

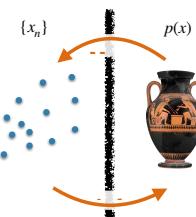
# Mathematical Tools for Neural and Cognitive Science

Fall semester, 2023

## Section 5: Statistical Inference and Model Fitting

### The sample average

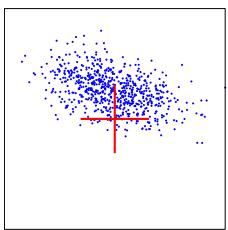
$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n$$



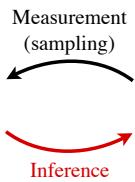
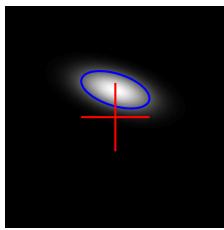
What happens as  $N$  grows?

- Variance of  $\bar{x}$  is  $\sigma_x^2/N$  (the “standard error of the mean”, or SEM), and so converges to zero *[on board]*
- “Unbiased”:  $\bar{x}$  converges to the true mean,  $\mu_x = \mathbb{E}(\bar{x})$  (formally, the “law of large numbers”) *[on board]*
- The distribution  $p(\bar{x})$  converges to a Gaussian (mean  $\mu_x$  and variance  $\sigma_x^2/N$ ): formally, the “Central Limit Theorem”

700 samples



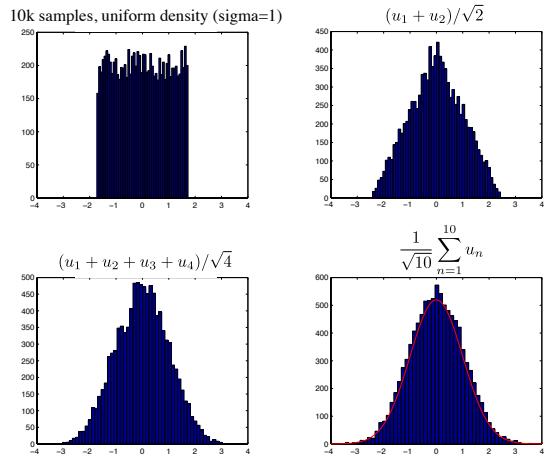
true density



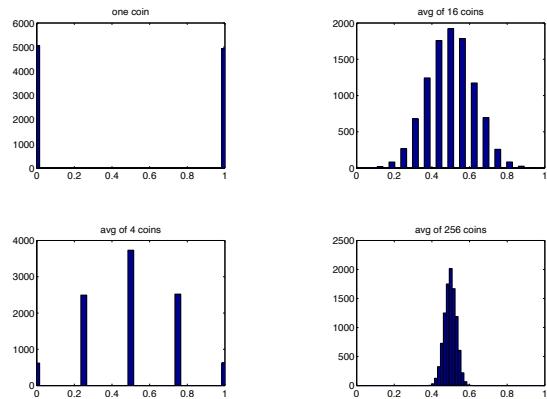
sample mean: [-0.05 0.83]  
sample cov: [0.95 -0.23  
-0.23 0.29]

true mean: [0 0.8]  
true cov: [1.0 -0.25  
-0.25 0.3]

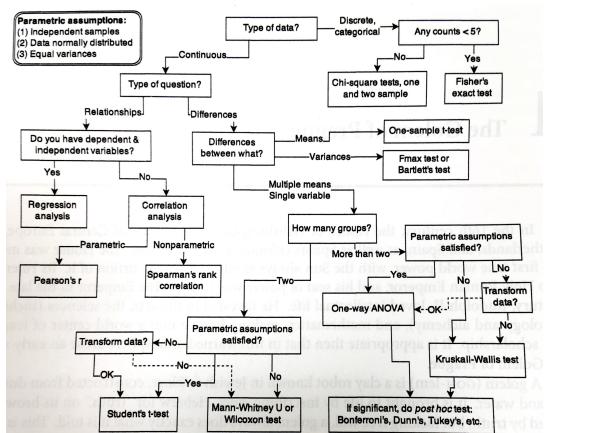
### Central limit for a uniform distribution...



