Lecture 6: Bootstrapping

36-402, Advanced Data Analysis

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The Big Picture

1. Knowing the sampling distribution of a statistic tells us about statistical uncertainty (standard errors, biases, confidence sets)
2. The bootstrap principle: *approximate* the sampling distribution by *simulating* from a good model of the data, and treating the simulated data just like the real data
3. Sometimes we simulate from the model we're estimating (parametric bootstrap)
4. Sometimes we simulate by re-sampling the original data (nonparametric bootstrap)
5. As always, stronger assumptions mean less uncertainty *if we're right*

Re-run the experiment (survey, census, ...) and we get more or less different data

$\therefore$ everything we calculate from data (estimates, test statistics, policies, ...) will change from trial to trial as well

This variability is (the source of) **statistical uncertainty**

Quantifying this is a way of being honest about what we do and do not know

Measures of Statistical Uncertainty

Standard error = standard deviation of an estimator

could equally well use median absolute deviation, etc.

p-value = Probability we'd see a signal this big if there was just noise

Confidence region = All the parameter values we can't reject at low error rates:

1. *Either* the true parameter is in the confidence region
2. *or* we are very unlucky
3. *or* our model is wrong

etc.

The Sampling Distribution Is the Source of All Knowledge

Data $X \sim P_{X,\theta_0}$, for some true θ_0
We calculate a statistic $T = \tau(X)$ so it has distribution P_{T,θ_0}
If we knew P_{T,θ_0}, we could calculate $\mathrm{Var}[T]$ (and so standard error), $\mathbf{E}[T]$ (and so bias), quantiles (and so confidence intervals or p-values), etc.
Problem 1: Most of the time, P_{X,θ_0} is very complicated
Problem 2: Most of the time, τ is a very complicated function
Problem 3: We certainly don't know θ_0
Upshot: We don't know P_{T,θ_0} and can't use it to calculate anything

The Solution

Classically ($\approx$ 1900–$\approx$ 1975): Restrict the model and the statistic until you can calculate the sampling distribution, at least for very large n

Modern ($\approx$ 1975–): Use complex models and statistics, but simulate calculating the statistic on the model

some use of this idea back to the 1940s at least

The Bootstrap Principle

1. Find a good estimate $\hat{P}$ for P_{X,θ_0}
2. Generate a simulation $\tilde{X}$ from $\hat{P}$, set $\tilde{T} = \tau(\tilde{X})$
3. Use the simulated distribution of the $\tilde{T}$ to approximate P_{T,θ_0}

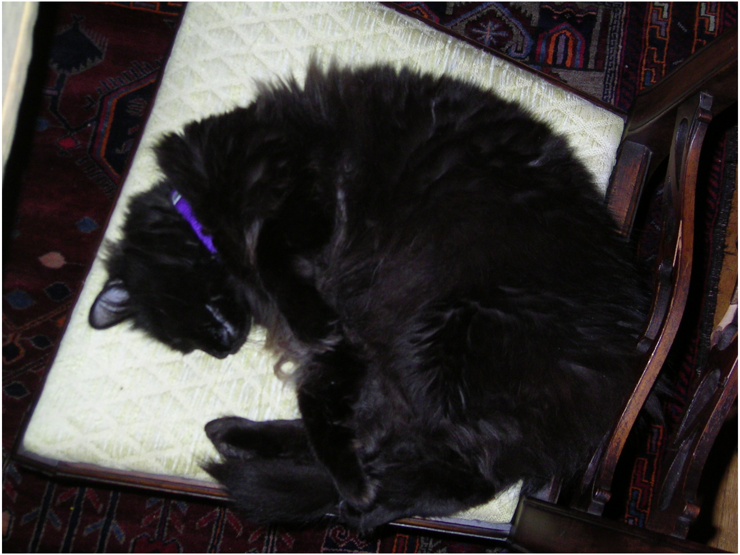
Refinements: improving the initial estimate $\hat{P}$
reducing the number of simulations or speeding them up
transforming τ so the final approximation is more stable
First step: find a good estimate $\hat{P}$ for P_{X,θ_0}

If we are using a model, our best guess at P_{X,θ_0} is $P_{X,\hat{\theta}}$, with our best estimate $\hat{\theta}$ of the parameters

THE PARAMETRIC BOOTSTRAP

1. Get data X, estimate $\hat{\theta}$ from X
2. Repeat b times:
    1. Simulate $\tilde{X}$ from $P_{X,\hat{\theta}}$ (simulate data of same size/"shape" as real data)
    2. Calculate $\tilde{T} = \tau(\tilde{X})$ (treat simulated data the same as real data)
3. Use empirical distribution of $\tilde{T}$ as P_{T,θ_0}

Concrete Example



Is Moonshine over-weight?

