ – or the distribution of $y \mid \boldsymbol{X}_0$
- Tools: logistic regression, regularization, classification trees/ensembles…
- Evaluate performance through cross-validation, **test set** performance (but maybe with AUC rather than misclass rate)

Considerations

- Almost all of the issues with regression apply to classification:
  - Transformation, Interactions, missings etc.
- Other issues: **multinomial outcomes** (logistic regression difficult here)
- **Very rare** (or very common) events
  - Where the "naïve model" is very good!
- There is less information per observation in the classification problem

Model Evaluation

- It is critical to evaluate your model on new data – not on the same data you used to build it
- Where possible, an independent **test set** should be used. If not, cross-validation
- In a time series set-up, test set might refer to data after a cutoff (or rolling horizons)
- In a voice-recognition problem, test set would contain **people** not in training set
  - Not just **observations** not in training set

Model Evaluation (cont'd)

- The measure of evaluation should be relevant to the problem at hand
- In regression, "mean square prediction error" (or its square root) is common

$$= \frac{1}{n_{\text{test}}} \sum (y - \hat{y}_i)^2$$

- In two-class classification, we often use **sensitivity** and **specificity**, compute AUC
- Alternatively, **precision** (= #true pos / #pred. pos) and **recall** (= sensitivity = #true pos/#actual pos), ignoring #true neg

Multinomial Classification

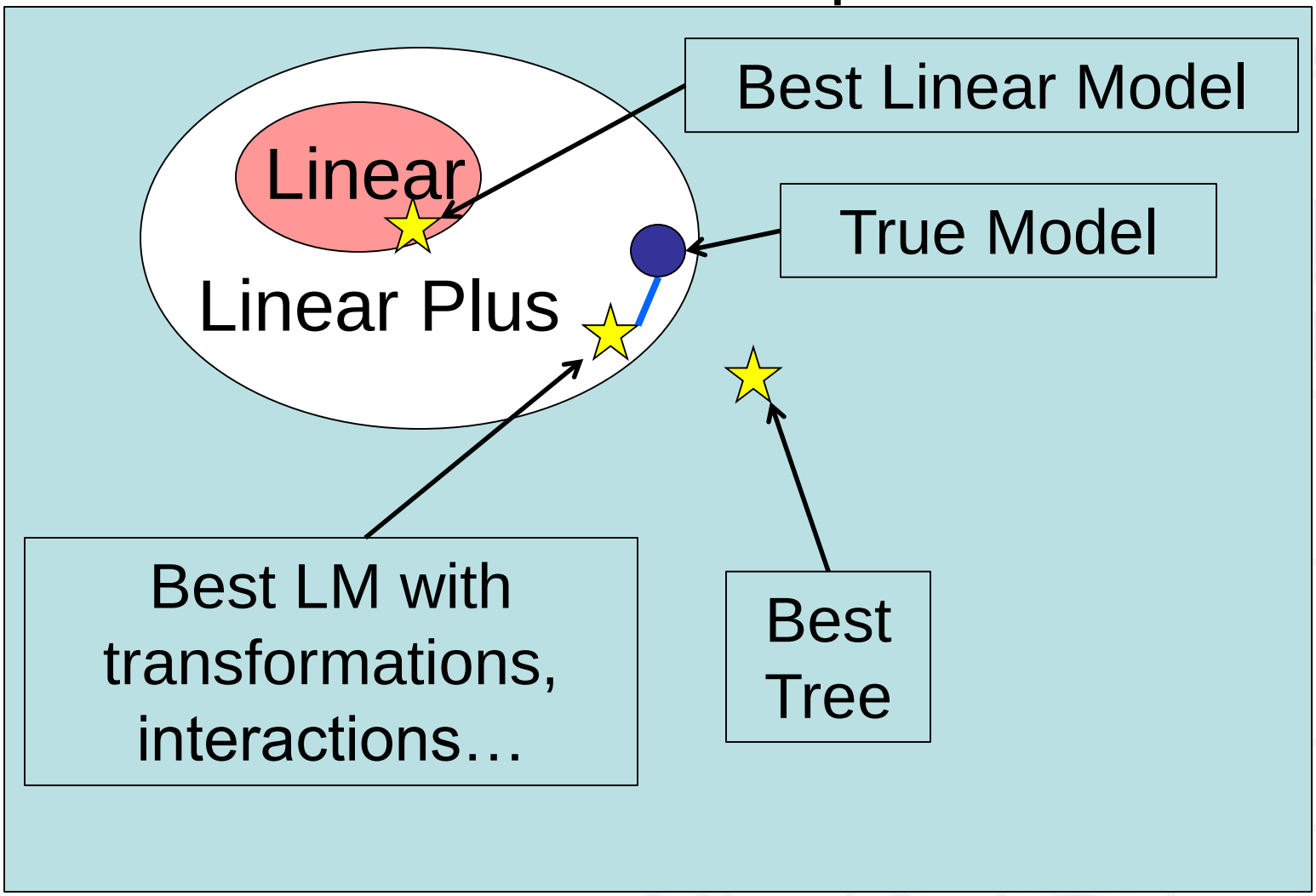
- In the multi-class case the approach is less clear
- The naïve model is often very bad
  - Mean of class-specific error rates? Maybe weighted by sample sizes?
  - $\sum_{i=1}^{n}\sum_{c=1}^{C}(y_{ic}-\hat{y}_{ic})^2$, where y_{ic} = 1 if obs. y is in class *c* and 0 otherwise? (Brier score)
  - Average of AUCs for “one-versus-all-other” classification models?
- I claim this problem is unsolved

Ensembles

- The two most exciting directions in machine learning over the last ten years have been in **ensembles** and neural networks
- We'll come back to neural networks
- Ensembles of automatically-generated "weak learners" can "vote" to produce classification or regression models that are very often better than our "one best model"

