CSC-591: Foundations of Data Science T/Th. 12:50-2:05pm. EBI-1005.

Ranga Raju Vatsavai

Chancellors Faculty Excellence Associate Professor in Geospatial Analytics Department of Computer Science, North Carolina State University (NCSU) Associate Director, Center for Geospatial Analytics, NCSU &

Joint Faculty, Oak Ridge National Laboratory (ORNL)

W4: 9/8-10/15

NC STATE UNIVERSITY

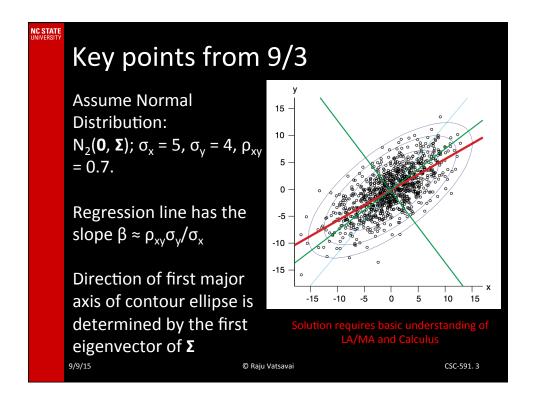
Administrative

• HW-1: Posted on Moodle

• Due: 9/21/15, 23:55pm

9/9/15

© Raju Vatsavai





So far

- We started with data (samples) drawn from a population
- We wanted to make inference (conclusions) about populations from noisy data that is drawn from it
- The randomness governing our data (samples) is given by densities and mass functions

9/9/15

© Raju Vatsavai

CSC-591. 5

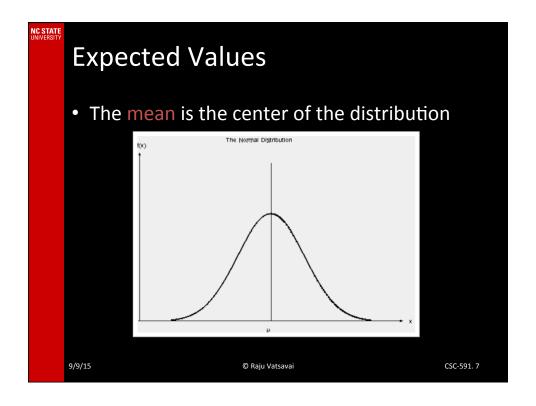
NC STATE

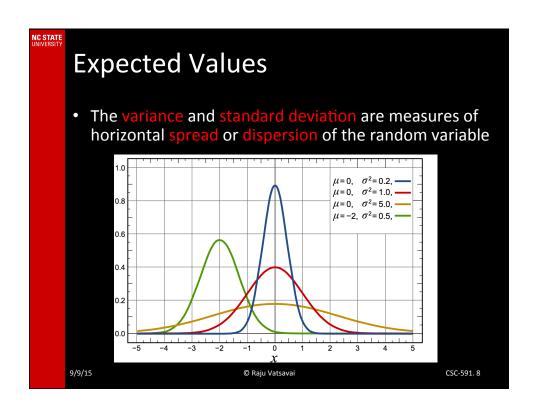
Expected Values

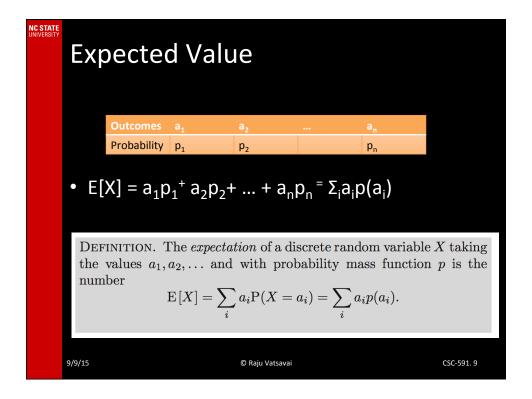
- Expected value of a random variable is intuitively the long-run average value of repetitions of the experiment it represents.
 - E.g., the expected value of a dice roll is 3.5
- The expected value is also known as the expectation, mathematical expectation, EV, mean, or first moment.

