THE UNIVERSITY OF TEXAS AT AUSTIN
Department of Statistics and Data Sciences
College of Natural Sciences

SDS 385: Stat Models for Big Data

Lecture 11: Bootstrap and subsampling

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Bootstrap

- So far we have talked about estimation, and ways to estimate statistical quantities quickly
- But often, you are interested in quantifying the variability of your estimate
- You can do this using the variance of your estimate or by producing a confidence interval
- What is a confidence interval?

Confidence Interval

- Data $X_1, \ldots, X_n \overset{\text{iid}}{\sim} P$
- Some estimator $\hat{\theta}$ of parameter of interest θ.
- For some coverage α, want to produce a lower and upper bound such that:

$$P\left(\hat{a} \leq \theta \leq \hat{b}\right) \geq 1 - 2\alpha,$$

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- Say you know the distribution of $(\hat{\theta} - \theta)/\hat{\sigma}$
- Then you will just return:

$$P\left(\hat{\theta} - \kappa_{1-\alpha}\hat{\sigma} \leq \theta \leq \hat{\theta} - \kappa_{\alpha}\hat{\sigma}\right) \geq 1 - 2\alpha,$$

  where $\kappa_\alpha, \kappa_{1-\alpha}$ are the quantiles of $(\hat{\theta} - \theta)/\hat{\sigma}$
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  where $\kappa_{\alpha}, \kappa_{1-\alpha}$ are the quantiles of $(\hat{\theta} - \theta)/\hat{\sigma}$
- The distribution of $(\hat{\theta} - \theta)/\hat{\sigma}$ depends on P.
- Often this distribution is normal, but with unknown parameters.

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- The trouble is we don't know P.
- What will we do if we did know P?

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- What will we do if we did know P?
- Draw B datasets of size n from P
- For the i^{th} dataset, calculate $\hat{\theta}^{(i)}$
- Now get the distribution of $\hat{\theta}^{(1)}, \ldots, \hat{\theta}^{(B)}$ and get the C.I.

Bootstrap

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- Drawing n points from this distribution boils down to?
- Sampling with replacement!

Bootstrap: plug in principle

True model	Bootstrapped model
$\hat{\theta}$	$\hat{\theta}^*$
$\hat{\sigma}$	$\hat{\sigma}^*$
$\dfrac{\hat{\theta} - \theta}{\hat{\sigma}}$	$\dfrac{\hat{\theta}^* - \hat{\theta}}{\hat{\sigma}^*}$

Empirical bootstrap

How do you estimate P?

Empirical Bootstrap $\hat{P} = \frac{1}{n}\sum_i \delta(x_i)$

Generate m samples $(X_1^*, \dots, X_n^*)^{(j)}$, $j = 1 : m$.
Each giving a $(\hat{\theta}^*, \hat{\sigma}^*)$ pair.
Compute the κ_α quantile
of the distribution of $\frac{\hat{\theta}^* - \hat{\theta}}{\hat{\sigma}^*}$

Parametric bootstrap $\hat{P} = P_{\hat{\theta}}$

Empirical bootstrap

Lets try the simplest setting with $\theta = \mu := E[X_1]$

- What is the expectation of the bootstrapped mean $\bar{X}^*$ given the data?

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\begin{aligned}
E[\bar{X}^*|X_1,\ldots,X_n] &= E\left[\frac{1}{n}\sum_i X_i^*|X_1,\ldots,X_n\right] \\
&= E[X_1^*|X_1,\ldots,X_n] \\
&= \sum_{i=1}^{n} X_i \times n = \bar{X}
\end{aligned}
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\mathrm{var}[\bar{X}^* | X_1, \ldots, X_n] &= \mathrm{var}\left[\frac{1}{n}\sum_{i=1}^{n} X_i^* | X_1, \ldots, X_n\right] \\
&= \frac{1}{n}\mathrm{var}\left[X_1^* | X_1, \ldots, X_n\right] \\
&= \frac{1}{n}\left(E[(X_1^*)^2 | X_1, \ldots, X_n] - \bar{X}^2\right) \\
&= \frac{1}{n}\underbrace{\left(\frac{1}{n}\sum_i X_i^2 - \bar{X}^2\right)}_{\text{Sample Variance}}
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\end{aligned}
$$

- This makes sense, since the sample variance converges to the true variance, and we all know that the variance of $\bar{X}$ is exactly σ^2/n

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- Its a normal, of course, like a lot of other estimators.
- With variance $\frac{1}{4nf(\tilde{\mu})^2}$, where $\tilde{\mu}$ is the population median and f is the density of P
- If we don't know P, we can't evaluate the above.

Empirical Bootstrap

Does it always work?

Empirical Bootstrap

Does it always work? Lets try the maximum of $X_1, \ldots, X_n \overset{\text{iid}}{\sim} U([0, \theta])$

- What is the true limiting distribution?

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- What is the true limiting distribution?

$$P\left(\frac{n(\theta - X_{(n)})}{\theta} > x\right) = P\left(X_{(n)} \leq \theta(1 - x/n)\right) = (1 - x/n)^n \to e^{-x}$$

- The bootstrapped limiting distribution

$$P\left(\frac{n(X_{(n)} - X^*_{(n)})}{X_{(n)}} = 0\right) = P(X^*_{(n)} = X_{(n)}) = \left(1 - (1 - 1/n)^n\right) \to 1 - 1/e$$

Empirical Bootstrap

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Empirical Bootstrap

Does it always work?

