Smoothing - part 3

- Penalized splines is not the only way to estimate $f(x)$ when $y = f(x) + \epsilon$
- Two others are kernel smoothing and the Lowess (Loess) smoother
- I'll only talk about Lowess
- The Lowess algorithm does the same thing as fitting a penalized spline
- Lowess is more ad-hoc. Only practical difference I've found is that Lowess includes an outlier detection/downweighting step
- Lowess is LOcally WEighted polynomial regreSSion
- Original paper is Cleveland, W.S. (1979) Robust locally weighted regression and smoothing scatterplots. JASA 74:829-836

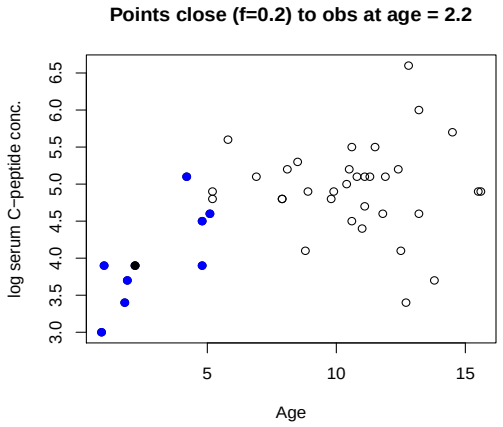
Lowess concepts

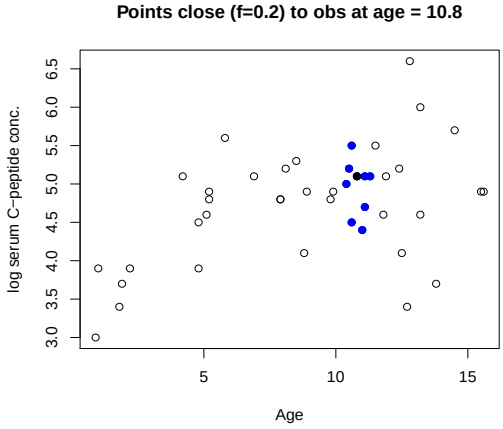
- any function, $f(x)$, is closely approximated by $\beta_0 + \beta_1 x$ over a small enough range of x
- so pick a point, x, may or may not be an x in the data
- fit a linear regression to the subset of the data with x values near x
- predict $f(x)$ from $\hat{\beta}_0 + \hat{\beta}_1 x$
- repeat for as many x's as needed to estimate $f(x)$
- A couple of refinements:
  - Use weighted regression with weights dependent on distance from x
  - "Robustify" the fit by downweighting the influence of regression outliers (far vertically from $\hat{f}(x)$)

- A simple algorithm that doesn't work well:
- Consider all points within specified distance d of x
- Fit OLS regression to these points
- Imagine fitting the curve to 5 points around x
- Then shifting to $x + 0.01$ that now includes 6 points
- that 6th point is within d of $x + 0.01$ but not within d of x
- Result is a very "jumpy" fitted curve
  because that 6'th point has a very large influence on the fitted value
- Lowess incorporates weighting so points $\approx d$ from x have some influence, but not much.
- Influence increases as x gets close to a data point
- Also hard to specify an appropriate d: depends on range of x values

Lowess details

- What is "close to x"?
  - Define close in terms of a fraction of the data points
  - f = smoothing parameter, $f \geq 0$.
  - For $0 \leq f \geq 1$, f is a fraction of data points.
  - For demonstration, consider small $f = 0.2$
  - For observation i, compute the n values: $d_{ij} = | x_i - x_j | \ \forall j$
  - The observations with the $f \times n$ smallest d_{ij} are "close" to d_{ij}.
    (Pictures on next two slides)
  - "close" means close if points dense in local neighborhood
    (e.g. $x_{43} = 10.8$)
    not so close if points sparse in local neighborhood ($x_{11} = 2.2$)
  - define h_i as the f quantile of d_{ij} for specified i
    $h_{11} = 2.94$, $h_{43} = 1.10$



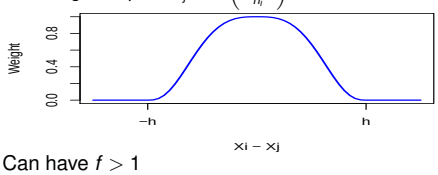


Lowess details

- How to weight points?
  - Cleveland proposed tricube function

$$T(t) = \begin{cases} (1-|t^3|)^3 & \text{for } |t| < 1 \\ 0 & \text{for } |t| \geq 1 \end{cases}$$

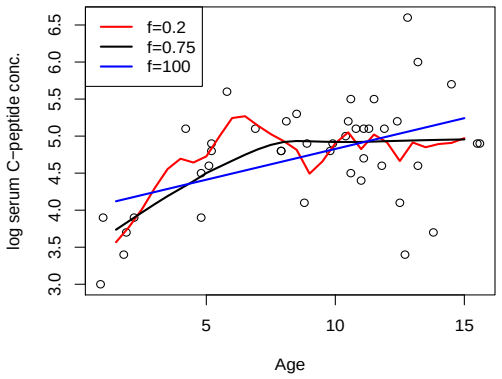
  - weight for point x_j is $T\left(\frac{x_i - x_j}{h_i}\right)$



- Can have $f > 1$
  In this case, $h_i = f^{1/p} \max(d_{ij})$, where $p = \#$ X variables
- large f, e.g. $f \approx 100$, give $w_i = 1$ to all points for all x_i

Lowess details

- What form of local polynomial to fit?
  - Default is often quadratic, can also use linear
- Putting together the pieces:
- estimate $f(x_i)$ by:
  - computing weights, $w_j(x_i)$, for each observation j based on closeness to x_i
  - fitting weighted regression with
    E $Y = \beta_0 + \beta_1 x$ or E $Y = \beta_0 + \beta_1 x + \beta_2 x^2$
  - estimating $f(x_i)$ as $\hat{\beta}_0 + \hat{\beta}_1 x_i$ or $Y = \hat{\beta}_0 + \hat{\beta}_1 x_i + \hat{\beta}_2 x_i^2$
  - Smoothness of estimated $\hat{f}(x_i)$ depends on smoothing parameter f



Loess to assess lack of fit

- Can use loess to assess lack of fit
  E $Y = \beta_0 + \beta_1 x$ is linear loess with $f \to \infty$
  E $Y = \beta_0 + \beta_1 x + \beta_2 x^2$: quadratic loess with $f \to \infty$
- Model comparison:
  - is a straight line appropriate?
    compare linear loess with $f = 100$ to linear loess with small f
  - is a quadratic curve appropriate?
    compare quadratic loess with $f = 100$ to quad. loess with small f
- Need to estimate model df and error df associated with a loess fit
- Intuitively depends on smoothing parameter
  - Smaller f means wigglier curve, larger model df, smaller error df
  - Very large f, e.g. ≈ 100 means model df = 2 or 3 and error df = $n-2$ or $n-3$
- Take same approach as we did with penalized regression splines

- $\hat{f}(x)$ is a linear combination of the observed y's, $\boldsymbol{l_i}\ \boldsymbol{y}$
- so $\hat{\boldsymbol{y}} = \boldsymbol{S}\boldsymbol{y}$ where each row of $\boldsymbol{S}$ is the appropriate $\boldsymbol{l_i}$
- $\boldsymbol{S}$ is a smoother matrix, equivalent to $\boldsymbol{P_X}$ for a Gauss-Markov model
- define model df as $tr(\boldsymbol{S})$
- define error df as $n - 2tr(\boldsymbol{S}) + tr(\boldsymbol{S}\boldsymbol{S}')$
- Degrees of freedom for diabetes data (n=43 obs.)

