ORIE 4580/5580: Simulation Modeling and Analysis

ORIE 5581: Monte Carlo Simulation

Unit 7: input modeling

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input modeling

we want to answer two related questions:

- how can we use data to define the probability distributions of the 'input sequences' to a stochastic model?
- how can we determine the distribution of our simulation output?

the basic question in both cases:

what distribution best models given data?

$\approx$ 3 cases depending on how much data we have

case 1: no data

- occurs when
  - no previous records
  - introduction of new operating policy
- **approach**: use the triangular distribution
  3 parameters: minimum, mode (i.e., most likely) and maximum
  note: most likely value $\neq$ mean!
- other distributions (uniform/exponential/beta) can be used in this context
- be creative!

case 2: huge amount of data

- nowadays, many settings are in the big data regime
- if lots of 'clean' data available:
  approach: use data directly in a simulation model via bootstrapping (i.e., resampling data uniformly with replacement)

the bootstrap

we are given dataset $(X_1, X_2, \ldots, X_n)$ of n iid observations
to get new samples $(Y_1, Y_2, \ldots, Y_\ell)$, we
– generate ℓ iid indices $(I_1, I_2, \ldots, I_\ell)$ uniformly from $\{1, 2, \ldots, n\}$
– output $(Y_1, Y_2, \ldots, Y_\ell)$ where $Y_k = X_{I_k}$
the histogram of $(Y_1, \ldots, Y_\ell)$ is called the bootstrap distribution.

warning: one should regard historical data with suspicion!

bootstrapping: example and comments

- mixture distributions often show up in real-world datasets – for example, the travel time of taxi trips from a hotel in Manhattan will typically comprise of trips to the airport (which can be modeled as a Normal rv about the mean travel time), and trips to nearby locations (which can be modeled as an Exponential rv)
  given past data, we want to use bootstrapping to sample from the travel time distribution (see notebook)

issues with using the bootstrap:

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case 3: moderate amount of data

- reasonable amount of data, but not enough for bootstrap
- **approach**:

– fit data to a parametric family of distributions
(Normal, exponential, Weibull, binomial, Poisson)
– determine parameters of selected distribution from the data
– use the fitted distribution to generate samples for simulation

- important questions:

1. how to choose the family of distributions?
2. how to select the parameters of the distribution?
3. how to assess the fit of the distribution and the parameters?

- simplifying and major (!) assumption – i.i.d. samples

choice of distribution families

to pick the appropriate family of distributions:

– **capture the physics**

'story' behind different distributions

– sum of iid rvs $\implies$ Normal distribution

– product of iid rvs $\implies$ Lognormal distribution

– max/min of iid rvs $\implies$ Wiebull (Extreme-value) distribution

– superposition of independent arrivals $\implies$ Poisson process

– use visual tests to guide distribution choice

physics of different distributions

normal distribution

- if X is the sum of a large number of other random quantities, i.e.

$$X = Y_1 + \ldots + Y_n$$

  then X can be approximately modeled as a normal random variable
- central limit theorem $\implies X \approx \mathcal{N}(0, 1)$ for large n
- *example* – total value of claims received by insurance company in one day

lognormal distribution

- if $W \sim \mathcal{N}(0,1) \implies e^W$ is log-normally distributed.
- moral – if X is the product of a large number of other random quantities, i.e.

$$X = Z_1 Z_2 \ldots Z_n,$$

  or alternately, $\ln X = \ln Z_1 + \ln Z_2 + \ldots + \ln Z_n$); then X can be approximately modeled as a log-normal random variable
- *example* – many financial asset models:
  $G_n =$ proportional change in asset value during time period n
  $W_n =$ net worth of an asset at the beginning of time period n

Weibull distribution

- system that is made up of n components with lifetimes $Y_1, \ldots, Y_n$
  let L be the lifetime of the system:
  - components are connected in series: $L = \min [Y_1, \ldots, Y_n]$
  - components are connected parallel: $L = \max [Y_1, \ldots, Y_n]$
- extreme value theory: approximate distribution of L when n is large and $Y_1, \ldots, Y_n$ are i.i.d. random variables.
  - L has approximately Weibull distribution when n is large.
- *example* – lifetime of complicated system is approximately Weibull