Bias vs Variance

All Relationships



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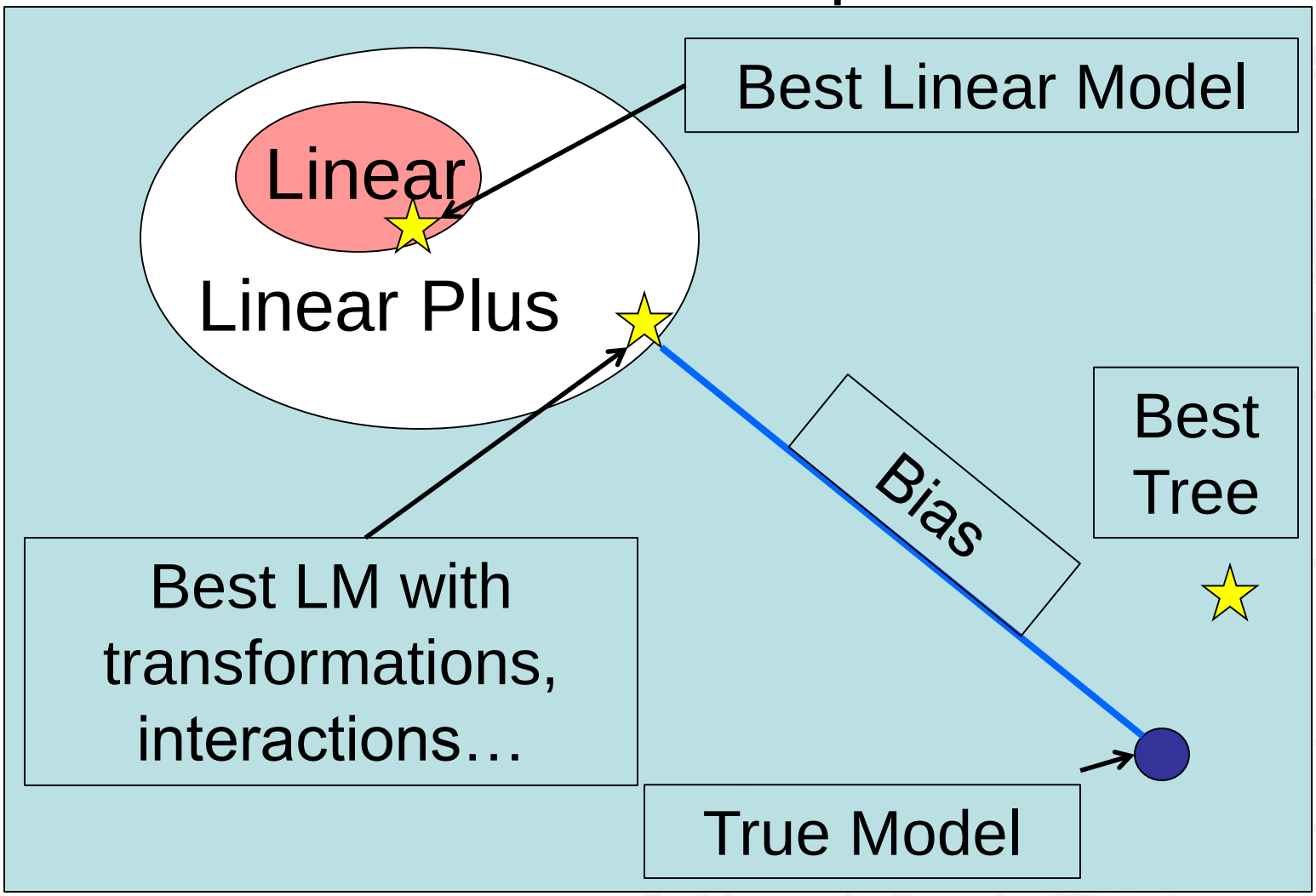
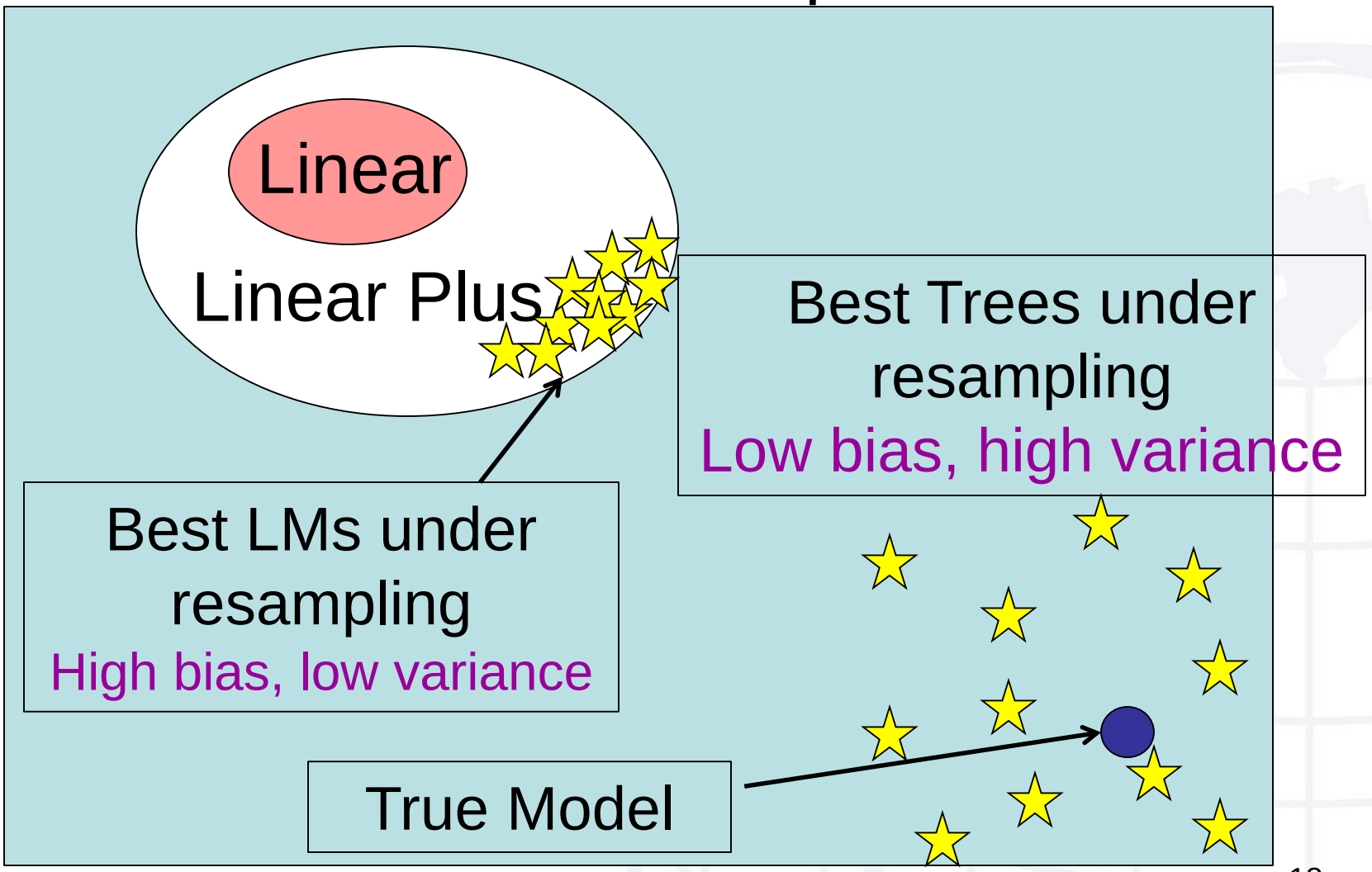


