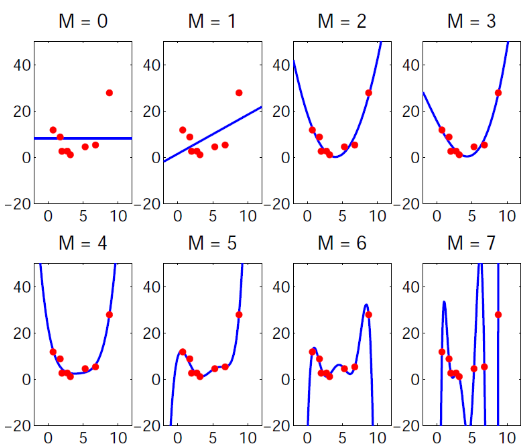
Mathematical Tools
for Neural and Cognitive Science

Fall semester, 2024

Section 6

Model fitting:
comparison, selection and regularization

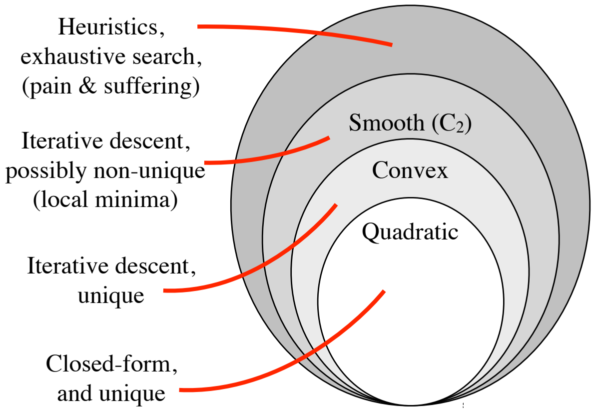


How do we avoid overfitting (i.e., concluding that M=7 is “best”)?

Taxonomy of model-fitting errors

- Unexplainable variability (e.g., due to noisy measurements)
- Overfitting (too many params, not enough data)
- Optimization failures (e.g., local minima)
- Model failures (what you’d really like to know)

Optimization...



Model Comparison

- If models are optimized according to some objective, it is natural to compare them based on the value of that objective…
  - for least squares regression, compare the residual squared error of two models (with different regressors).
  - for ML estimates, compute the likelihood (or log likelihood) ratio, and compare to 1 (or zero).
  - for MAP estimates, common to compute the posterior ratio
- **Problem**: evaluating the objective with the same data used to optimize the model leads to over-fitting!

Bayesian Model Comparison

- Eg: Is the coin fair? Compared to what?
- Consider two models: $M_1 : p = 0.5 \quad M_2 : p = 0.6$

$$p(M_k \mid D) = \frac{p(D \mid M_k) P(M_k)}{p(D)}$$

Compare their *posterior ratio*:

$$\frac{p(M_1 \mid D)}{p(M_2 \mid D)} = \frac{p(D \mid M_1) P(M_1)}{p(D \mid M_2) P(M_2)}$$

Comparing models' predictive performance

Option 1: Include a penalty for number of parameters:

For an ML estimate: $\hat{\theta} = \arg\min_{\theta} \left[-\ln p(\vec{d}|\theta) \right]$

a. Akaike information criterion (AIC) [Akaike, 1974]

$$E_{\mathrm{AIC}}(\vec{d}, \hat{\theta}) = 2\ \dim(\hat{\theta}) - 2 \ln p(\vec{d}|\hat{\theta})$$

b. Bayesian information criterion (BIC) [Schwartz, 1978]

$$E_{\mathrm{BIC}}(\vec{d}, \hat{\theta}) = \dim(\hat{\theta})\ \ \ln \left[\dim(\vec{d}) \right] - 2 \ln p(\vec{d}|\hat{\theta})$$

valid when $\dim(\vec{d}) >> \dim(\hat{\theta})$

Option 2: Cross-validation
(evaluate generalization to held-out data)

Cross-validation

A resampling method for estimating predictive error of a model. Widely used to identify/avoid over-fitting, and to provide a fair comparison of models.

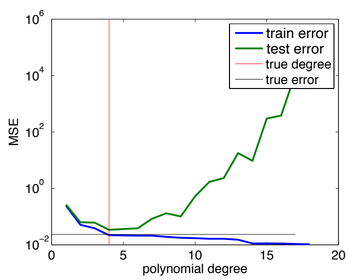
(1) Randomly partition data into a "training" set, and a "test" set.

(2) Fit model to training set. Measure error on test set.

(3) Repeat (many times).

