Course Overview – Nonparametric Regression and Classification

STAT/BIOSTAT 527, University of Washington

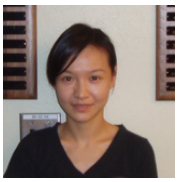
Emily Fox

April 2nd, 2013

Course Staff

- Instructor: **Emily Fox**

- TA: **Shirley You Ren**



Content: What is the course about?

Course Structure

- 3 Primary Tasks:
  - **Regression**
  - **Classification**
  - **Density Estimation**
- 5 Modules:
  - **Nonparametric Preliminaries**
  - **Splines and Kernels**
  - **Bayesian Nonparametrics**
  - **Nonparametrics for Multivariate Covariates**
  - **Classification**

Task 1: Regression

- Assume a sample
- Model:

- Task involves estimating the function *f*

- Goals of nonparametric approach:
  - Make few assumptions about *f*
  - Use a large number of parameters, but constrained in some way to avoid overfitting the data
  - Complexity can grow with the sample size

Task 2: Classification

- Assume a sample $(x_1, Y_1), \ldots, (x_n, Y_n)$

- Task involves estimating a predictive model of *Y* given *x*

- Goals of nonparametric are as before, but now for link between *x* and *Y* with *Y* discrete-valued

Task 3: Density Estimation

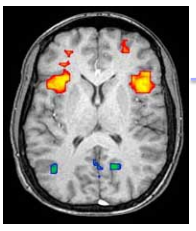
- Assume a sample

- Task involves estimating the density *p*

- Goals of nonparametric approach are as before, but applied to the estimation of *p*

fMRI Prediction Task

- **Goal:** Predict word stimulus from fMRI image



Classifier
(logistic regression, kNN, …)

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or
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fMRI

fMRI

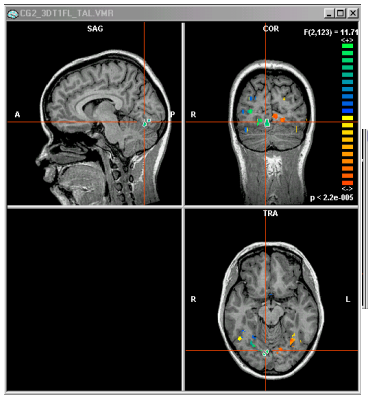
~1 mm resolution

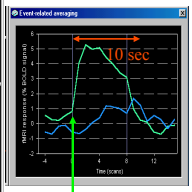
~1 image per sec.

20,000 voxels/image

safe, non-invasive

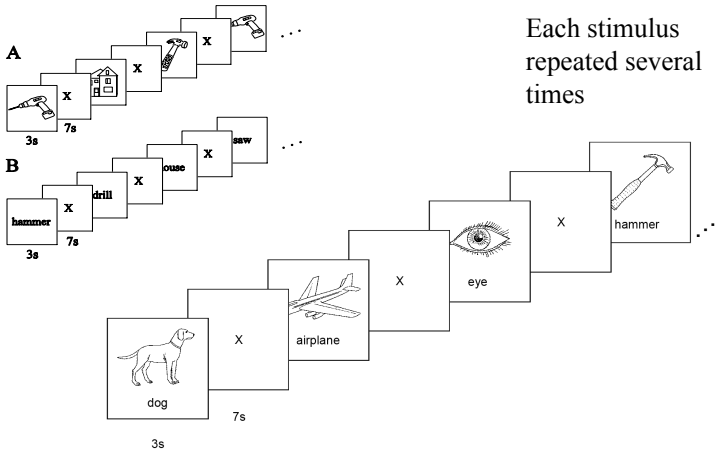
measures Blood Oxygen Level Dependent (BOLD) response





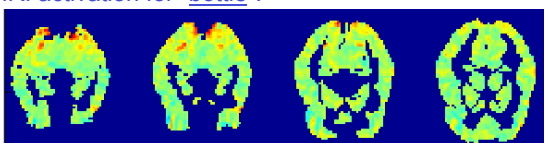
Typical fMRI response to impulse of neural activity