	Linear loess			Quadratic loess		
span	model	error	total	model	error	total
0.2	11.00	27.89	38.89	17.49	21.8	39.33
0.75	3.04	39.02	42.06	4.61	37.51	42.12
100	2.00	41.00	43.00	2.99	39.99	42.98

- Both df are approximate because $\boldsymbol{S}$ usually not idempotent

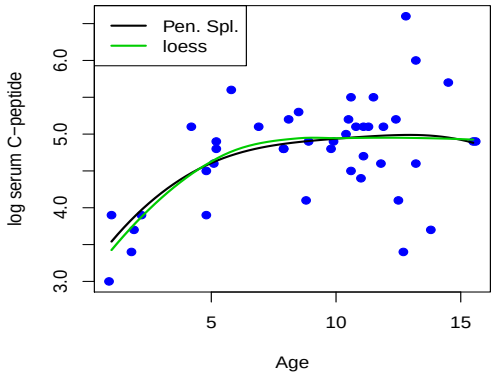
"Robustifying" the fit

- Regression outliers (unusually large or small Y given the X value) can have a big influence, especially when considering only a few points in a local neighborhood
- Idea derived from "M-estimation", a type of robust regression
  goal: general pattern, less (or not) affected by individual values
- Provides a mechanism to reduce the infleuence of one (or more) outliers without deleting any observations
- Concept: (for either linear regression or smoothing)
  wt. regr. where the wt's depend on the size of the residual
- Downweight points with large absolute residuals
- A common choice is the bisquare weight function

$$B(t) = \begin{cases} (1-t^2)^2 & t \le 1 \\ 0 & t > 1 \end{cases}$$

- Cleveland suggests $\delta_i = B(e_i/6m)$,
  m is the median of $| e_1 |, | e_2 |, \cdots, | e_n |$

- M estimation fits very well with local estimation by weighting
- The loess algorithm to estimate $\hat{f}(x_i)$:
  - fit preliminary regression and calculate residuals, e_i
  - calculate $w_j(x_i)$ for each obs. based on f, fraction of points
  - calculate δ_i for downweighting residuals
  - WLS with weights = $w_j(x_i) \times \delta_i$
  - repeat last three steps, once or until convergence
  - estimate $\hat{y}(x_i)$
- In my experience, the choice of smoothing parameter is crucial
  choice of loess or penalized splines much less
  both give similar smooths, when similar amounts of smoothing



Computing for loess

```
# at least two functions to smooth using the loess algorithm
#  lowess()  older version, still used
#  loess()   what I use and will demonstrate

# use the diabetes data to illustrate
diabetes <- read.csv('diabetes.csv')

# basic call
diab.lo <- loess(y ~ age, data=diabetes)

# printing the object provides useful info
diab.lo

# and summary() provides more
summary(diab.lo)
```


Computing for loess

```
# the equivalent # parameters is not trace(S).
#   I don't understand what additional calculation is being done or why.

# default fit is local quadratic (degree = 2) with f = 0.75 (called span)

# useful helper functions:
#  predict, residuals both behave as you would expect.
#  Can specify newdata=  in usual way

plot(diabetes$age,diabetes$y)
lines(seq(0,16,0.5),predict(diab.lo,newdata=data.frame(age=seq(0,16,0.5))))

# can change span or default degree
temp <- loess(y~age,data=diabetes, span=100, degree=2)
lines(seq(0,16,0.5),predict(temp,newdata=data.frame(age=seq(0,16,0.5))))
```

Computing for loess

```
temp <- loess(y~age,data=diabetes, span=100, degree=1)
lines(seq(0,16,0.5),predict(temp,newdata=data.frame(age=seq(0,16,0.5))))

# can also use anova to do model comparison
anova(temp, diab.lo)

# one catch is that both models must be loess objects
diab.lm <- lm(y~age,data=diabetes)
anova(diab.lm, diab.lo)    # doesn't work

# so fit linear using loess() with degree=1 and large span
# or quadratic using degree=2 and large span
```


Computing for loess

```
# default is no outlier downweighting.  add this by specifying
#  family='symmetric'  (Default is family='gaussian'

diab.lo2 <- loess(y~age, data=diabetes, family='symmetric')

plot(diabetes$age,diabetes$y,col=4,pch=19)
lines(seq(0,16,0.5),predict(diab.lo,newdata=data.frame(age=seq(0,16,0.5))))
lines(seq(0,16,0.5),predict(diab.lo2,newdata=data.frame(age=seq(0,16,0.5))),
  col=4)
# very similar fits in this case because no really obvious outliers
```


Methods for large P, small N problems

- Regression has (at least) three major purposes:
  1. Estimate coefficients in a pre-specified model
  2. Discover an appropriate model
  3. Predict values for new observations
- Regression includes classification
  because classification can be viewed as a logistic regression
- Up to now (500, 511), have worked with data with small to moderate number of observations, small number of potentially important variables.
- What if many potential variables?
- e.g. 10,000 variables and 100 observations, $p >> n$
- Linear regression with all 10,000 variables will not work ($\boldsymbol{X}'\boldsymbol{X}$ singular)
- Forward stepwise or all subsets regression will not work well when predictors are highly correlated

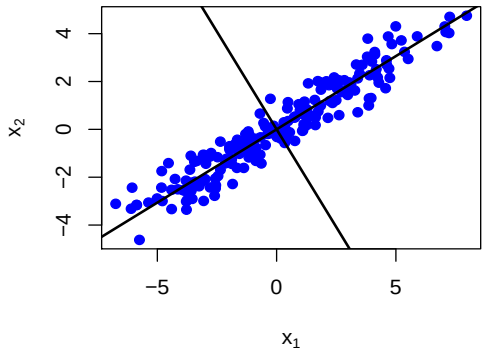
- Often prediction is the most important goal,
  but need 1) and 2) to do prediction
- Practical methods sometimes called data mining.
- Huge area of current research: Statistics, Computer Science
- Large number of potential methods
- We look very quickly at four methods
  1. Principal Components Regression
  2. Partial Least Squares Regression
  3. Ridge Regression
  4. Lasso
- Support Vector Machines, Neural Networks, and elastic nets are other popular (or upcoming) techniques that we will not talk about.
- Hastie, Tibshirani, and Friedman, 2009, *The Elements of Statistical Learning* is my primary source for this material. Also discusses SVM's, NN's, and EN's.