Averaging (Ensembles) Might Help



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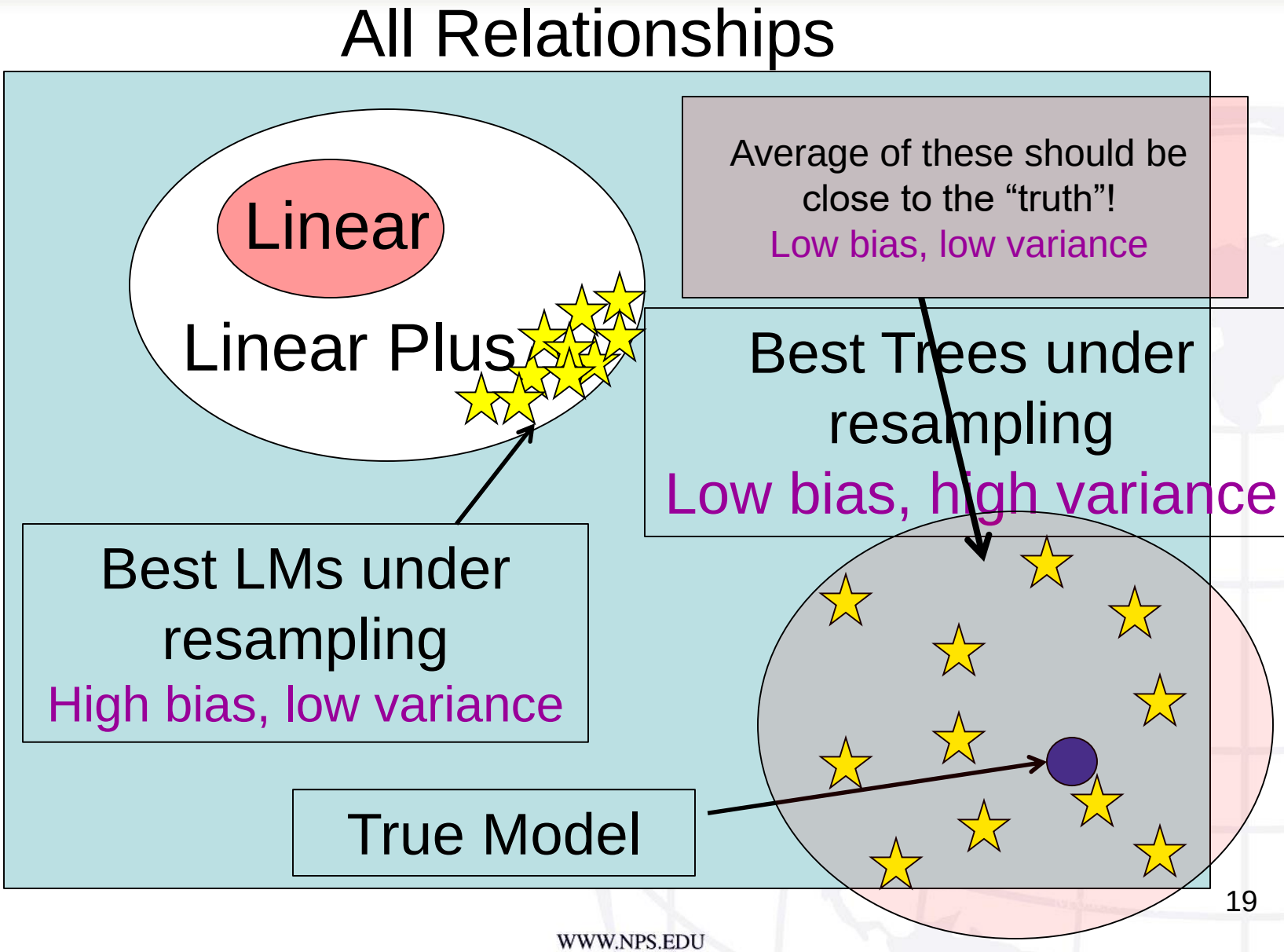