(4) Choose model that minimizes the average cross-validated ("**test**") error

Using cross-validation to select the degree of a polynomial model:



Ridge regression

(a.k.a. L_2 regularization)

Ordinary least squares regression:

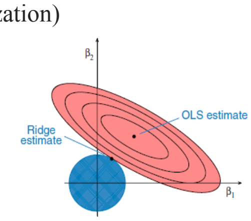
$$\arg\min_{\vec{\beta}} ||\vec{y} - X\vec{\beta}||^2$$

"Regularized" least squares regression:

$$\arg\min_{\vec{\beta}} ||\vec{y} - X\vec{\beta}||^2 + \lambda ||\vec{\beta}||^2$$

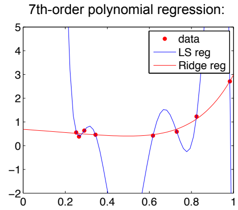
Equivalent formulation: MAP estimate, assuming Gaussian likelihood & prior!

$$\hat{\beta}_{\mathrm{ridge}} = (X^T X + \lambda I)^{-1} X^T \vec{y}$$

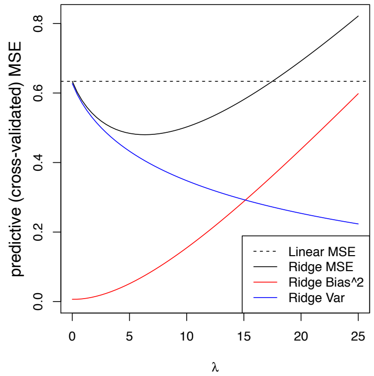


Choose lambda by cross-validation:

7th-order polynomial regression:



Ridge Regression trades off bias and variance:



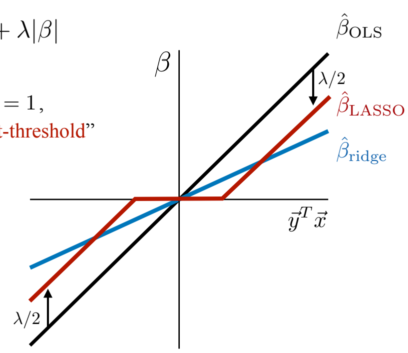
[from http://www.stat.cmu.edu/~ryantibs/datamining/]

L_1 regularization

(a.k.a. "least absolute shrinkage and selection operator" - LASSO)

$$\arg\min_{\beta} ||\vec{y} - \vec{x}\beta||^2 + \lambda|\beta|$$

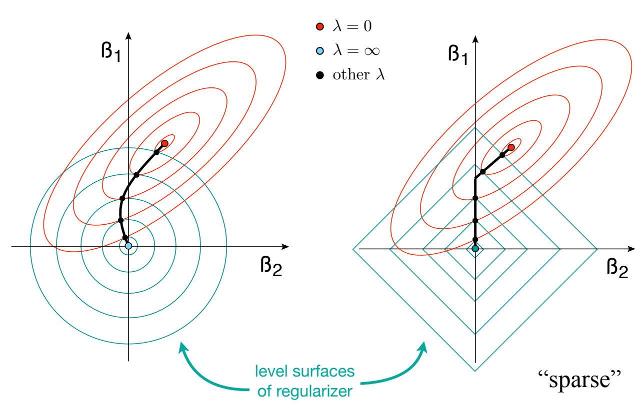
Assuming $\|\vec{x}\|^2 = 1$,
solution is a "soft-threshold"
on $\vec{y}^T\vec{x}$



MAP interpretation:
Gaussian noise, with
"Laplacian" prior

Ridge regression vs. LASSO (2-dimensional) solutions

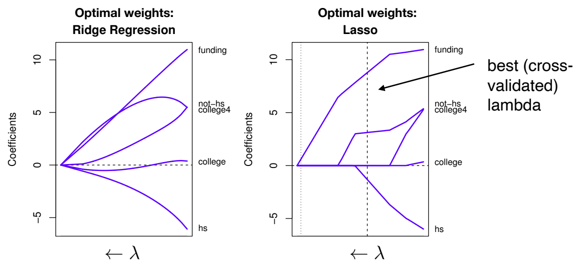
Ridge (L_2) LASSO (L_1)



LASSO vs. ridge regression

Table 2.1 *Crime data: Crime rate and five predictors, for $N = 50$ U.S. cities.*

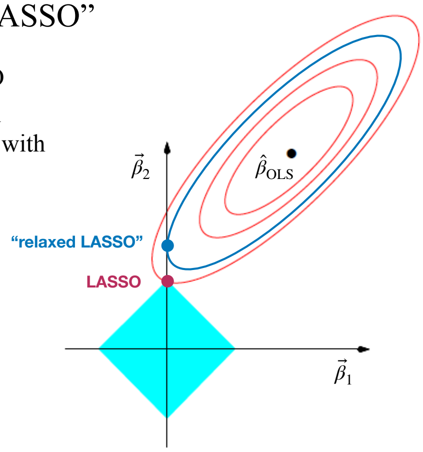
city	funding	hs	not-hs	college	college4	crime rate
1	40	74	11	31	20	478
2	32	72	11	43	18	494
3	57	70	18	16	16	643
4	31	71	11	25	19	341
5	67	72	9	29	24	773
⋮	⋮	⋮	⋮	⋮		
50	66	67	26	18	16	940



[From Hastie, Tibshirani, Wainwright 2015]

The "Relaxed LASSO"

1. Solve for LASSO
2. Eliminate unused regressors (those with zero coefficients)
3. Re-fit (using LS regression)



Clustering

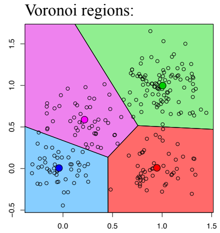
- K-Means (Lloyd, 1957)
- "Soft-assignment" version of K-means
  (a form of Expectation-Maximization - EM)
- In general, alternate between:
  1) Estimating cluster assignments (classification)
  2) Estimating cluster parameters
- Coordinate descent: converges to (possibly local) minimum
- Need to choose K (number of clusters) - cross-validation!