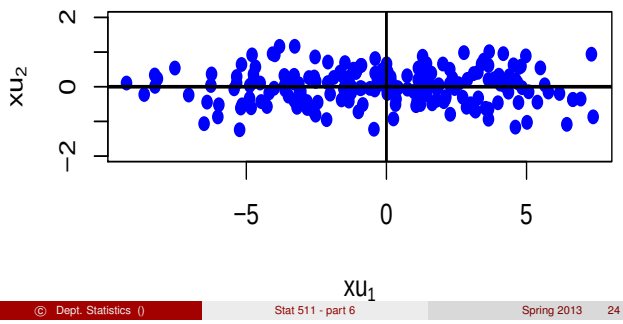
Examples

- Arcene data:
  - Use abundance of proteins in blood to predict whether an individual has cancer (ovarian or prostate).
  - Training data: 10,000 variables, 100 subjects: 44 with cancer, 56 without
  - Validation data: to assess performance of model on new data (out-of-sample prediction) 100 subjects
- Corn grain data:
  - Use the near-infrared absortion spectrum to predict % oil in corn grain
  - Data from ISU grain quality lab, provided by Dr. Charlie Hurbugh
  - Training Data 1: 20 samples from 2008
  - Training Data 2: 337 samples from 2005 - 2008
  - Validation Data: 126 samples from 2009, 2010
  - 38 variables, all highly correlated: pairwise 0.79 - 0.9999

Principle Components Regression

- Useful for:
  - Reducing # X variables
  - Eliminating collinearity
- Example:
  - Corn Grain data, training set 2
  - 337 samples, 38 X variables
- X variables highly correlated: large off-diagonal elements of $\boldsymbol{X}'\boldsymbol{X}$.
- Remember the spectral (aka eigen) decomposition: $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{U}'$, where $\boldsymbol{U}'\boldsymbol{U} = \boldsymbol{I}$
- Center all X variables: $X_i^c = X_i - \mu_i$
- Apply decomposition to $\boldsymbol{X}^{c'}\boldsymbol{X}^c = \boldsymbol{U}\boldsymbol{D}\boldsymbol{U}'$
- Compute new X variables: $\boldsymbol{X}^* = \boldsymbol{X}\boldsymbol{U}$
- This is a rigid rotation around (0,0)

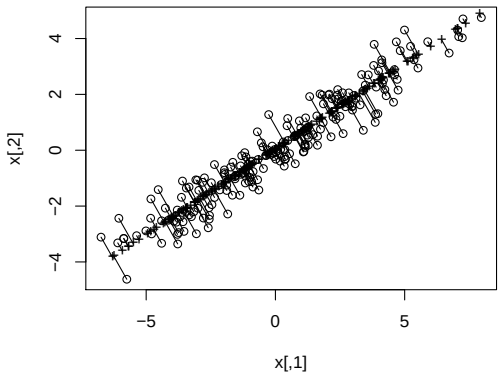




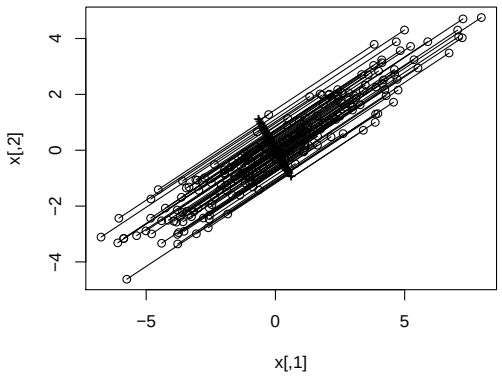
- Why use $\boldsymbol{X}^*$? They are uncorrelated!
- So no multicollinearity problem.
- Estimate $\hat{\beta}^* = (\boldsymbol{X}^{*'}\boldsymbol{X})^{-}\boldsymbol{X}'\boldsymbol{y}$
- Now, want $\hat{\beta}$ for original X variables
- $\hat{\beta} = \boldsymbol{U}\hat{\beta}^*$ because E $Y = \boldsymbol{X}^*\boldsymbol{b}^* = \boldsymbol{X}\boldsymbol{U}\boldsymbol{b}^*$
- If use k PCA axes, obtained from k X variables, can show that the $\hat{\beta}$ are the same as the $\hat{\beta}$ from OLS regression, assuming no numerical issues due to multicollinearity
- However, principal components have a second use.

- Subsets of the k PCA axes provide a reduced rank approximation of $\boldsymbol{X}$
- Some background:
- If X's are centered, $\boldsymbol{X}'\boldsymbol{X}/(N-1)$ is the variance-covariance matrix of the X's
- If X's are centered and scaled (so var $X_i = 1$), $\boldsymbol{X}'\boldsymbol{X}/(N-1)$ is the correlation matrix of the X's
- "Total variance" = $\sum_{i=1}^{k} VarX_i = tr(\boldsymbol{X}'\boldsymbol{X})/(N-1)$
- If $\boldsymbol{X}$ centered, total variance $= tr(D)/(N-1)$, because $tr(\boldsymbol{X}'\boldsymbol{X}) = tr(\boldsymbol{U}\boldsymbol{D}\boldsymbol{U}') = tr(\boldsymbol{D}\boldsymbol{U}'\boldsymbol{U}) = tr(\boldsymbol{D}\boldsymbol{I}) = tr(\boldsymbol{D})$
- If $\boldsymbol{X}$ centered and scaled, $tr(D) = k(N-1)$
- Eigenvalues (diagonal elements of D) customarily sorted from largest (D_{11} to smallest D_{kk}
- A subset of the k eigenvalues and associated eigenvectors provides a reduced rank approximation to $\boldsymbol{X}'\boldsymbol{X}$.