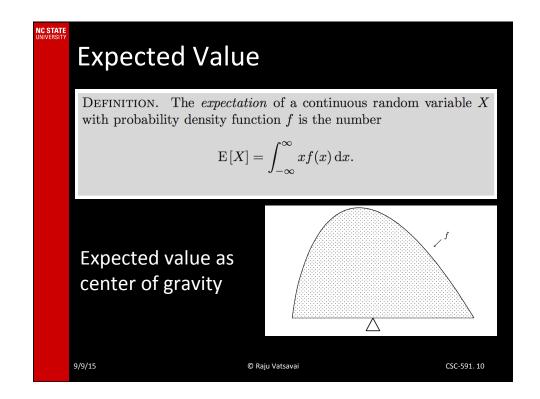
9/9/15

© Raju Vatsavai









Variance

Definition. The $variance\ \mathrm{Var}(X)$ of a random variable X is the number

$$\operatorname{Var}(X) = \operatorname{E}\left[(X - \operatorname{E}[X])^{2}\right].$$

AN ALTERNATIVE EXPRESSION FOR THE VARIANCE. For any random variable $\boldsymbol{X},$

$$\operatorname{Var}(X) = \operatorname{E}[X^{2}] - (\operatorname{E}[X])^{2}.$$

9/9/15

© Raju Vatsavai

CSC-591. 11

NC STATE

Example

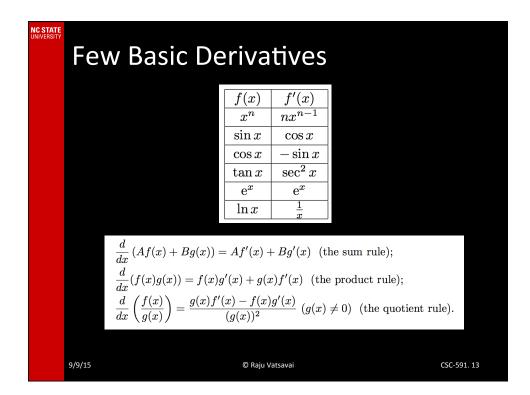
• The random variable is given by the following PDF. $(2(1-x)) \text{ if } 0 \le x \le 1$

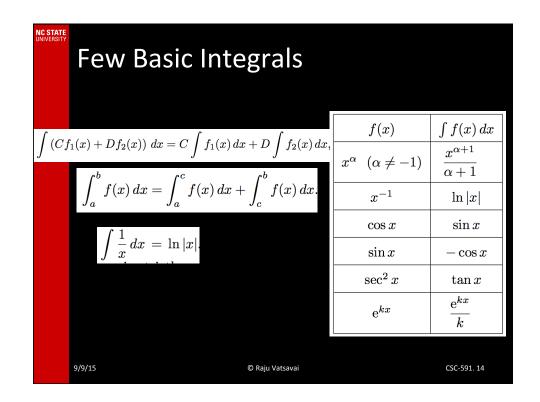
 $f(x) = \begin{cases} 2(1-x) & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise} \end{cases}$

- First verify that f(x) is valid PDF.
 - $-2(1-x) = 2 2x \ge 0$ precisely when $x \le 1$; thus f(x) is everywhere nonnegative

9/9/15

© Raju Vatsavai





Example

• Check if f(x) has unit area under its graph

$$\int_{-\infty}^{\infty} f(x)dx = 2\int_{0}^{1} (1-x)dx = 2\left(x - \frac{x^{2}}{2}\right)\Big|_{0}^{1} = 1$$