others

- *Geometric*(p): number of coin tosses before heads/number of independent trials till success, with $p = \mathbb{P}[\text{success}]$
(only memoryless discrete distn)
- *Binomial*(n, p): number of successes in n independent trials, where $p = \mathbb{P}[\text{success}]$
- *Poisson*(λ): number of outcomes in a very large number of independent trials ($n \to \infty$), where $\mathbb{P}[\text{outcome}] = \lambda/n$ is very small (for example, spontaneous radioactive emissions in a material over a day, positive COVID tests in a large population, etc.); mean number of successes λ
- *Exponential*(λ): good model for 'holding' times/inter-arrival times/delays, with mean $1/\lambda$ (only memoryless continuous distn)

visualizing fit: histograms and Q-Q plots

hypothesis: data comes from a distribution with cdf $F(\cdot)$

method 1: (visually) compare empirical histogram to hypothesized pdf

note: scale appropriately

- Δ: bin width, n: # of data points $\implies$ area under histogram $= n\Delta$
- must scale pdf by $n\Delta$ to compare
- discrete data: $\hat{p}(i) =$ fraction of times observe outcome i in data set

method 2: compare cdfs (how?)

Q-Q Plots

- more informative visual tool
- helps understand **tails** of the distribution

QQ plot

- order data in increasing order $Y_1 \leq Y_2 \leq \ldots \leq Y_n$
  - fraction of observations $\leq Y_j$ is j/n
- empirical cdf can be defined as $\hat{F}(Y_j) = \left(\frac{j-0.5}{n}\right)$
- for test cdf $F(\cdot)$, compute 'quantiles' $Z_j = F^{-1}\left(\frac{j-0.5}{n}\right)$
- Q-Q plot $\implies$ $[(Y_j, Z_j) : j = 1, \ldots, n]$

QQ plots: notes

- observed values will never fall exactly on the straight line
- ordered values are not independent, because we ordered them
  if one point lies above the line, the next is likely to do the same...
- values at extremes have much higher variance than those in the middle

parameter fitting

parameter estimation

hypothesis: data $X_1, \ldots, X_n$ comes from parametric distribution family with cdf $F(\cdot)$

how do we choose parameters of $F(\cdot)$?

two methods:

- method of moments
- maximum likelihood estimation

method of moments: definition

want to fit data to cdf $F(\cdot)$ with p unknown parameters

method of moments

1. using data $(X_1, X_2, \ldots, X_n)$, estimate the first p empirical moments. Let $m_1, \ldots, m_p$ be the estimated moments, where

$$m_k =$$

2. compute the first p moments of the hypothesized p.d.f
let $\mu_1, \ldots, \mu_p$ be these exact moments, where

$$\mu_k =$$

3. set $\mu_k = m_k$ for $k = 1, \ldots, p$, and solve these p equations for the p unknown parameters

MOM for exponential rv

- given 5 interarrival times: 3, 1, 4, 3, 8
- want to model this as being from an exponential distribution
- recall: mean of $Exp(\lambda)$ rv is $1/\lambda$.

MOM for Normal rv

example – hypothesis: $X_1, \ldots, X_n$ are i.i.d. samples from $\mathcal{N}(a, b^2)$

MOM estimator: pros and cons

- advantage: easy to setup, and most of the time gives *some* answer
- con: answers not always very meaningful
- tl;dr: use MoM when more sophisticated procedures fail!

maximum likelihood estimation

fit i.i.d data $D = (X_1, X_2 \ldots, X_n)$ to cdf $F(\cdot)$ with unknown parameters Θ

likelihood function

$L(\Theta|D)$: measure of how well parameters Θ 'explain' given data D

– function of Θ (not a probability distribution)

– for discrete r.v., $L(\Theta|D) = \Pi_{i=1}^{n} p(X_i|\Theta)$

– for continuous r.v., $L(\Theta|D) = \Pi_{i=1}^{n} f(X_i|\Theta)$

maximum likelihood estimation

1. using data $D = (X_1, X_2, \ldots, X_n)$, define likelihood function $L(\Theta|D)$
2. find Θ which maximizes the log-likelihood, i.e.

$$\Theta^{\star} =$$

MLE: exponential rv

hypothesis: interarrival times $3, 1, 4, 1, 8$ are i.i.d. samples from $Exp(\lambda)$

MLE for exponential

hypothesis: interarrival times $X_1, X_2, \ldots, X_n$ are i.i.d. samples from $Exp(\lambda)$