- Consider just $(XU)_1$ in the 2 X example:
- tr$(\boldsymbol{X}'\boldsymbol{X})) = 2718.7$, $diag(D) = [2669.1,\ 49.6]$
- Most (98.2% = 2669.1/2718.7 of the total variability in the two variables is "explained" by the first rotated variable
- To see this, consider reconstructing $\boldsymbol{X}$ from just the first column of $\boldsymbol{X}^*$.
- Since $\boldsymbol{X}^* = \boldsymbol{X}\boldsymbol{U}$, $\boldsymbol{X}^*\boldsymbol{U}^{-1} = \boldsymbol{X}$
- The 'one axis' reconstruction of $\boldsymbol{X}$ is $\boldsymbol{X}_1 = \boldsymbol{X}_1^*\boldsymbol{U}_1$, where $\boldsymbol{X}_1^*$ is the first column of $\boldsymbol{X}^*$ and $\boldsymbol{U}_1$ is the first row of $\boldsymbol{U}$
- Aside: when $\boldsymbol{U}$ is full rank, it has a unique inverse. Since $\boldsymbol{U}'\boldsymbol{U} = \boldsymbol{I}$, that inverse is $\boldsymbol{U}'$.



- Another way to think about PCA, motivated by previous plot.
- The X^* values for PCA axis 1 are the projections of $\boldsymbol{X}$ onto a vector. Could project onto any vector.
- An extreme choice on next page
- Would like to identify the vector for which the variance of the projected values is maximized.
- PCA axis $\nu_m = \boldsymbol{\alpha}$ for which Var($\boldsymbol{X\alpha}$) is maximized subject to:
  1. $||\boldsymbol{\alpha}|| = 1$, avoids trivial changes; Var $\boldsymbol{X}$ $2\boldsymbol{\alpha}$ = 4 Var $\boldsymbol{X\alpha}$.
  2. $\boldsymbol{\alpha}'\nu_i = 0$, $\forall i = 1, \ldots, m-1$, ensures that axis m is orthogonal to all previous axes (1, 2, . . ., m-1)
- The set of ν_m is the matrix of eigenvectors $\boldsymbol{U}$!



- Would have a problem if tried to use $\boldsymbol{X}_1$ as two X variables in a regression! $\boldsymbol{X}_1'\boldsymbol{X}_1$ is singular.
- Don't need to: use only $\boldsymbol{X}_1^*$ (one column) in the regression
- Suggests a way to fit a regression with more X variables than observations (e.g. Corn data from 2008 only: 20 obs, 38 X variables)
- Do a PCA on $\boldsymbol{X}'\boldsymbol{X}$ to create $\boldsymbol{X}^*$. Fit a sequence of regressions:
  - only first column of X^*, i.e. X_1^*
  - first two columns of X^*, i.e. $[X_1^*, X_2^*]$
  - first three columns, . . . many columns
- Use cross validation or GCV to choose optimum number of PCA axes to include in the regression.

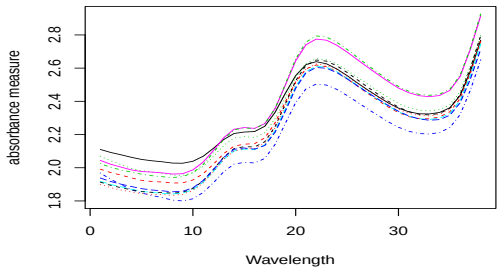
Partial Least Squares (PLS) regression

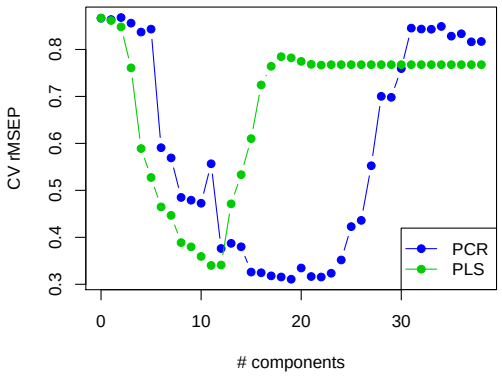
- The PCA at the center of PC Regression only considers the variability in $\boldsymbol{X}$.
- No reason that the linear combination of $\boldsymbol{X}$ that has the largest variance (PCA axis 1) also has to be effective at predicting $\boldsymbol{Y}$
- PCA axes 5 and 7 may be the most highly associated with Y.
- PLS finds axes that simulaneously explain variation in $\boldsymbol{X}$ and predict Y
- The PLS axis ν_m is the $\boldsymbol{\alpha}$ that maximizes

$$Corr^2(\boldsymbol{y}, \boldsymbol{X\alpha})\ Var(\boldsymbol{X\alpha}),$$

subject to:
  1. $||\boldsymbol{\alpha}|| = 1$, avoids trivial changes; Var $\boldsymbol{X}$ $2\boldsymbol{\alpha}$ = 4 Var $\boldsymbol{X\alpha}$.
  2. $\boldsymbol{\alpha}'\nu_i = 0$, $\forall i = 1, \ldots, m-1$, ensures that axis m is orthogonal to all previous axes (1, 2, . . ., m-1)
- Contrast with PCA problem: max Var($\boldsymbol{X\alpha}$)

- Including the correlation with y seems appealing.
- My practical experience is that the max Var aspect of the problem dominates the max Corr, so PLS often very similar to PCR.
- Example: Predicting %Oil in corn grain.
- X is absorbance at 38 wavelengths in the Near Infrared. Data for 10 samples:





Ridge Regression

- An old idea (Hoerl and Kennard, 1970, Techn.) currently in revival
- Originally proposed as a solution to multicollinearity
- Problem is that two or more X variables are correlated
- i.e. some off diagonal elements of $\boldsymbol{X}'\boldsymbol{X}$ are large relative to the diagonal elements
- The ridge regression fix: add an arbitrary constant to the diagonal elements
- i.e. estimate $\hat{\beta}$ by

$$\hat{\beta} = (\boldsymbol{X}'\boldsymbol{X} + \lambda \boldsymbol{I})^{-1}\boldsymbol{X}'\boldsymbol{Y}$$

- Choice of λ changes $\hat{\beta}$ and fit of model
- No justification for one choice or another
- But, we've seen expressions like $(\boldsymbol{X}'\boldsymbol{X} + \lambda \boldsymbol{I})^{-1}\boldsymbol{X}'\boldsymbol{Y}$ very recently when we talked about penalized least squares.