- Therefore, f(x) is a valid PDF.
- Now compute Expected value

$$\operatorname{E}[X] = \int_{-\infty}^{\infty} x f(x) \, \mathrm{d}x.$$

9/9/15

© Raju Vatsavai

CSC-591. 15

NC STATE

Example

Mean

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x f(x) dx$$

$$= \int_{0}^{1} x \left[2(1-x) \right] dx$$

$$= 2 \int_{0}^{1} \left(x - x^{2} \right) dx$$

$$= 2 \left(\frac{x^{2}}{2} - \frac{x^{3}}{3} \right) \Big|_{0}^{1}$$

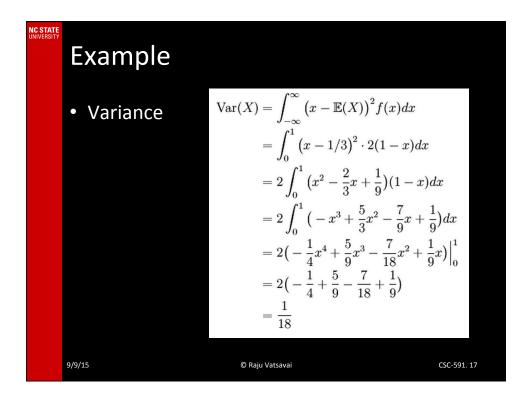
$$= 1/3$$

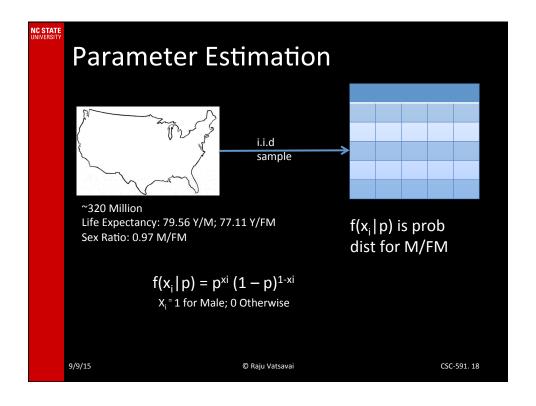
• Compute Variance $Var(X) = E[(X - E[X])^2]$

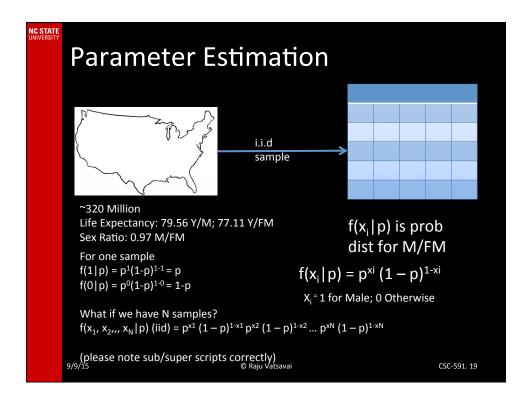
$$Var(X) = E[(X - E[X])^{2}]$$

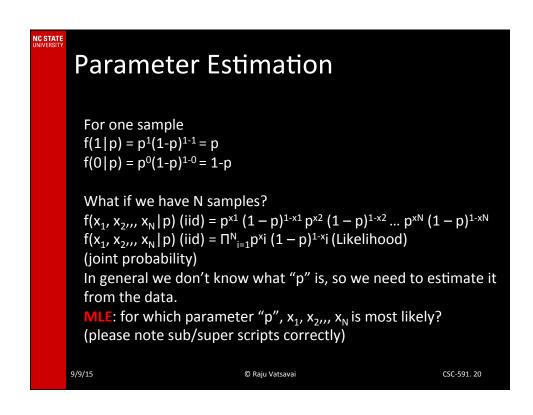
9/9/15

© Raju Vatsavai









Maximum Likelihood Estimation

- General outline for single parameter
 - Write down the likelihood function: $L(\theta)$
 - Maximize likelihood (difficult due to product)
 - · Log-likelihood (monotonic)
 - Take In (natural log)
 - Differentiate $I(\theta)$ with respect to the parameter (θ)
 - Set derivative 0 and solve resulting equation
 - Check this is maximum (by taking 2nd derivative) (generally we don't need, e.g., uni-modal Gaussian)

9/9/15

© Raju Vatsavai

CSC-591. 21

UNIVERSIT

Likelihood function

Let X_1, \ldots, X_n have joint pmf or pdf

$$f(x_1, x_2, ..., x_n; \theta_1, ..., \theta_m)$$
 (7.6)

where the parameters $\theta_1, \ldots, \theta_m$ have unknown values. When x_1, \ldots, x_n are the observed sample values and (7.6) is regarded as a function of $\theta_1, \ldots, \theta_m$, it is called the **likelihood function**. The maximum likelihood estimates $\hat{\theta}_1, \ldots, \hat{\theta}_m$ are those values of the θ_i 's that maximize the likelihood function, so that

$$f(x_1, x_2, \dots, x_n; \hat{\theta}_1, \dots, \hat{\theta}_m) \ge f(x_1, x_2, \dots, x_n; \theta_1, \dots, \theta_m)$$
 for all $\theta_1, \dots, \theta_m$

When the X_i 's are substituted in place of the x_i 's, the **maximum likelihood** estimators (mle's) result.