Typical Stimuli



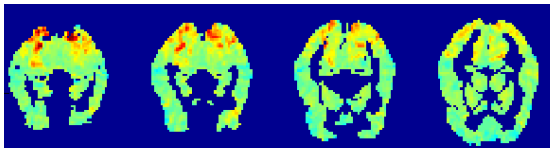
fMRI Activation

fMRI activation for "bottle":

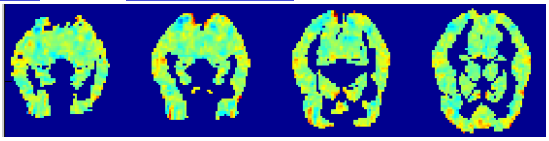


bottle

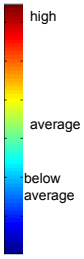
Mean activation averaged over 60 different stimuli:



"bottle" minus mean activation:

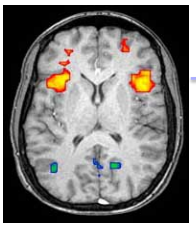


fMRI activation



fMRI Prediction Task

- **Goal:** Predict word stimulus from fMRI image
- **Challenges:**
  - p >> n (covariate dimension >> sample size)
  - Cost of fMRI recordings is high
  - Only have a few training examples for each word



Classifier
(logistic regression, kNN, …)

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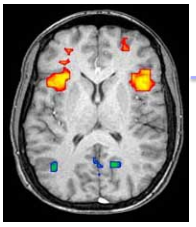
or
HOUSE

Zero-Shot Classification

- **Goal:** Classify words not in the training set
- **Challenges:**
  - Cost of fMRI recordings is high
  - Can't get recordings for every word in the vocabulary



Classifier
(logistic regression, kNN, …)

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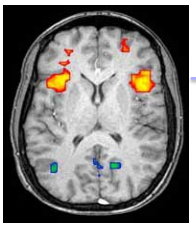
Zero-Shot Classification

- **Goal:** Classify words not in the training set
- **Challenges:**
  - Cost of fMRI recordings is high
  - Can't get recordings for every word in the vocabulary
- We don't have many brain images, but we have a lot of info about the words and how they relate (co-occurrence, etc.)
- How do we utilize this "cheap" information?



Classifier
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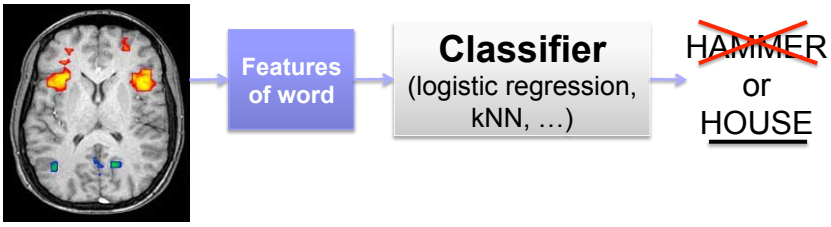
Semantic Features

Semantic feature values: "**celery**"	Semantic feature values: "**airplane**"
0.8368, eat	0.8673, ride
0.3461, taste	0.2891, see
0.3153, fill	0.2851, say
0.2430, see	0.1689, near
0.1145, clean	0.1228, open
0.0600, open	0.0883, hear
0.0586, smell	0.0771, run
0.0286, touch	0.0749, lift
…	…
…	…
0.0000, drive	0.0049, smell
0.0000, wear	0.0010, wear
0.0000, lift	0.0000, taste
0.0000, break	0.0000, rub
0.0000, ride	0.0000, manipulate

Zero-Shot Classification

- From training data, learn two mappings:
  - S: input image → semantic features
  - L: semantic features → word
- Can use "cheap" co-occurrence data to help learn L



Assumed Background

- **[Stat 502 and Stat 504] or [Biostat 514 and Biostat 515]**
- **Comfortable with:**
  - Linear algebra
  - Probability
  - R (or Matlab, Python, etc.)
- **Computational and mathematical maturity**

Logistics: How is the course going to run?