- Penalized splines: $(\boldsymbol{X}'\boldsymbol{X} + \lambda^2 \boldsymbol{D})^{-1}\boldsymbol{X}'\boldsymbol{Y}$ is the solution to the penalized LS problem:

$$min(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta) + \lambda^2 \sum u_j^2$$

- The ridge regression estimates are the solution to a penalized LS problem!

$$min\left[(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta) + \lambda\beta'\beta\right]$$

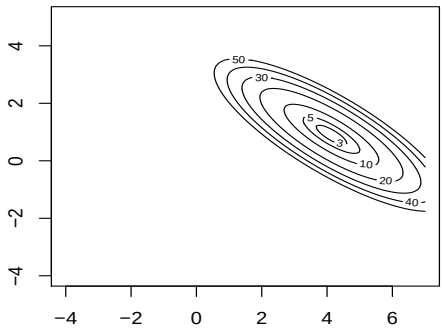
- This insight has lead to the recent resurgence of interest
- Concept of the penalty makes sense. One consequence of multicollinearity is large variance in β. The penalty helps keep β's closer to zero.
- Another version of penalized regression:
- Instead of using $\lambda \sum \beta_i^2$ as the penalty, use $\sum |\beta|$.
- The first is called an L_2 penalty; the second an L_1 penalty

The LASSO

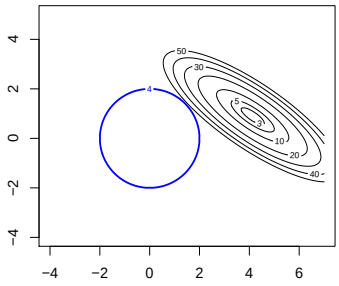
- The LASSO: find β that minimize:

$$(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta) + \lambda\beta'\mathbf{1}$$

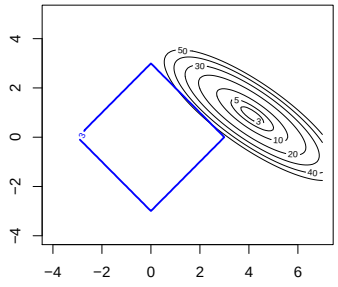
- Seems like a trivial change.
- Turns out to have major and useful consequences
- Because of the shape of the surface of constant penalty
- Consider a regression with 2 X variables. Y, X_1 and X_2 have mean 0.
- Correct model is E $Y = \beta_1 X_1 + \beta_2 X_2$, $\beta_1 = 4, \beta_2 = 0.5$
- Consider the contours of $SS = (Y - \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2)^2$ for a grid of (β_1, β_2)



- Now, think about penalized LS by considering the penalty as a constraint
- What is the LS estimate of (β_1, β_2) given the constraint that $\beta_1^2 + \beta_2^2 = 4$
- Given by the (β_1, β_2) on the constraint surface for which the LS surface is a minimum

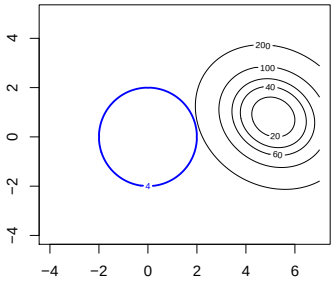


- Changing to L1 penalty changes the shape of the constraint surface



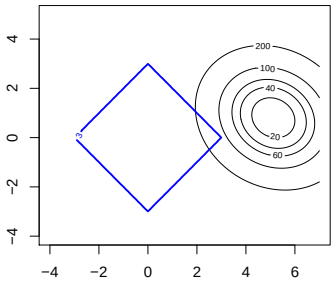
- In this case, $\hat{\beta}_1 \approx 2$, $\hat{\beta}_2 \approx 1$

- The shape of the LASSO (L1 penalty) tends to force $\hat{\beta}$ to 0
- 2nd data set, $\beta_1 = 5,\ \beta_2 = 1$



- $\hat{\beta}_1 \approx 1.9,\ \hat{\beta}_2 \approx 0.7$

- But, the L1 penalty forces $\hat{\beta}_2$ to 0

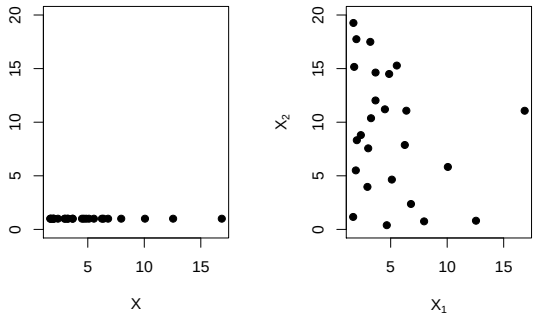


- In this case, $\hat{\beta}_1 = 3,\ \hat{\beta}_2 = 0$

- In practice, the LASSO seems to give better prediction equations than do PCR and PLS.
- Provides a mechanism to do variable selection .
- This has been just a quick introduction to all these methods. There are many details that I have omitted.

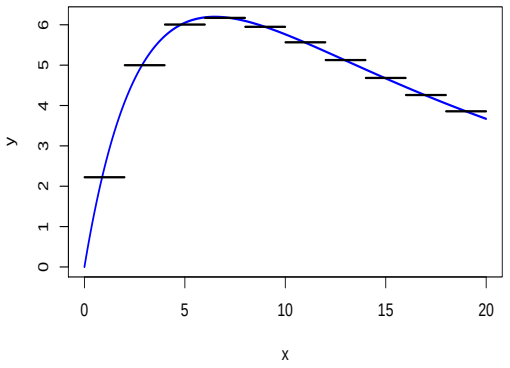
Classification and Regression Trees

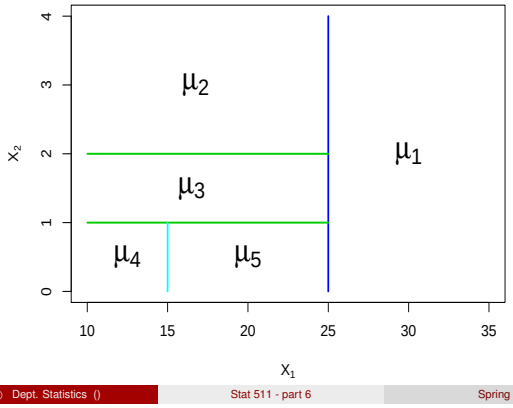
- Another option for problems with complicated interactions
- A very quick way to get a boat-load of X variables is to consider all possible interactions:
  10 X's: 45 cross-products and 120 three-variable interactions!
- Could imagine estimating
  $f(X_1, X_2, \ldots, X_k, X_1X_2, \ldots X_{k-1}X_k, X_1, X_2, X_3, \ldots X_{k-2}X_{k-1}X_k \ldots)$
- Gets hard beyond $k = 4$: "Curse of dimensionality"
- In high dimensions, every point is isolated (see next slide)
- Solutions:
  1. Assume effects are additive E $Y = f(X_1) + f(X_2) + \ldots + X_k$
  2. What if you expect interactions or contingent response to a variable?
     - Contingent response:
       if $X_1 \geq$ e.g. 25, Y unrelated to X_2
       if $X_2 <$ e.g. 25, Y depends on X_1 and X_2
- Tree models provide a way to model contingent responses parsimoniously