MLE: Geometric rv

hypothesis: $X_1, \ldots, X_n$ are i.i.d. samples from $Geom(p)$ distribution

MLE: Normal rv

hypothesis: $X_1, \ldots, X_n$ are i.i.d. samples from $N(\mu, \sigma^2)$

MLE: uniform rv

hypothesis: $X_1, \ldots, X_n$ are i.i.d. samples from $U[0, \alpha]$

MLE: uniform rv

Clicker question: MLE for uniform

given data $(X_1, X_2, \ldots, X_n)$ with sample moments m_1 and m_2, the MLE for α assuming the data comes from a uniform distribution over $(-\alpha, \alpha)$ is

(a) $\alpha = \sqrt{3m_2}$

(b) $\alpha = \max_i X_i$

(c) $\alpha = \min_i X_i$

(d) $\alpha = \max_i |X_i|$

(e) No MoM estimator is possible

MLE: notes

- sometimes (rarely) MLE can be computed in closed-form
- usually: compute MLE via numerical optimization
- why use MLE's?
  - they contain *all* the available statistical information about parameters in the data
  - they (asymptotically) have the smallest variance of any possible parameter estimator

goodness of fit

goodness of fit tests

- fitting distributions = hypothesis testing

$$H_0 : \text{data come from the hypothesized distribution}$$
$$H_1 : \text{data do not come from the hypothesized distribution.}$$

chi-square goodness of fit test

- can be used for discrete or continuous distributions
- compare histogram of data with expected frequencies under hypothesized distribution

chi-square goodness of fit test

chi-square test

1. choose k: number of bins

$[b_{i-1}, b_i)$: i-th bin

$[b_0, b_k]$ should cover the whole range.

2. compute $O_i =$ observed number in bin i
   $E_i =$ expected number in bin i (under hypothesis)

3. compute the test statistic $D^2 = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$.

4. under the null hypothesis, D^2 has (approximately) a chi-squared distribution with $df = k - s - 1$ degrees of freedom
   (s is the number of parameters estimated from the data)

4. compute $\chi^2_{df,1-\alpha} = F^{-1}_{\chi^2_{df}}[1 - \alpha]$

chi-square test: example

example – chi-sqared test for car interarrival times.

bin	cumulative	observed	expected	$(O-E)^2/E$
0, 0.05	33	33	27.674	1.024
0.05, 0.1	58	25	24.330	0.018
0.1, 0.15	80	22	21.389	0.017
0.15, 0.2	90	10	18.804	4.122
0.2, 0.3	121	31	31.066	0.000
0.3, 0.5	165	44	42.570	0.048
0.5, ∞	229	64	63.163	0.011

$s = 1, \quad D^2 = 5.242, \quad \text{d.f.} = 5, \quad \chi^2_{5,1-0.05} = 11.070.$

chi-square test:notes

how many bins

- range of a continuous distribution can be divided into any number of bins
- too many $\implies$ expected frequencies become small
  too few $\implies$ test has little power of discrimination
- desirable to divide the continuous range bins with equal probabilities.
  $E_i = E_j$ for all $i, j = 1, \ldots, k$.
  then, k is the only decision.
- the size of the bins should be such that $E_i \geq 5$.

p-value: $\mathbb{P}\left[X > D^2\right]$, where X is a chi-squared distributed random variable with $k - s - 1$ d.f., and D^2 is the test statistic

Kolmogorov-Smirnov (KS) test

- chi-square test:
  histogram of the data $\iff$ pdf of the hypothesis
- KS:
  empirical cdf of the data $\iff$ cdf of the hypothesis
- advantages:
  - more discriminating power than Chi-square
  - does not require grouping the data into bins