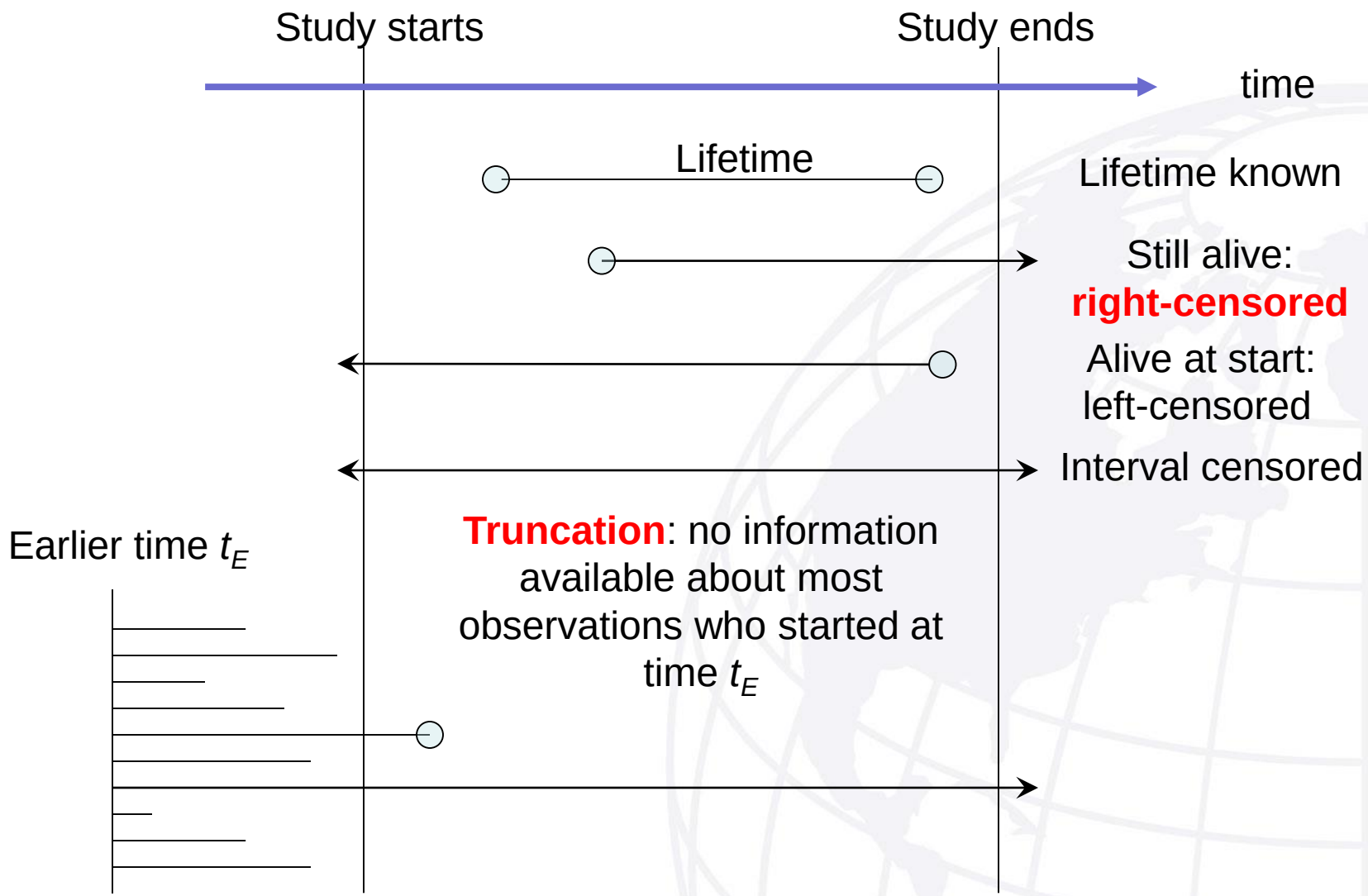
Other Important Problems

- **Time Series**, where observations share time dependency
  - This is a huge subject about which you saw some good info in OS 4106
- **Spatial Statistics**, where there is correlation, possibly directional, between observations close together
  - We will look briefly at some elementary aspects of this, especially making maps

Other Problems (cont'd)

- **Survival Analysis**: analysis of lifetime data
  - Issues: lots of the lifetimes are "right-censored," that is, not completely observed (observations are still living)
  - There can be left-censoring (birth dates / starting times unknown)….
  - Maybe more often we have "truncation," where we haven't observed all the people who were alive when we started

Survival Analysis



Supervised Learning

- **Supervised** learning is when there are known *y*'s
  - Classification and regression
  - With perhaps a linguistic stretch, time series, spatial analysis and survival analysis
- As opposed to **unsupervised**, in which there is just a bunch of *x*'s with no known *y*'s
  - Examples to follow, but the primary example is always clustering – dividing into groups

Learning, cont'd

- In **semi-supervised** learning we have a small amount of supervised data, plus lots of unsupervised data to help out
- In **reinforcement learning**, the algorithm gets "rewarded" for smart guesses
  - Like when your sibling hides something…
  - An important foundation for Artificial Intelligence algorithms and one very much worthy of serious study…
  - …but not in this course

Unsupervised Learning

Unsupervised learning: techniques with no specified response variable

1.) Principal Components (PCA)

- For numeric data, reduce dimensionality
- Remove noise; can also compress data

- Projection Pursuit (different criteria)
- Blind Source Separation
  - "Cocktail party problem"
- No Y variable

Unsupervised Learning

Unsupervised learning: techniques with no specified response variable

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Details to Follow

Unsupervised Learning

Techniques with no specified response variable, cont'd

2.) Clustering

- Find structure ("lumps") in observations
  - Group X's without knowing their y's
  - Usually we don't know number of clusters
- Important questions:
  - How do we measure the **distance** between observations – or clusters – if our measures are on different scales or categorical?

Unsupervised Learning

Techniques with no specified response variable, cont'd

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Details to follow

Unsupervised Learning

3.) Association rules (market baskets)

- Given a set of categorical data, deduce rules like "if a $\in$ A and b $\in$ B, then c $\in$ C"
- Each rule carries **coverage** (proportion of pop'n for which a $\in$ A and b $\in$ B) and **confidence** (proportion of obs with a $\in$ A and b $\in$ B for which c $\in$ C)
- No particular response specified; any variable can be "predictor" or "response"

Unsupervised Learning

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Details to follow

Unsupervised Learning

4.) Density Estimation

- Given data, what density might it have come from?
- One form: “Bump hunting”
- Particularly tough in high dimensions where data is very sparse
- Can sometimes be cast as a classification problem

- Anomaly / outlier detection

Unsupervised Learning

5.) Multidimensional scaling

- Map high-d data into 2 (or 3) dimensions while preserving inter-point distances (or maybe their ordering) to the extent possible

Details to follow, briefly

- Self-Organizing (Kohonen) Map

6.) Search

- PageRank
- Recommender Systems (Amazon, Pandora…)

Principal Components

- **Goals**:
  - Reduce dimensionality, maybe de-noise
  - Explore linear dependence among predictors
  - Produce uncorrelated X's for use in regression
- Basic idea: replace original measurements by a set of specially chosen weighted averages ("linear combinations")
- Basic PC is for **numeric data only**

Example

- Defense Language Institute study concerning program effectiveness
- $x_1, x_2, \ldots, x_6$ is a sequence of quarterly exam scores
- Do we need all six values?
- Maybe replace the six exam scores with
  - z_1 = average of the six exam scores
  - z_2 = (avg. of last 3) – (avg. of first 3)
  - This creates a **two-dimensional** data set
  - Some information is lost