### Central limit for a binary distribution...



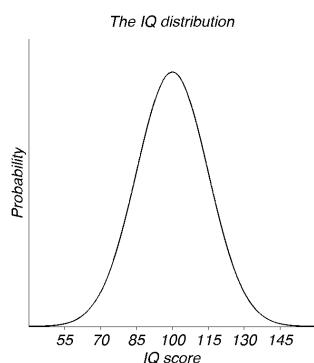
### Classical “frequentist” statistical tests



Statistical Rethinking, Richard McElreath

## Classical/frequentist approach - $z$

- In the general population, IQ is known to be distributed normally with
  - $\mu = 100$ ,  $\sigma = 15$
- We give a drug to 30 people and test their IQ
- $H_1$ : NZT improves IQ
- $H_0$  ("null"): it does nothing



## Test statistic

- We calculate how far the observed value of the sample average is away from its expected value.
- In units of standard error.
- In this case, the test statistic is

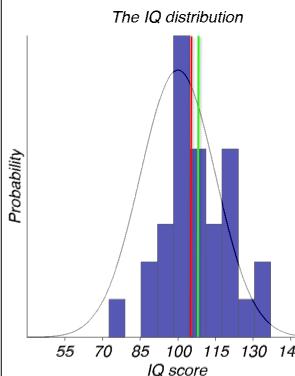
$$z = \frac{\bar{x} - \mu}{SE} = \frac{\bar{x} - \mu}{\sigma / \sqrt{N}}$$

- Compare to a distribution, in this case  $z$  or  $N(0,1)$

## Does NZT improve IQ scores or not?

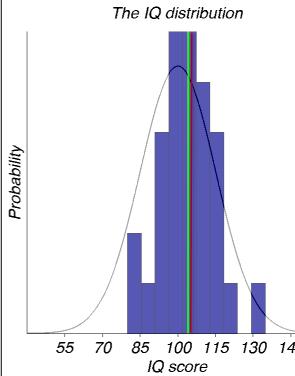
		Reality	
		Yes	No
Decision	Yes	Correct	Type I error $\alpha$ -error "False alarm"
	No	Type II error $\beta$ -error "Miss"	Correct

## The $z$ -test



- $\mu = 100$  (Population mean)
- $\sigma = 15$  (Population standard deviation)
- $N = 30$  (Sample contains scores from 30 participants)
- $\bar{x} = 108.3$  (Sample mean)
- $z = (\bar{x} - \mu)/SE = (108.3 - 100)/SE$  (Standardized score)
- $SE = \sigma / \sqrt{N} = 15/\sqrt{30} = 2.74$
- Error bar/CI:  $\pm 2$  SE
- $z = 8.3/2.74 = 3.03$
- $p = 0.0012$
- Significant?
- One- vs. two-tailed test

What if the measured effect of NZT had been half that?



- $\mu = 100$  (Population mean)
- $\sigma = 15$  (Population standard deviation)
- $N = 30$  (Sample contains scores from 30 participants)
- $\bar{x} = 104.2$  (Sample mean)
- $z = (\bar{x} - \mu)/SE = (104.2 - 100)/SE$
- $SE = \sigma / \sqrt{N} = 15/\sqrt{30} = 2.74$
- $z = 4.2/2.74 = 1.53$
- $p = 0.061$
- Significant?

## Significance levels

- Are denoted by the Greek letter  $\alpha$ .
- In principle, we can pick anything that we consider unlikely.
- In practice, the consensus is that a level of 0.05 or 1 in 20 is considered as unlikely enough to reject  $H_0$  and accept the alternative.
- A level of 0.01 or 1 in 100 is considered “highly significant” or “really unlikely”.