- Best known method is the Classification and Regression Tree (CART)
- Breiman et al. (1984), *Classification and Regression Trees*
- Concept: (for 1 X variable)
  - Any E $Y = f(X)$ can be approximated by a sequence of means

$$f(X) = \begin{cases} \mu_1 & X \leq k_1 \\ \mu_2 & k_1 > X \leq k_2 \\ \vdots & \vdots \\ \mu_K & k_{K-1} \leq X < k_K \\ \mu_{K+1} & k_K \leq X \end{cases}$$





- Given Y, assumed continuous, and a set of p potentially useful covariates $\{\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_p\}$, how do we find a subset of k $\boldsymbol{X}$'s and a set of split points $\boldsymbol{s}$ that define an optimal partition of regions $R = \{R_1, R_2, \ldots R_M\}$.
- Criterion: for continuous $\boldsymbol{Y}$, least squares

$$\sum_{j=1}^{M} \sum_{i \in R_j} (Y_i - \mu_j)^2 \qquad (1)$$

  - Focus is on finding the partition.
  - If partition R known, the region means $\{\mu_1, \mu_2, \ldots \mu_M\}$ that minimize (1) are easy to estimate
  - They are the sample average for each region
- Difficult part is finding the optimal partition into regions
- i.e. (previous picture): how to discover which covariates are $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$, and where to split each covariate?

- use a greedy algorithm: make a series of locally optimal choices (best next step), in the hope that together they provide the globally optimal solution.
- Given all the data, 1st step is to split into two half-planes based on variable $\boldsymbol{X}_j$ and split point s:

$$\begin{aligned} R_1(j,s) &= \{X : X_j \leq s\} \\ R_2(j,s) &= \{X : X_j > s\} \end{aligned}$$

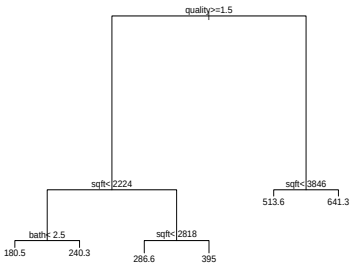
  that minimize

$$SS = \sum_{i:X \in R_1(j,s)} (Y_i - \bar{Y}_1)^2 + \sum_{i:X \in R_2(j,s)} (Y_i - \bar{Y}_2)^2$$

- This search is quite fast,
  because the model is constant mean within region
- If $\boldsymbol{X}_j = 1, 1.2, 1.6, 2, 5$, any s between 1.6 and 2 has same SS. Only need to consider one s, e.g. s= average of two adjacent X values.

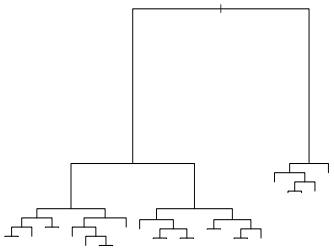
- Now consider R_1 alone: split into two half planes, R_{11} and R_{12}
- Consider R_{11} alone: split into two half planes R_{111} and R_{112}
- Continue until either:
  - reduction in SS after splitting is small
  - small number of points in region
    5 is a commonly used minimum number of points.
    will not split a region with 5 or fewer points
- Back up one level and consider the other side of the split
- Split it as appropriate
- Result is a tree giving the partition into regions and the associated $\hat{Y}$ for each region

- Example: Minneapolis housing price data from Kutner et al.
- Data: Sale price of a house and 11 characteristics (e.g. size, lot size, # bedrooms, ...
- Goal: predict expected sale price given the characteristics

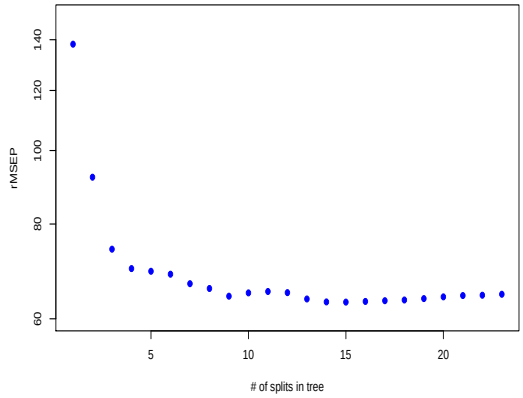


- Suggests # bathrooms important for small houses, not others

- How large/complex a tree should you produce?
- A tree allowing smaller decrease in SS per split



- What is “out of sample” prediction error for each size of tree (# of splits)?
- estimate by ten-fold cross-validation



- Familiar pattern from model selection in multiple regression:
- Simple models have large rMSEP: mostly bias
- Models that are too complex have slightly larger rMSEP: overfitting the training data set
- General advice: fit too large a tree then prune it back
  Increases the chance that find good global optimum (details in Hastie, Tibshirani and Friedman, 2009, *The Elements of Statistical Learning*, p 308.)
- Other general advice: If you believe two (or more variables) have additive effects, don’t use a tree.
  - Split on X_1, then each subset of the data is split on X_2
  - Same X_2 split in both sides. Tree can’t take advantage.
  - Use a GAM
- Trees are low bias, high variance predictors / classifiers

Classification Tree

- response is 0/1 or 1/2/. . ./K
- Want to classify an observation given X
- Same strategy: divide covariate space into regions
- For each region and class, calculate $\hat{p}_{mk}$, the proportion of observations in region m in class k
- Classify the region as type k if k is the most frequent class in the region
- Replace SS (node impurity for continuous data) with one of
  - Misclassification rate: $1 - \sum \hat{p}_{mk^*}$, where k^* is the set of classes other than the true class
  - Gini index: $\sum \hat{p}_{mk}(1 - \hat{p}_{mk})$
  - Deviance: $-\sum \hat{p}_{mk} \log \hat{p}_{mk}$

Random Forests

- Crazy-seeming idea that works extremely well for a low bias, high variance classifier (like a tree)
  - Draw a NP bootstrap sample of observations (resample with replacement)
  - Construct classification or regression tree T_b
  - Repeat B times, giving $T_1,\ T_2,\ \ldots T_B$
- For a specified set of covariates, $\boldsymbol{X}$, each tree gives a prediction $\hat{Y}_b$
- The Random Forest prediction is
  - regression: Average of the B tree-specific predictions
  - classification: most frequent predicted class among the B trees.
- Example of a general technique called *Bootstrap Aggregation* or *bagging*

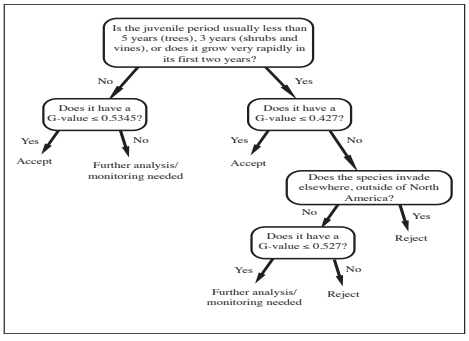
- Why this works: Consider a regression. Assume $\hat{Y} \sim (Y, \sigma^2)$
- If tree predictions are independent, Var $\bar{\hat{Y}} = \sigma^2/B$
- If some positive pair-wise correlation, ρ, Var $\bar{\hat{Y}} = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$
- Still less than σ^2, but better if ρ close to 0
- One final detail that reduces correlation between trees (and hence between their predictions)
  - At each split in each bootstrap tree, randomly choose $m \leq p$ variables as splitting candidates. Often $m \approx \sqrt{p}$
- Does this work: Minneapolis house data, 10 fold c.v.