Website and Discussion Board

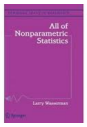
- Course website:
  http://stat.washington.edu/courses/stat527/s13

- Catalyst:
  - Used for all discussions
  - Post all questions there (unless personal)
  - See website for sign-up details

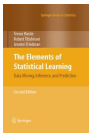
Reading

- No required textbook
- Three suggested textbooks (on website):
  - Wakefield, “Bayesian and Frequentist Regression Methods", Springer 2012

  - Wasserman, “All of Nonparametric Statistics”, Springer 2005



  - Hastie, Tibshirani, Friedman “The Elements of Statistical Learning”, Springer 2009



- Papers linked on course website

Homework

- 7 HWs total
- Assigned and due weekly on *Thursdays*
- Collaboration allowed, but write-ups and coding must be done individually
- Submitted at beginning of class
- Allowed 2 “late days” for entire quarter

Project

- Options:
  - Choose project from specified list
  - Re-implement existing paper from specified list
  - Propose own project idea
- Individual
- New work, but can be connected to research
- Schedule:
  - Proposal (1 page) – April 25
  - Progress report (3 pages) – May 16
  - Poster presentation – June 6
  - Final report (8 pages, NIPS format) – June 11

Grading

- HWs 1, 2, 4, 5, 6 (10% each)
- HWs 3, 7 (5%) – short, due dates coincide with project due dates
- Final project (40%)

Support/Resources

- Office Hours
  - TA: W 2-4pm in Padelford A-316
  - Emily: Th 11am-12pm in Padelford B-305
- Recitations
  - Optional tutorial/example-based sections will be held *every other* week
  - Choose from:
    - Monday, 2-3pm
    - Monday, 5-6pm
    - Tuesday, 4-5pm
  - Location TBD

Module 1: Nonparametric Preliminaries

Intro, What to Report?

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The Optimal Prediction

- Assume we *know* the data-generating mechanism
- If our task is prediction, which summary of the distribution $Y \mid x$ should we report?

- Taking a decision-theoretic framework, consider the ***expected loss***

Continuous Responses

- Expected loss $E_X \left\{ E_{Y|X} \left[L(Y, f(x)) \mid X = x \right] \right\}$

- Example: L_2

  Solution:

- Example: L_1

  Solution:

- More generally: L_p

General Responses

- Expected loss $E_X \left\{ E_{Y|X} \left[L(Y, f(x)) \mid X = x \right] \right\}$
- Example: log-likelihood

When Gaussian:

When Laplacian:

Incorporating Models into Prediction

- We don't actually know the data-generating mechanism
- Need an estimator $\hat{f}_n(\cdot)$ based on a random sample $Y_1, \ldots, Y_n$, also known as ***training data***

- Statistical models can be used to encode knowledge about aspects of the data-generating mechanism

- Models can provide simplifying assumptions
  - Can help cope with estimation issues due to limited data

Incorporating Models into Prediction

- Assume some form for how the data are generated
  - E.g., $Y = f(x) + \epsilon \qquad E[\epsilon] = 0 \quad \text{var}(\epsilon) = \sigma^2$
  - For non-constant variance, can consider GLMs
- Then, typically assume some form for *f(x)*
- Model + loss function → some estimator

Parametric Regression

- *Parametric* inference assumes parametric form for $f(x)$
- Advantages:
  - Efficient estimation
  - Concise summarization
- What is the right parametric form for $f(x)$?

Goals of Nonparam Regression

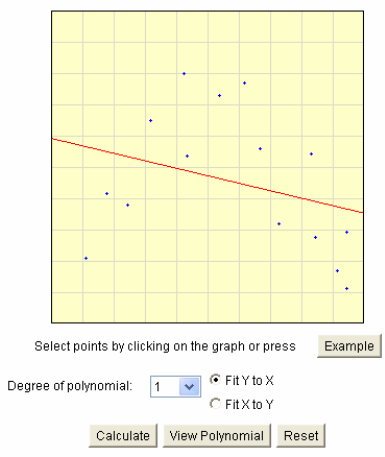
- Goals of *nonparametric* inference:
  - Assume little prior knowledge of data-generating mechanism
  - More flexibly model *f* (i.e., relationship between *x* and *Y*)
  - Maintain "reasonable" efficiency of estimation
- Often actually assume parametric forms with large numbers of parameters
  - Constrained to avoid overfitting the data
- Particularly useful when task is prediction
  - Focus on accuracy of prediction rather than parameter values
- Let's discuss this idea of "complexity" more…

Model Complexity

- How complex of a function should we choose?
  - To increase flexibility, using many parameters is attractive
  - However, wide prediction intervals…
  - Leads to wild predictions

Example: Polynomial Regression

- For added flexibility, allow for high order polynomial, right?