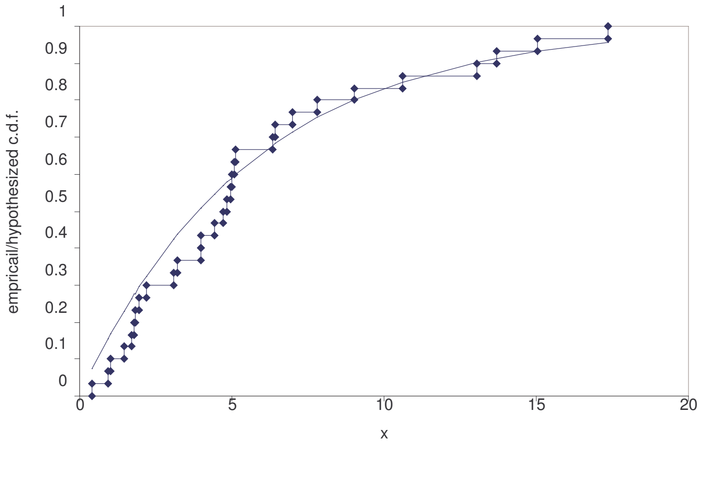
Kolmogorov-Smirnov test

KS goodness-of-fit test

- data: $(X_1, \ldots, X_n)$, hypothesis distribution with cdf $F(\cdot)$.
- construct the empirical cdf function from the data (Without continuity correction)
- KS test statistic is $D = \max_x |F(x) - \hat{F}(x)|$
- reject the null hypothesis if $D > D_{n,\alpha}$
  - $\lim_{n\to\infty} \sqrt{n}D \sim$ Kolmogorov distribution
  - $D_{n,\alpha}$: confidence level of Kolmogorov distribution
  - $n =$ sample size, $\alpha =$ is the level of significance
  - values of $D_{n,\alpha}$ are tabulated

Kolmogorov-Smirnov test

- $\hat{F}(\cdot)$ is a step function.
- to compute test statistic $D = \max_x |F(x) - \hat{F}(x)|$:
  enough to evaluate $|F(x) - \hat{F}(x)|$ only at the "jump" points



Kolmogorov-Smirnov Test

- the test needs to be adjusted if:
  - used for a discrete rv
  - if one uses the data to estimate any parameters
- with adjustments, distribution of D depends on the particular distribution that is hypothesized
- tables of percentiles are available for many common distributions

goodness-of-fit tests: final remarks

- little data $\implies$
  all goodness of fit tests will have trouble rejecting any distribution
- enormous data $\implies$
  theoretical families of distributions may not be broad enough to accurately reflect the data
- should not have blind faith in goodness of fit tests
- software fits all distributions and ranks them based on p-values
  don't trust those rankings completely

parameter estimation error

parameter estimation error

we have now seen how to
– choose a **distribution family**
– fit **parameters**
– visualize/measure **goodness-of-fit**

even if we do everything right, $\exists$ errors in parameter estimates

- how can we estimate the magnitude of this error?
- can this error affect our simulations?

parameter estimation error: example

given $n = 200$ inter-arrival times of people arriving to a COVID testing site

- distribution guess:
- MLE estimate:
- parameter estimation error: $\hat{\lambda} - \lambda =$

parameter estimation error: example

given $n = 200$ inter-arrival times of people arriving to a COVID testing site

- distribution guess: Exponential(λ)
- MLE estimate: $\hat{\lambda} = 200/\sum_{i=1}^{2} 00A_i$
- parameter estimation error: $|\hat{\lambda} - \lambda|$

suppose there is one tester, and each test time is iid, with mean $\mu = 20s$, standard deviation $\sigma = 20s$

- service rate $= \mu = 3$ per minute
- set $\rho = \lambda/\mu = \lambda/3$
- average number of people in test center?
  Pollaczek-Khintchine formula:

$$L = \rho + \frac{\rho^2 + \lambda^2\sigma^2}{2(1-\rho)} = \frac{\lambda}{3} + \frac{\lambda^2}{9 - 3\lambda},$$

parameter estimation error: example

suppose our estimate $\hat{\lambda} =$ is accurate to ± 0.25.

- we can use PK formula to compare the expected number of cars when $\mu = 3$ and $\mu = 6$.
- Much less variability in *L* as μ increases

bootstrapping

- pretend we knew the **true** cdf F
- mimic the sampling process:
  generate many samples, each of size n, from F
- get an estimate of λ, $\hat{\lambda}_i$ say, from the ith sample
- plot a histogram of the $\hat{\lambda}_i$s
- **problem:** don't know F
- **solution:** replace it with a good guess

parametric bootstrap

1. given data $X_1, X_2, \ldots, X_n$ and family of distributions with one or more parameters θ
2. compute parameter estimate $\hat{\theta}_0$ using MoM/MLE
   let $\hat{F}$ be the cdf with this parameter
3. for $i = 1, 2, \ldots, m$
   3.1 generate sample $Y_1(i), Y_2(i), \ldots, Y_n(i)$ from $\hat{F}$
   (note: sample size same as in the original data)
   3.2 use same estimation procedure as in step 2 to get new estimate $\hat{\lambda}_i$ from the generated sample
4. plot a histogram of the m estimates $\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_m$ to get a sense of the distribution of the estimation error in $\hat{\lambda}_0$