9/9/15

© Raju Vatsavai

Poisson Example

$$P(X = x) = \frac{\lambda^x e^{-\lambda}}{x!}$$

For $X_1, X_2, ..., X_n$ iid Poisson random variables will have a joint frequency function that is a product of the marginal frequency functions, the log likelihood will thus be:

$$l(\lambda) = \sum_{i=1}^{n} (X_i log \lambda - \lambda - log X_i!)$$

= $log \lambda \sum_{i=1}^{n} X_i - n\lambda - \sum_{i=1}^{n} log X_i!$

We need to find the maximum by finding the derivative:

$$l'(\lambda) = \frac{1}{\lambda} \sum_{i=1}^{n} x_i - n = 0$$

9/9/15

© Raju Vatsavai

CSC-591. 23

UNIVERSITY

Exponential Distribution

Suppose X_1, \ldots, X_n is a random sample from an exponential distribution with parameter λ . Because of independence, the likelihood function is a product of the individual pdf's:

$$f(x_1,\ldots,x_n;\lambda)=(\lambda e^{-\lambda x_1})\cdot\cdots\cdot(\lambda e^{-\lambda x_n})=\lambda^n e^{-\lambda \sum x_i}$$

The ln(likelihood) is

$$\ln[f(x_1,\ldots,x_n;\lambda)] = n\ln(\lambda) - \lambda \sum x_i$$

Equating $(d/d\lambda)[\ln(\text{likelihood})]$ to zero results in $n/\lambda - \Sigma x_i = 0$, or $\lambda = n/\Sigma x_i = 1/\bar{x}$. Thus the mle is $\hat{\lambda} = 1/\bar{X}$;

9/9/15

© Raju Vatsavai

Normal Distribution

If $X_1, X_2, ..., X_n$ are iid $\mathcal{N}(\mu, \sigma^2)$ random variables their density is written:

$$f(x_1, \dots, x_n | \mu, \sigma) = \prod_{i=1}^{n} \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2} \left[\frac{x_i - \mu}{\sigma}\right]^2\right)$$

Regarded as a function of the two parameters, μ and σ this is the likelihood:

$$\ell(\mu, \sigma) = -nlog\sigma - \frac{n}{2}log2\pi - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2$$

$$\frac{\partial \ell}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \mu)$$

$$\frac{\partial \ell}{\partial \sigma} = -\frac{n}{\sigma} + \sigma^{-3} \sum_{i=1}^{n} (x_i - \mu)^2$$

so setting these to zero gives \bar{X} as the mle for μ , and $\hat{\sigma}^2$ as the usual.

9/9/15

© Raju Vatsavai

CSC-591. 25

UNIVERSIT

Why MLE

- Widely regarded as the best method of point estimation
- MLE provides a feasible solution
- MLE has nice asymptotic properties
 - Consistent
 - Asymptotically normal
 - Efficiency

9/9/15

© Raju Vatsavai

Properties

- Consistency: means that having a sufficiently large number of observations n, it is possible to find the value of θ_0 with arbitrary precision.
- Asymptotically Normal: means that the estimated parameter is equal to the true parameters plus a random error that is approximately normal (given sufficient data), and the error's variance decays as 1/n

CSC-591. 27

9/9/15 © Raju Vatsavai

NC STATE UNIVERSITY

Least Squares Estimators

- Instead of maximizing the likelihood of the observed outcome, we can construct an estimator by looking at the distance of the observed outcome and the outcome that we would expect with a particular parameter value.
- The value that minimizes this distance is then an estimate for the parameter.

9/9/15 © Raju Vatsavai CSC-591. 28

Confidence Intervals

- Properties of estimators provide valuable information for comparing and choosing an estimator, but no quality information
 - E.g., consistency guarantees that the estimated value will approach the true value in the limit, but does not give information on how close it is to the true value, given some data with a certain number of samples.
- For quantifying the quality of a particular estimate, we can compute a *confidence interval* (*CI*) around the estimate θ^{n} , such that this interval covers the true value θ with some high probability 1α . The narrower this interval, the closer we are to the true value, with high probability.

9/9/15 © Raju Vatsavai

CSC-591. 29

UNIVERSITY

Acknowledgements

- Vipin Kumar (Minnesota)
- Jiawei Han (UIUC)
- Hanspeter Pfister (Harvard)
- Larry Wasserman (CMU)

9/9/15

© Raju Vatsavai