K-Means clustering algorithm

Alternate between two steps:

1. Estimate cluster assignments: given class centers, assign each point to closest one:

Voronoi regions:

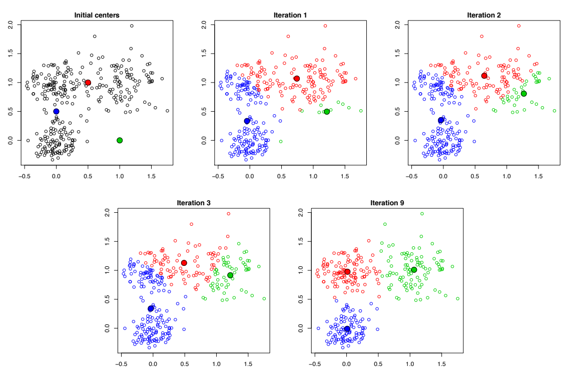


Soap bubbles:

2. Estimating cluster parameters: given assignments, re-estimate the centroid of each cluster.

K-means example

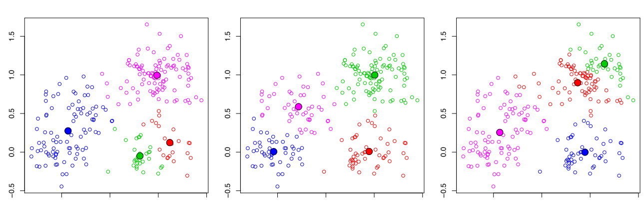
$N = 300$, and $K = 3$



[from R. Tibshirani, 2013]

K-means optimization failures

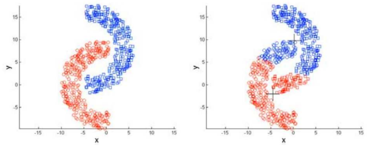
Initialization matters (due to local minima) …
Three solutions obtained with different random starting points:



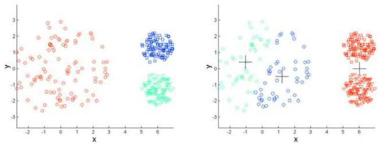
[from R. Tibshirani, 2013]

K-means systematic failures

Non-convex/non-round-shaped clusters



Clusters with different densities



Picture courtesy: Christof Monz (Queen Mary, Univ. of London)

ML for discrete mixture of Gaussians: soft K-means

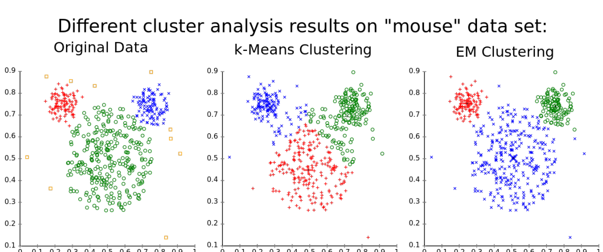
$$p(\vec{x}_n | a_{nk}, \vec{\mu}_k, \Lambda_k) \propto \sum_k \frac{a_{nk}}{\sqrt{|\Lambda_k|}} e^{-(\vec{x}_n - \vec{\mu}_k)^T \Lambda_k^{-1} (\vec{x}_n - \vec{\mu}_k)/2}$$

a_{nk} = assignment *probability*

$\{\vec{\mu}_k, \Lambda_k\}$ = mean/covariance of class *k*

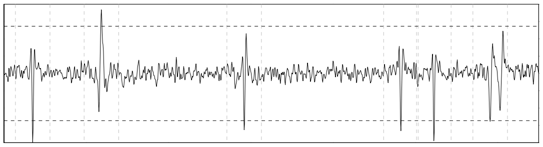
Intuition: alternate between maximizing these two sets of variables (“coordinate descent”)

Essentially, a version of K-means with “soft” (i.e., continuous, as opposed to binary) assignments!



[wikipedia]

Application to neural "spike sorting"

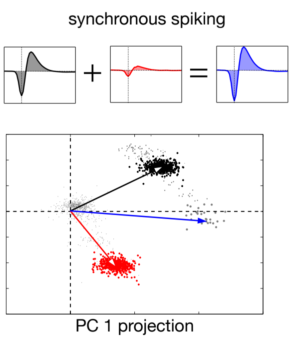


Standard solution:

1. Threshold to find segments containing spikes
2. Reduce dimensionality of segments using PCA
3. Identify spikes using clustering (e.g., K-means)

Note: Fails for overlapping spikes!

Failures of clustering for near-synchronous spikes



[Pillow et. al. 2013]