Principal Components

- In principal components, we first find p orthogonal linear combinations of the p original regressors
  - "Orthogonal" means both "at right angles" and also "uncorrelated" here
  - No information created or destroyed, although…
  - We often then drop some of the new combinations, achieving…
  - **Dimensionality reduction**

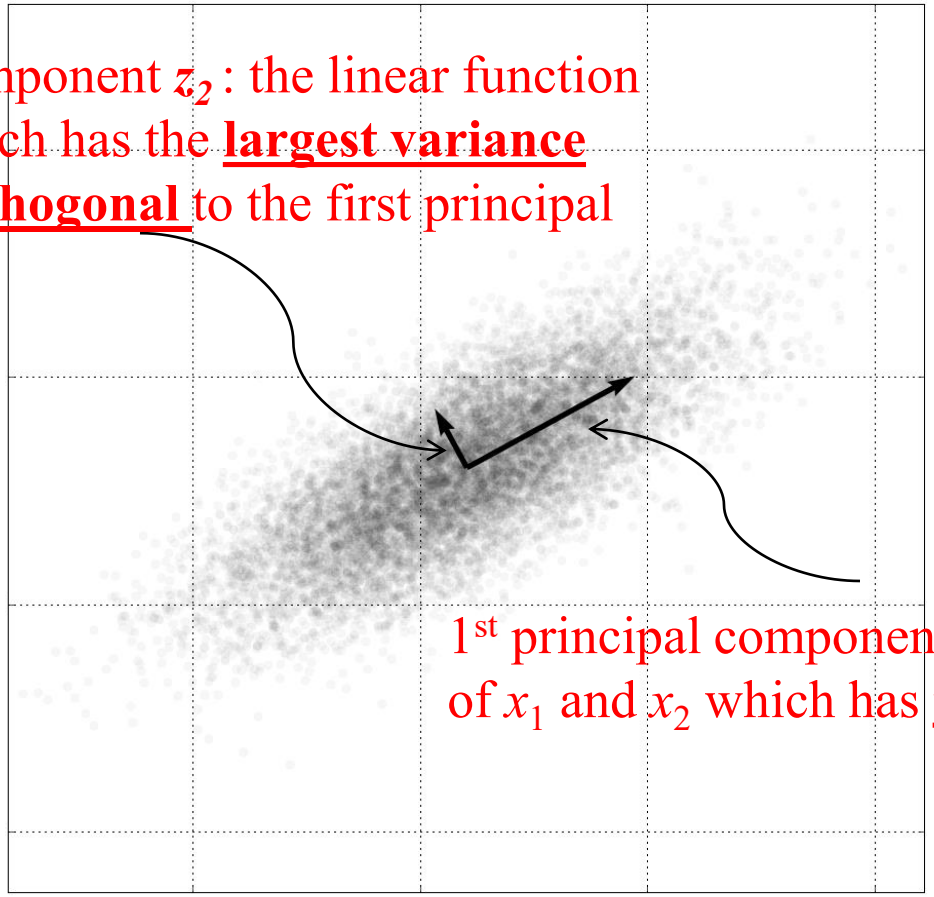
Principal Components

- These new linear combinations are the principal components – i.e. we re-express our X's in terms of p orthonormal basis vectors
- The first principal component points in the direction of the principal axis of the data – the direction in which there is most spread (that is, the "largest variance")

Two-dimensional Example

If we were to replace x_1 and x_2 with **one** variable, z_1 would be a natural choice; it has more variablity than either variable x_1 or x_2.

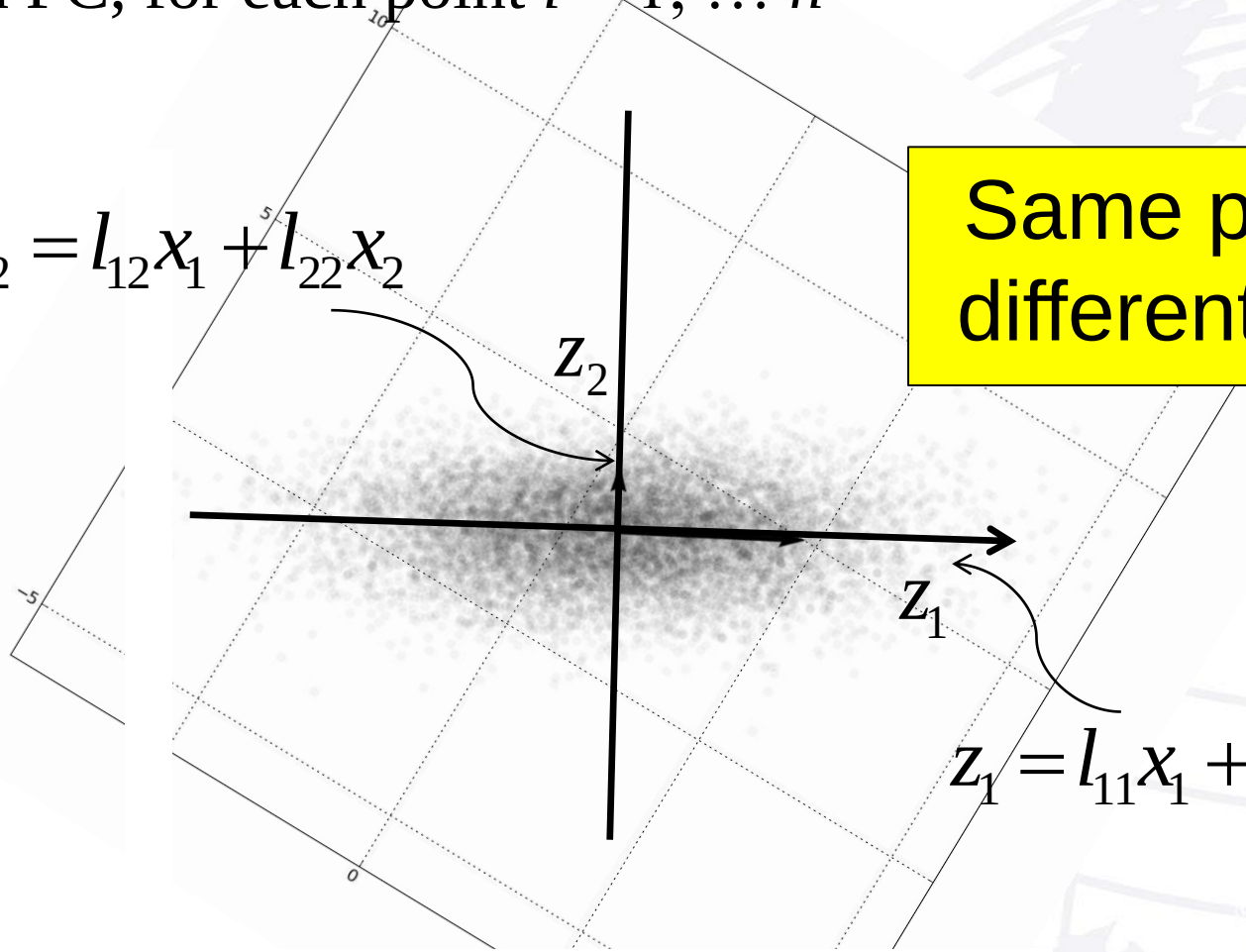
2nd principal component z_2 : the linear function of x_1 and x_2, which has the **largest variance** among those **orthogonal** to the first principal component z_1 .