Method	rMSEP
Tree	64.86
Forest	55.39

- Disadvantage:
  no convenient way to summarize / describe the model

Forests or trees?

- One of my current research collaborations: predicting invasiveness of woody trees and shrubs
- The horticulture industry wants to import shrubs and trees from other countries.
  - Showy flowers, interesting form, survives in nasty places
- Some, e.g. buckthorn, become invasive pests, invading native forests.
- The USDA Ag and Plant Health Inspection Service (APHIS) has to decide whether to permit importation of new plants.
- The million $ question: will it be invasive. ????
  - Various “seat-of-the-pants” models
  - A CART model beats all of them in predicting invasiveness in IA
  - And Chicago, and northern IN, and southern MN, and northern MO.
  - Nice, clean tree that we have published so others can use our results
    (See next slide)



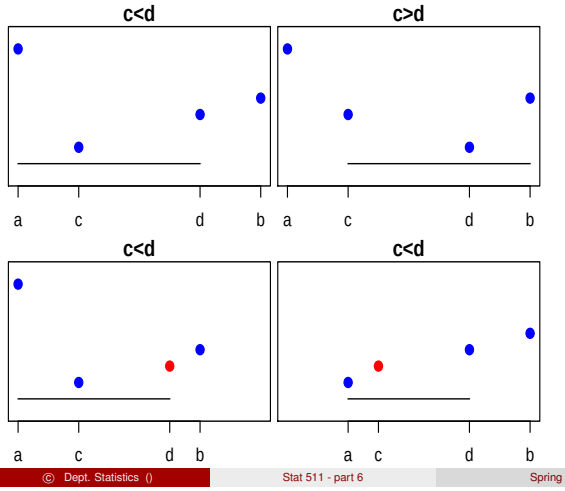
- A random forest makes even better predictions
- But, have 1000 trees. Can't show them.
- The model lives in a computer.
- We're currently writing a proposal to put the RF model on a web server, so everyone can use it.

Numerical Optimization

- Huge field, many different techniques, active research area
- Has impact in just about every scientific field
- Applied statisticians need a basic familiarity with optimization
- and how to help it when the usual doesn't work
- That's my goal in this section
- Will talk about:
  - golden section search
  - Gauss-Newton (have already done this)
  - Newton-Raphson
  - "derivative-free" methods (e.g. BFGS)
  - Nelder-Mead
  - the Expectation-Maximization (EM) algorithm
- Will talk about minimization (max f = min $-f$)

Golden section search

- For a unimodal function of a scalar (univariate) function
- Requires two starting values, a and b. Finds location of the minimum of $f(x)$ in $[a, b]$
- The concept:
  - Choose two points c and d s.t. $a < c < d < b$
  - Calculate $f(a)$, $f(b)$, $f(c)$ and $f(d)$
  - if $f(c) < f(d)$, minimum is somewhere between a and d replace b with d
  - if $f(c) > f(d)$, minimum is somewhere between c and b replace a with c
- A picture will make this much clearer



- So, how to pick c and d?
- Convergence is faster when:
  - $c - a + d - c = b - c$ i.e. $d - a = b - c$
  - ratios of distances between points in "old" and "new" configurations are equal
- result is when $\left(\frac{c-a}{d-b}\right)^2 = \frac{c-a}{d-b} + 1$
- i.e. $\frac{c-a}{b-d} = \frac{1+\sqrt{5}}{2}$
- This is the "golden ratio" of mathematical fame, which gives this method its name.
- Iterate until the bracketing region is sufficiently small
- Usually defined relative to minimum achievable precision for the operating system
- N.B. Only works for univariate problems!

Practical issues

- This algorithm is very robust. It has always worked for me.
- If you have multiple minima in $[a, b]$, algorithm finds one of them Not necessarily the correct (smallest) minimum.
- Variation finds roots of a function, i.e. x s.t. $f(x) = 0$
  - Need to choose a and b s.t. $f(a)$ and $f(b)$ have opposite signs
  - i.e. $f(a) > 0$ and $f(b) < 0$
  - Which guarantees (for a continuous function) there is a root in $[a, b]$
- I find profile likelihood confidence intervals by finding roots of $\log L(\theta_{mle}) - \log L(\theta) - \chi^2_{1-\alpha,DF}/2 = 0$
- find one endpoint by finding root between $[small, \theta_{mle}]$ and the other by finding root between $[\theta_{mle}, large]$

Minimization for functions of vectors

- We've already seen one algorithm for minimization of a function of vectors: Gauss-Newtown (see part 5, slides 47, 48)
- Another way to write one step of the Gauss-Newton iteration:
  - $\beta^{(i+1)} = \beta^{(i)} + (\boldsymbol{D}'\boldsymbol{D})^{-1}\boldsymbol{D}'(\boldsymbol{y} - f(\boldsymbol{x}, \beta))$
  - where $\boldsymbol{D}$ is the matrix of derivatives of f w.r.t. each element of β evaluated at each X
- A related algorithm: Newton-Raphson
  - to find a root of a function, i.e. x s.t. $f(x) = 0$
  - If $f(x)$ is linear, the root is $x - \frac{f(x)}{f'(x)}$, where $f'(x) = \frac{df}{dx} \mid x$
  - If $f(x)$ is non-linear, can find the root by successive approximation
    $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$
    $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}, \ldots$
  - We need to find the minimum/maximum of a function, i.e. where $f'(x) = 0$, so our iterations are:
    - $x_1 = x_0 - \frac{f'(x_0)}{f''(x_0)}$ $\quad x_2 = x_1 - \frac{f'(x_1)}{f''(x_1)}, \ldots$