Example: Polynomial Regression

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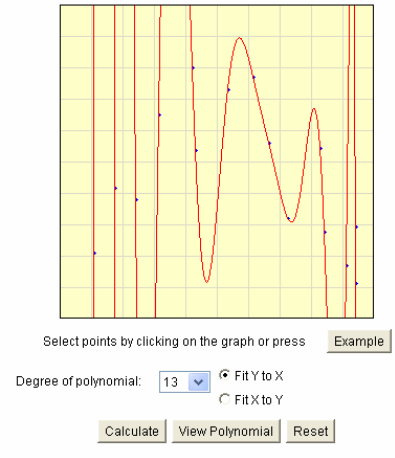

Measuring Predictive Performance

- Assume estimate $\hat{f}_n(\cdot)$ based on training data $y_1, \ldots, y_n$
- The ***generalization error*** provides a measure of predictive performance

$$GE(\hat{f}_n) = E_{Y,X}\left[L(Y, \hat{f}_n(X))\right]$$

Measuring Predictive Performance

- Assume L_2 loss
- Averaging over repeat training sets $\mathbf{Y}_n = Y_1, \ldots, Y_n$ we get the ***predictive risk*** at x^*

$$E_{Y^*,\mathbf{Y}_n}\left[(Y^* - \hat{f}_n(x^*))^2\right] =$$

- Recall $MSE[\hat{f}_n(x)] = \text{bias}(\hat{f}_n(x))^2 + \text{var}(\hat{f}_n(x))$

Measuring Predictive Performance

- Finally, let's average over covariates *x*
  - ***Integrated MSE***
  - ***Average MSE***
- Note: ***avg. pred. risk =*** σ^2 + ***avg. MSE***

Bias-Variance Tradeoff

- Minimizing risk = balancing bias and variance
- Note: *f(x) is unknown, so cannot actually compute MSE*

More on Nonparam Regression

- Often framed as learning functions with a complexity penalty
  - Regular behavior in small neighborhoods of the input
  - E.g., locally linear or low-order polynomial…estimator results from averaging over these local fits
- Choice of neighborhood = strength of constraint
  - Large neighborhood can lead to linear fit (very restrictive) whereas small neighborhoods can lead to interpolation (no restriction)

More on Nonparam Regression

- Different restrictions lead to different nonparametric approaches
  - Roughness penalty → ***splines***
  - Weighting data locally → ***kernel methods***
  - Etc.
- Each method has associated ***smoothing*** or ***complexity*** param
  - Magnitude of penalty
  - Width of kernel (defining "local")
  - Number of basis functions
  - …
- Bias-variance tradeoff
- Will explore methods for choosing smoothing parameters

Module 1: Nonparametric Preliminaries

Review of Regression, Linear Smoothers

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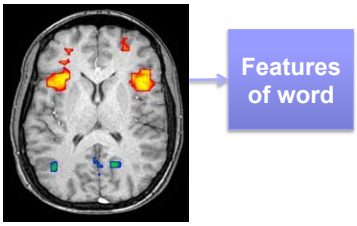
fMRI Prediction Subtask

- **Goal:** Predict semantic features from fMRI image



Linear Regression – *review*

- Model:
- ***Design matrix***:
- Rewrite in matrix form:

Linear Regression – *review*

- Least squares estimation:
  - Minimize ***residual sum of squares***
  - Take gradient and set = 0
- In Gaussian case, LS est. = maximum likelihood est.

Linear Regression – *review*

- ***Fitted values***
- Number of parameters
- For any *x*, we can write

Linear Smoothers

- Definition:
  $\hat{f}_n$ of f is a ***linear smoother*** if, for each *x*, there exists
  $$\ell(x) = (\ell_1(x), \ldots, \ell_n(x))^T$$
  such that
- Matrix form
  - Fitted values
  - Smoothing or "hat" matrix
- Effective degrees of freedom:

Linear Smoothers

- Note 1:

  A linear smoother does ***not*** imply that $f(x)$ is linear in *x*

- Note 2:

  If $Y_i = c$ for all *i*, then $\hat{f}_n(x) = c$ for all *x*