1st principal component z_1 : the linear function of x_1 and x_2 which has **the largest variance**

Transforming Rotates the Axes

Here we plot (z_{i1}, z_{i2}) where $z_{i1} = l_{11}x_{i1} + l_{21}x_{i2}$ are the scores from the first PC and $z_{i1} = l_{11}x_{i1} + l_{21}x_{i2}$ are the scores from the second PC, for each point $i = 1, \ldots n$



Same points, different axes

For p variables there are p p.c.'s

- The p principal components are:

$$z_1 = l_{11}x_1 + l_{21}x_2 + \ldots + l_{p1}x_p = \mathbf{l_1}^{\mathrm{T}}\mathbf{x}$$
$$z_2 = l_{12}x_1 + l_{22}x_2 + \ldots + l_{p2}x_p = \mathbf{l_2}^{\mathrm{T}}\mathbf{x}$$
$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$
$$z_p = l_{1p}x_1 + l_{2p}x_2 + \ldots + l_{pp}x_p = \mathbf{l_p}^{\mathrm{T}}\mathbf{x}$$

loadings

where the vectors of **loadings** are orthogonal to one another and have length 1

- The loadings are just weights; we take p weighted averages of our p variables

PC Scores Have Maximal Variance

- The **scores** are the values of the PCs for each observation
- E.g., $z_{i1} = l_{11}x_{i1} + \ldots + l_{p1}x_{ip}$ is the **score** of the i^{th} observation on the first PC
- We choose the loadings so that the first PC scores have the largest variance among all linear functions of the x's
  - (for which the coefficient vector has length 1)
- The second PC scores have the largest variance among all linear functions (w/len 1) which are orthogonal to the first…etc.

Why Variance?

- A direction with no variability is uninformative; maybe one in which there is lots of variability is very informative
- Choosing scores with maximum variance leads to straightforward computation
- Other indices of “interestingness” can be used
- PCs widely used, seem to be successful

Finding PCs in Practice

- In R, use `prcomp()` or `princomp()`
  - `prcomp()` (stronger but less friendly) uses the *n* – 1 divisor for variances, calls scores `x`
  - `princomp()` uses *n*, calls scores `scores`
  - Both **center** the data by subtracting means; we'll need those values for scoring new observations
  - Neither **scales** by default; we usually do that
- Remember: we convert data to scores
- Start with *p* columns, convert to *p* scores

How do we find the loadings?

- Let *S* be the (sample) cov. matrix of the x's
- cov (*X*) =

$$\begin{bmatrix} s_{x_1}^2 & \widehat{\text{cov}(x_1, x_2)} & \cdots & \widehat{\text{cov}(x_1, x_p)} \\ \widehat{\text{cov}(x_2, x_1)} & s_{x_2}^2 & \cdots & \widehat{\text{cov}(x_2, x_p)} \\ \vdots & \vdots & \ddots & \vdots \\ \text{cov}(x_p, x_1) & \widehat{\text{cov}(x_p, x_2)} & \cdots & s_{x_p}^2 \end{bmatrix}$$

$$s_{x_j}^2 = \frac{\sum_{i=1}^{n} (x_{ij} - \bar{x}_j)^2}{n-1} \qquad \hat{\text{cov}}(x_j, x_k) = \frac{\sum_{i=1}^{n} (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)}{n}$$

Some programs divide by *n* rather than *n*– 1 when computing PC's

Finding Loadings

- We want to find l such that $l\,S\,l^T$ is maximized, subject to the constraint that $l\,l^T = 1$
- Method of Lagrange multipliers: construct $f = l\,S\,l^T - \lambda\,(l\,l^T - 1)$, take derivatives...
- Solution: we want $l\,S = \lambda\,l$
- **That is**, the first principal component is precisely the first eigenvector of the matrix S
- Subsequent eigenvectors give subsequent principal components

Decomposing the S Matrix

- The loadings are the eigenvectors of S
- $S = L\,\Lambda\,L^T$
- $[\boldsymbol{L}_1, \boldsymbol{L}_2, \ldots, \boldsymbol{L}_p] \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_p \end{bmatrix} \begin{bmatrix} \boldsymbol{L}_1 \\ \boldsymbol{L}_2 \\ \vdots \\ \boldsymbol{L}_p \end{bmatrix}$

Column eigenvectors are the loadings for each PC

The j^{th} eigenvalue is the sample variance of the scores corresponding to the j^{th} PC.

i.e. $\lambda_j = s_{z_j}^2$ for $j = 1, \ldots, p$

And $\lambda_1 \geq \lambda_2 \ldots \lambda_p \geq 0$

$\sum s_{x_j}^2 = \sum \lambda_j = \sum s_{z_j}^2$

Scaling the X's

- The sum of the original data columns' variances is equal to the sum of the score columns' variances
  - But differently apportioned
  - Some have lots, some have hardly any
- If the x's are in different units, like lb and °F, their variances won't be additive
  - The analysis doesn't care, but we do, because changing to kg and °C shouldn't change anything