Switch to R

Data on weights of 144 cats; fit Gaussian, find 95th percentile

```
library(MASS); data(cats); summary(cats)
(q95.gaussian <- qnorm(0.95,mean=mean(cats$Bwt),sd=sd(cats$Bwt)))
```

Switch to R

Simulate from fitted Gaussian; bundle up estimating 95th percentile into a function

```
rcats.gaussian <- function() {
  rnorm(n=nrow(cats),mean=mean(cats$Bwt),sd=sd(cats$Bwt))
}

est.q95.gaussian <- function(x) {
  m <- mean(x)
  s <- sd(x)
  return(qnorm(0.95,mean=m,sd=s))
}
```

Simulate, plot the sampling distribution from the simulations

```
sampling.dist.gaussian <- replicate(1000, est.q95.gaussian(rcats.gaussian()))
plot(hist(sampling.dist.gaussian,breaks=50),freq=FALSE)
plot(density(sampling.dist.gaussian))
abline(v=q95.gaussian,lty=2)
```

Switch to R

Find standard error and a crude confidence interval

```
sd(sampling.dist.gaussian)
quantile(sampling.dist.gaussian,c(0.025,0.975))
```

Improving on the Crude Confidence Interval

The crude confidence interval uses the distribution of $\tilde{\theta}$ under $\hat{\theta}$
But really we want the distribution of $\hat{\theta}$ under θ
Observation: Generally speaking,

$$\Pr_{\hat{\theta}}\left(\tilde{\theta} - \hat{\theta} \leq a\right) \rightarrow \Pr_{\theta_0}\left(\hat{\theta} - \theta_0 \leq a\right)$$

faster than

$$\Pr_{\hat{\theta}}\left(\tilde{\theta} \leq a\right) \rightarrow \Pr_{\theta_0}\left(\hat{\theta} \leq a\right)$$

(errors converge faster, as in CLT)
$\hat{\theta} - \theta_0$ is (nearly) "pivotal"

The Basic, Pivotal CI

$q_{\alpha/2}, q_{1-\alpha/2} =$ quantiles of $\tilde{\theta}$

$$
\begin{aligned}
1-\alpha &= \Pr_{\hat{\theta}}\left(q_{\alpha/2} \leq \tilde{\theta} \leq q_{1-\alpha/2}\right) \\
&= \Pr_{\hat{\theta}}\left(q_{\alpha/2} - \hat{\theta} \leq \tilde{\theta} - \hat{\theta} \leq q_{1-\alpha/2} - \hat{\theta}\right) \\
&\approx \Pr_{\theta_0}\left(q_{\alpha/2} - \hat{\theta} \leq \hat{\theta} - \theta_0 \leq q_{1-\alpha/2} - \hat{\theta}\right) \\
&= \Pr_{\theta_0}\left(q_{\alpha/2} - 2\hat{\theta} \leq -\theta_0 \leq q_{1-\alpha/2} - 2\hat{\theta}\right) \\
&= \Pr_{\theta_0}\left(2\hat{\theta} - q_{1-\alpha/2} \leq \theta_0 \leq 2\hat{\theta} - q_{\alpha/2}\right)
\end{aligned}
$$

Basically: re-center the simulations around the empirical data

Switch to R

Find the basic CI

```
2*q95.gaussian - quantile(sampling.dist.gaussian,c(0.975,0.025))
```

As always, if the model isn't right, relying on the model is asking for trouble

How good is the Gaussian as a model for the distribution of cats' weights?