- Rule of thumb: when the asymptotic distribution is normal.
- Another con is it will take forever if n is large, even if you parallelize
- What do you do when its not?

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- What to do? You will need to analytically correct the variability.

Subsampling - pros and cons

Pros

- Very fast, specially you have a super-linear estimation algorithm
- Works for statistics which bootstrap doesnt work for, i.e. requires far less conditions, as long as b grows to infinity with n, but at a slower rate.

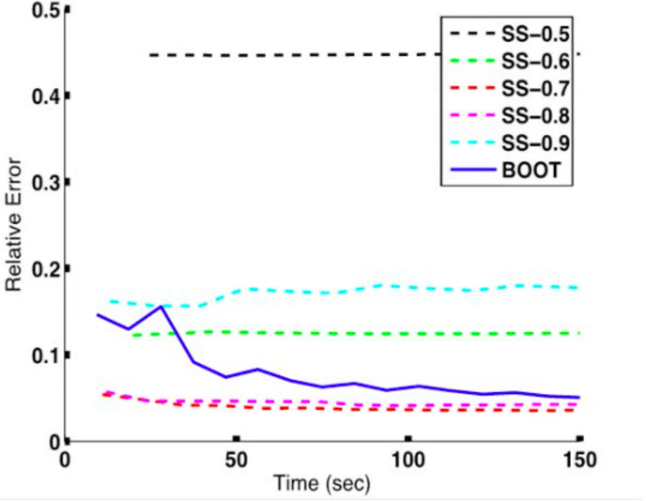
Cons

- Very sensitive to the choice of b (next two slides)
- You need to know the scaling factor to correct for using $b < n$

Subsampling - cons [See "Bag of little Bootstraps" paper]

- Multivariate linear regression with d = 100 and n = 50,000 on synthetic data.
- x coordinates sampled independently from StudentT(3).
- $y = w^T x + \varepsilon$, where w in R^d is a fixed weight vector and ε is Gaussian noise.
- Estimate $\theta_n = w_n$ in R^d via least squares.
- Compute a marginal confidence interval for each component of w_n and assess accuracy via relative mean (across components) absolute deviation from true confidence interval size.
- For subsampling, use $b(n) = n^\gamma$ for various values of γ.
- Similar results obtained with Normal and Gamma data generating distributions, as well as if estimate a misspecified model.

Subsampling - cons



Bag of little bootstraps

- In between subsampling and bootstrap
- Draw size m w/o replacement samples from the data
- Draw size n with replacement samples from each subsample

Summary

- Three main parts+ϵ
- Large scale optimization:
    - Gradient descent, Newton Raphson
    - Stochastic gradient descent, proximal methods, subgradients, dual coordinate ascent, etc.

Summary

- Three main parts+ϵ
- Large scale optimization:
    - Momentum methods:
        - SGD has trouble navigating ravines, i.e. areas where the surface curves much more steeply in one dimension than in another , which are common around local optima.
        - Momentum helps accelerate SGD in the correct direction by damping oscillation
        - It does this by adding a fraction of the update vector of the past time step to the current update vector:

Summary

- Three main parts
- Large scale optimization:
  - Adaptive methods:
    - John Duchi, Elad Hazan, Yoram Singer. "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization." Journal of Machine Learning Research 2011
    - Adaptively learn learning rates for different coordinates – slow learning rates for frequent features, and large ones for infrequent features
    - Unfortunately the squared gradients keep accumulating and eventually learning rate goes to zero.
    - Diederik, Kingma; Ba, Jimmy (2014), "Adam: a Method for Stochastic Optimization"
    - ADAM uses exponentially decaying average of past squared gradients, and also does bias correction by estimating moments.

Summary

- Large scale optimization:
  - Stochastic gradient descent
    - Rie Johnson and Tong Zhang. Accelerating stochastic gradient descent using predictive variance reduction. In Advances in neural information processing systems, pages 315–323, 2013
    - Main point: Talks about dual coordinate ascent and shows how this leads to variance reduction

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- Large scale optimization:
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    - Main point: Talks about dual coordinate ascent and shows how this leads to variance reduction
    - Wilson et al., The Marginal Value of Adaptive Gradient Methods in Machine Learning (NeurIPS 2017)
    - Talks about pitfalls of Adaptive methods using a simple overparameterized problem
    - Feng Niu, Benjamin Recht, Christopher Re, Stephen J. Wright, Hogwild!: A Lock-Free Approach to Parallelizing Stochastic Gradient Descent", NIPS 2011.
    - Asynchronous SGD without locks–use the sparsity in data

Summary

- Nearest neighbor methods: locality sensitive hashing, random projections and Johnson-Lindenstrauss, tree structures
  - Random Features for Large-Scale Kernel Machines, Ali Rahimi, Ben Recht, NIPS 2007
  - Random hash functions to project data to a low dimensional space so that the inner products of the transformed data are approximately equal to those in the feature space of a kernel.
  - Weinberger, Kilian, et al. "Feature hashing for large scale multitask learning." ICML, 2009.
  - Random projection type hash functions to bring high dimensional data down to lower dimensional space while not affecting the dot products (which are important for a various number of tasks).

Summary

- PCA, Spectral clustering
- Semisupervised learning, Pagerank, connection using random walks
- Power method for eigenvectors
- Networks: blockmodels, mixed membership models, connections to spectral clustering
- Topic models: connection to mixed membership models and corner finding algorithms
- Bootstrap and subsampling