Scaling the X's

- "If the x's are in different units, their variances won't be additive"
- In that case, it's usual to **scale** the columns by dividing each by its SD
  - In practice we will usually do this, with `scale = TRUE` for `prcomp`
  - Loadings are **`rotation`**, scores are **`x`**
- After scaling, the total variance across the score columns will add up to p
- Example 0: Made-up, low-d data
- Example 1: The iris data

Iris Example

```
> (iris.pc <- prcomp (iris[,-5])) # extra () says "print"
```

I didn't scale here because all the measurements all already in inches

```
Standard deviations:
[1] 2.0562689 0.4926162 0.2796596 0.1543862
```

```
> round (prcomp (iris[,-5])$rotation, 3)
```

	PC1	PC2	PC3	PC4
Sepal.Length	0.361	-0.657	0.582	0.315
Sepal.Width	-0.085	-0.730	-0.598	-0.320
Petal.Length	0.857	0.173	-0.076	-0.480
Petal.Width	0.358	0.075	-0.546	0.754

Signs within a column can all be reversed and still give the same answer

We hope for a few interpretable components, but interpretation is often difficult

Interpreting Coefficients

- Each iris is described by four numbers
- Suppose you wanted one number – one weighted average – for each flower, such that those numbers were as spread out as possible. How would you do that?
- Answer: .361 (Sepal Len) – .085 (Sepal Wid) + .857 (Petal Len) + .358 (Petal Wid)

  $-.361^2 + (-.085)^2 + .857^2 + .358^2 = 1$
- That linear combination accounts for 92% of all the variability in all 4 original columns

Scores

- Scores (`x`) are returned automatically
- The score columns are uncorrelated, as are the columns of loadings
- Using `library (rgl)`, compare:
- `cc <- rep (c("red", "blue", "black"), each=50)`
- `plot3d (iris[,1:3], col=cc)`
- `plot3d(iris.pc$x[,1:3], col=cc)`

How Many PCs Should Be Kept?

```
> summary (iris.pc)
Importance of components:
                          PC1     PC2     PC3     PC4
Standard deviation     2.0563 0.49262 0.2797 0.15439
Proportion of Variance 0.9246 0.05307 0.0171 0.00521
Cumulative Proportion  0.9246 0.97769 0.9948 1.00000
```

Standard deviations of Score Columns s_j for $j = 1, \ldots, p$

Proportion of Variance of Score Columns: $s_j^2 / \sum_k s_k^2$

Rules of Thumb:

Keep the PCs as long as

- Proportion of the Variance > .10
- Cumulative Proportion > .90, .99
- If scaling, keep any w/ $s > 1$

Or

- Look for a "knee" in the scree plot

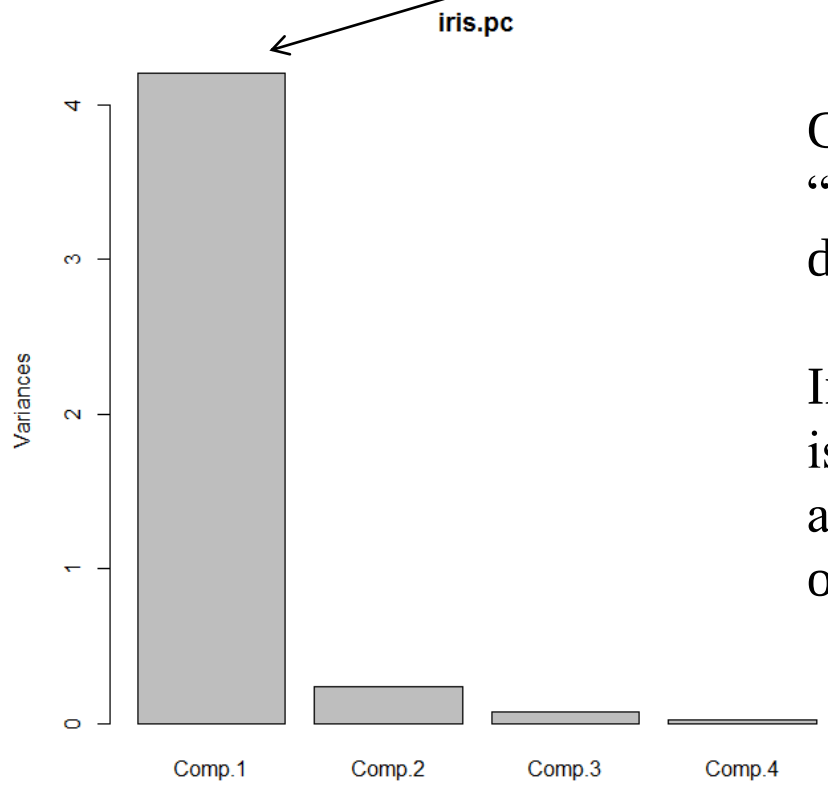
Cumulative Proportion of Variance

$$\frac{\sum_{i=1}^{j} s_{z_i}^2}{\sum_{i=1}^{p} s_{z_i}^2} \quad \text{for } j = 1, \ldots, p$$

Scree plot

```
> plot(iris.pc)
```

$s^2_{z1} = 4.2$



Common rule: look for a "knee" in the plot, where the descent slows

In the iris example, 1 or 2 PCs is enough to capture "almost all" of the variability in the original data

State Example

- Built in `state.x77` data
- Why is scaling necessary?
- R uses %*% for matrix multiplication
- Standardized data <- (data – center) / scale
  - Remember R acts columnwise; see example
- Then `stddata %*% rotation = scores`, and `scores %*% t(rotation) = stddata`
  - No information lost or created, but…
  - What if we drop a few PCs here?