Switch to R

Compare histogram to fitted Gaussian density and to a smooth density estimate

```
plot(hist(cats$Bwt),freq=FALSE)
curve(dnorm(x,mean=mean(cats$Bwt),sd=sd(cats$Bwt)),add=TRUE,col="purple")
lines(density(cats$Bwt),lty=2)
```

Problem: Suppose we don't have a trust-worthy parametric model
Resource; We do have data, which tells us a lot about the distribution
Solution: **Resampling**, treat the sample like a whole population

THE NONPARAMETRIC BOOTSTRAP

1. Get data X, containing n samples
2. Repeat b times:
    1. Generate $\tilde{X}$ by drawing n samples from X *with replacement* (resample the data)
    2. Calculate $\tilde{T} = \tau\tilde{X}$ (treat simulated data the same as real data)
3. Use empirical distribution of $\tilde{T}$ as $P_{T,\theta}$

Is Moonshine Overweight, Take 2

Model-free estimate of the 95th percentile is the 95th percentile of the data
How precise is that?

Switch to R

Resampling, re-estimating, and finding sampling distribution, standard error, bias, CIs

```
(q95.np <- quantile(cats$Bwt,0.95))
resample <- function(x) {
  sample(x,size=length(x),replace=TRUE)
}
est.q95.np <- function(x) {
  quantile(x,0.95)
}
sampling.dist.np <- replicate(1000, est.q95.np(resample(cats$Bwt)))
plot(density(sampling.dist.np))
abline(v=q95.np,lty=2)
sd(sampling.dist.np)
mean(sampling.dist.np - q95.np)
quantile(sampling.dist.np,c(0.025,0.975))
2*q95.np - quantile(sampling.dist.np,c(0.975,0.025))
```

Bootstrapping Regressions

A regression is a model for Y conditional on X

$$Y = m(X) + \text{noise}$$

Silent about distribution of X, so how do we simulate?
Options, putting less and less trust in the model:

1. Hold x_i fixed, set $\tilde{y}_i = \hat{m}(x_i) + \text{noise}$ from model's estimated noise distribution (e.g., Gaussian)
2. Hold x_i fixed, set $\tilde{y}_i = \hat{m}(x_i) +$ a resampled residual
3. Resample (x_i, y_i) pairs (resample data-points or resample cases)

The `cats` data set has weights for cats' hearts, as well as bodies

Much cuter than an actual photo of cats' hearts

Source: `http://yaleheartstudy.org/site/wp-content/uploads/2012/03/cat-heart1.jpg`

How does heart weight relate to body weight?

(Useful if Moonshine's vet wants to know how much heart medicine to prescribe)

Switch to R

Plot the data with the regression line

```
plot(Hwt~Bwt, data=cats, xlab="Body weight (kg)", ylab="Heart weight (g)")
cats.lm <- lm(Hwt ~ Bwt, data=cats)
abline(cats.lm)
```

Switch to R

Coefficients and "official" confidence intervals:

```
coefficients(cats.lm)
confint(cats.lm)
```

Switch to R

The residuals don't look very Gaussian:

```
plot(cats$Bwt,residuals(cats.lm))
plot(density(residuals(cats.lm)))
```

Switch to R

Find CIs for coefficients by resampling cases:

```
coefs.cats.lm <- function(subset) {
  fit <- lm(Hwt~Bwt,data=cats,subset=subset)
  return(coefficients(fit))
}
cats.lm.sampling.dist <- replicate(1000, coefs.cats.lm(resample(1:nrow(cats))))
(limits <- apply(cats.lm.sampling.dist,1,quantile,c(0.025,0.975)))
```

Sources of Error in Bootstrapping

Simulation Using only b bootstrap replicates
Make this small by letting $b \to \infty$
Costs computing time

Approximation Using $\hat{P}$ instead of P_{X,θ_0}
Make this small by careful statistical modeling

Estimation Only a finite number of samples
Make this small by being careful about what we simulate (e.g., basic interval vs. crude interval)

Generally: for fixed n, nonparametric boostrap shows more uncertainty than parametric bootstraps, but is less at risk to modeling mistakes

yet another bias-variance tradeoff

Summing Up

1. Standard errors, biases, confidence regions, p-values, etc., could all be calculated from the sampling distribution of our statistic
2. The bootstrap principle: simulate from a good estimate of the real process, use that to approximate the sampling distribution
   - Parametric bootstrapping simulates an ordinary model
   - Nonparametric bootstrapping resamples the original data

   Simulations get processed *just like* real data
3. Bootstrapping works for regressions and for complicated models as well as distributions and simple models