Newton-Raphson and Fisher scoring algorithms

- For functions of vector valued parameters, the scalar derivatives are replaced by gradient vectors and Hessian matrices:
  - $\boldsymbol{X}_1 = \boldsymbol{X}_0 - \boldsymbol{H}_0^{-1}\boldsymbol{D}_0$
    $\boldsymbol{X}_2 = \boldsymbol{X}_1 - \boldsymbol{H}_1^{-1}\boldsymbol{D}_1, \ldots,$
  - where $\boldsymbol{D}_i$ is the gradient vector evaluated at $\boldsymbol{X}_i$ and $\boldsymbol{H}_i$ is the Hessian matrix evaluated at $\boldsymbol{X}_i$.
- Fisher scoring: replace the observed Hessian matrix with its expected value
  - E $-\boldsymbol{H}^{-1}$ is the Fisher information matrix from Stat Theory
  - Requires calculating the expectation
  - In expectation, E $\boldsymbol{H}$ = E $\boldsymbol{D}'\boldsymbol{D}$
  - Historically useful because gave simple expressions for hand-worked iterative calculations for many discrete distributions
  - In many cases, Newton-Raphson works better than Fisher scoring

Practical considerations

- i.e. does it matter which method choose?
  - Newton-Raphson requires the Hessian (2nd derivative) matrix
  - Easy to compute if have analytic second derivatives
  - If have to compute gradient and/or Hessian numerically, considerably numerical inaccuracy in Hessian (more below)
  - To me, not much of a practical difference
  - Numerical analysts focus on this sort of issue; I don't.
  - For me: what is provided / used by software trumps theoretical concerns.
  - John Tukey: practical power = product of statistical power and probability a method will be used.

"Derivative-free" methods

- What if you don't (or don't want to) calculate an analytic gradient vector or Hessian matrix?
- For Gauss-Newton: replace the analytic gradient with a numeric approximation
  - Two possibilities:
    - "forward" differences: $\frac{df}{dx} \mid x_0 \approx \frac{f(x_0+\delta)-f(x_0)}{\delta}$
    - "central" differences: $\frac{df}{dx} \mid x_0 \approx \frac{f(x_0+\delta)-f(x_0-\delta)}{2\delta}$
  - "central" differences are better approximations, but require more computing when $\boldsymbol{X}$ is large
- For Newtown-Raphson, also need to approximate the Hessian (2nd derivative) matrix
  numerical accuracy issues are a serious concern: differences of differences are subject to serious roundoff error
- various algorithms reconstruct the Hessian matrix from a sequence of estimated derivatives
- The Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is the most popular (for good reasons).

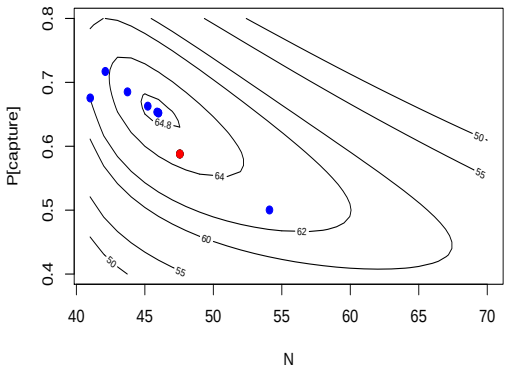
Take home message for an applied statistican: BFGS is a

Dealing with problems

- What if the algorithm doesn't converge?
  - First, and foremost, check that any analytic quantities (derivatives, Hessian matrices) are correct.
    - Many times I've made a sign error in one of my calculations
    - Has serious consequences; usually stops algorithm from making progress!
    - Compare analytic derivatices (or Hessian) to numerical approximations.
    - Should be close
  - Consider different starting values
    - if start at a "bad" place, e.g. gradient essentially flat there, will not make progress
- Working on the above two things usually fixes problems.
- If not, consider a different algorithm, e.g. Nelder-Mead, which does not depend on derivatives

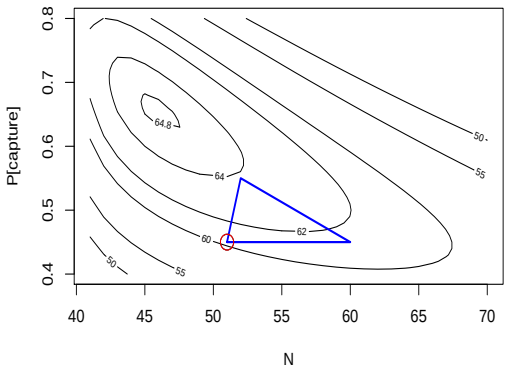
Step-halving

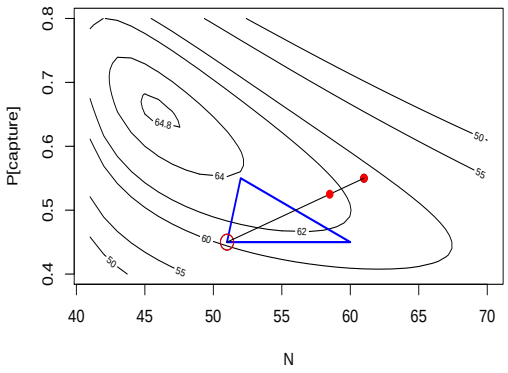
- One practical detail
- G-N, N-R, and BFGS all have the form:
  $\boldsymbol{X}^{(i+1)} = \boldsymbol{X}^{(}i) +$ "step"
- Step specifies both the direction to move and the amount to move.
- Sometimes the direction is reasonable, but the amount is not.
- Picture on next slide (NR iterations), started at (50,0.2)
- Practical solution: Step-halving
  - when $f(\boldsymbol{X}^{i+1}) > f(\boldsymbol{X}^{i})$, i.e. algorithm 'getting worse'
  - replace "step" with "step"/2
  - if that's still too much, repeat (so now 1/4 original step)
- N-R step starting at (54, 0.5) goes to (41, 0.68)
  lnL from 62.9 down to 62.0
- Red dot would be the 'step-halved' next try, lnL > 64

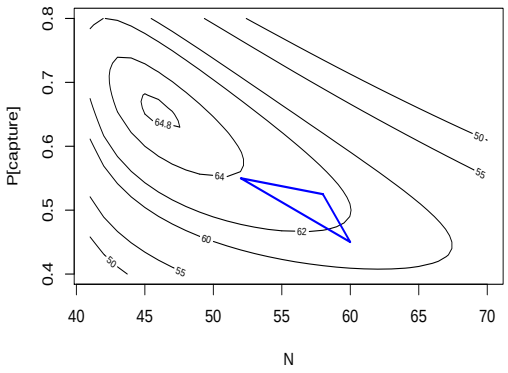


Nelder-Mead algorithm

- Concepts, not details
- N is the length of the parameter vector
- Construct a $N + 1$ simplex in the parameter space (picture on next slide)
- Find the worst vertex (largest if minimizing, smallest if maximizing)
- Replace it by a new point
  - Basic step is reflection (another picture)
  - But also expansion, contraction and reduction
  - (As I said, details don't matter)
- Fundamentally different algorithm from others
- Doesn't directly use any gradient information
- So, what do I use?
  - BFGS is my standard default choice
  - If that struggles, I switch to Nelder-Mead



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