PC Recap: States Example

- In the `state.x77` example, data is 50 × 8
  - 50 points lying in an 8-dimensional space
- Full set of PC loadings was 8 × 8
  - Instructions for converting from one space to another
- Scores = data `%*%` loadings
  - 50 points' coordinates in the new 8-d space
  - Sometimes we explicitly scale and/or center; then scores are (data – center)/scale `%*%` loadings

PC Recap: States Example

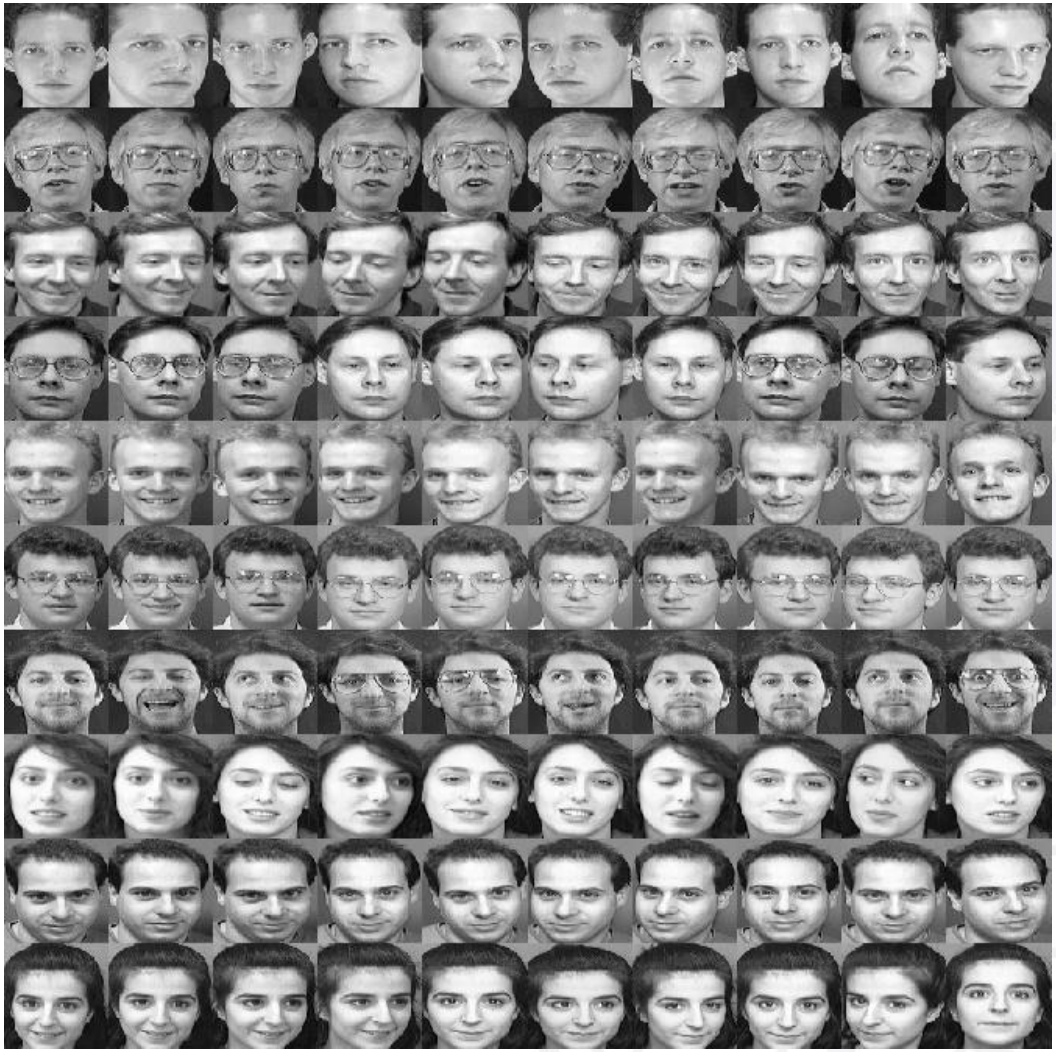
- Scores = data %*% loadings (weights)
- data = Scores %*% t(loadings)
  - Or (Scores %*% t(loadings)) * scale + center
  - No information gained or lost, until…
- We reduce dimensionality by using only a subset of scores, and a subset of the columns of loadings
- Then we lost a little information but may still have a decent approximation

Principal Comp Bigger Example

- Here's one example of a way that principal components can be used in practice: facial recognition
- Training set: Olivetti Research Lab, Cambridge UK (1994)[1]
- 40 subjects × 10 images/subject × (92×112) pixels/image × 255 gray levels per pixel
- Task 1: Read 400 images into R object `faces`
  - I used `read.pnm()` from `library (pixmap)`
  - Plot method available
  - This produces an S4 object; use `@` to extract
  - This data has 400 rows and 10,304 columns
  - We can keep fewer columns and still do well

1. F. Samaria and A. Harter, "Parameterisation of a stochastic model for human face identification," 2nd IEEE Workshop on Applications of Computer Vision, December 1994, Sarasota (Florida).

Examples



The Approach

- Computing distances between a training 10,000-vector and a test one is expensive, and the pixels are highly correlated
- Let's reduce the dimensionality by finding 382 PCs and keeping, say, 200 or so
- Each training set picture can be represented **exactly** with a score vector of 382 numbers, or approximately with 200
- For a test set item we get its 200-vector of scores and compare it to training set scores

The Eigenfaces

- Use `prcomp()` to get loadings, scores
- The loadings are called **eigenfaces** here
- Each "real" face is a linear combination of eigenfaces
- Perhaps we only need to keep a "small" number of these, $m' < m$ – perhaps 200?
- Test set: Subject 17 plus some randoms
- For a new face, convert it into a vector of 200 scores, compare it to all other vectors of scores, and see where it falls

Let's Do This Thing

- Lots of typing, so just follow along
- But the story is:
  - Create training and test sets
  - Compute PCs for training set; keep 200
  - Use those loadings to compute PC scores for test set, too
  - For each test set item, measure its distance to each of the training set items
  - Assign the test set item to the person depicted in the nearest-neighbor within the training set

Or some other reasonable number

Experiment

- How well did we do?
- What happens if you project a random pixel vector into face space?
- Answer: you get a vaguely face-like thing, a weird combination of eigenfaces
- Its scores won't be near any actual faces'
- "Rule": if distance to some picture is small, this is a face we've seen; if it's medium, this is a new face; if it's large, this isn't a face at all

Final Thoughts

- PC not well-suited to categorical data…
  - …Or data that varies with time and space
- In many problems we represent our data with a rich set of basis functions
  - Original measurements
  - Polynomials and products (interactions)
  - Transformations like log, sin/cos…
- In PC we select a small set of basis functions from a large original set, but..
- Lots of good choices aren't in the PC basis