## Common misconceptions



Is “Statistically significant” a synonym for:

- Substantial
- Important
- Big
- Real

Does statistical significance gives the

- probability that the null hypothesis is true
- probability that the null hypothesis is false
- probability that the alternative hypothesis is true
- probability that the alternative hypothesis is false

Meaning of  $p$ -value. Meaning of CI.

---

---

---

---

---

---

## Student’s $t$ -test

- $\sigma$  not assumed known
- Use 
$$s^2 = \frac{\sum_{i=1}^N (x_i - \bar{x})^2}{N-1}$$
- Why  $N-1$ ?  $s$  is unbiased (unlike ML version), i.e.,  $\mathbb{E}(s^2) = \sigma^2$
- Test statistic is 
$$t = \frac{\bar{x} - \mu_0}{s / \sqrt{N}}$$
- Compare to  $t$  distribution for CIs and NHST
- “Degrees of freedom” reduced by 1 to  $N-1$

---

---

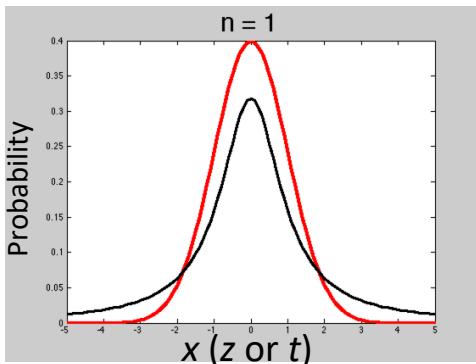
---

---

---

---

The  $t$  distribution approaches the normal distribution for large  $N$



---

---

---

---

---

---

## The $z$ -test for binomial data

- Is the coin fair?
- Lean on central limit theorem
- Sample is  $n$  heads out of  $m$  tosses
- Sample mean:  $\hat{p} = n / m$
- $H_0: p = 0.5$
- Binomial variability (one toss):  $\sigma = \sqrt{pq}$ , where  $q = 1 - p$
- Test statistic: 
$$z = \frac{\hat{p} - p_0}{\sqrt{p_0 q_0 / m}}$$
- Compare to  $z$  (standard normal)
- For CI, use 
$$\pm z_{\alpha/2} \sqrt{\hat{p}\hat{q} / m}$$

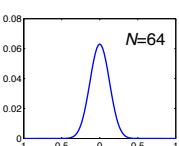
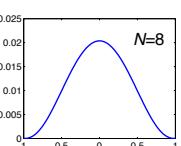
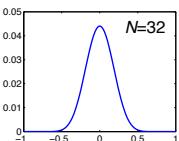
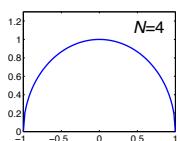
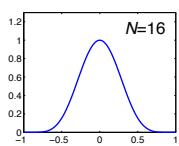
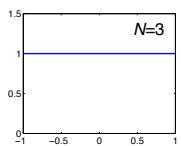
## Other frequentist univariate tests

- $\chi^2$  goodness of fit
- $\chi^2$  test of independence
- test a variance using  $\chi^2$
- $F$  to compare variances (as a ratio)
- Nonparametric tests (e.g., sign, rank-order, etc.)

Lack of correlation is favored in  $N > 3$  dimensions

Null Hypothesis:  
Distribution of normalized dot product of pairs of Gaussian random vectors in  $N$  dimensions:

$$(1 - d^2)^{\frac{N-3}{2}}$$



## Estimation of model parameters (outline)

- How do I compute estimates from data?
- How “good” are my estimates?
- How well does my model explain data to which it was fit? Other data (prediction/generalization)?
- How do I compare models?

## Estimation

- An “estimator” is a function of the data, intended to provide an approximation of the “true” value of a parameter
- One can evaluate estimator quality in terms of squared error,  $MSE = \text{bias}^2 + \text{variance}$
- Traditional statistics often aims for an unbiased estimator, with minimal variance (“MVUE”)
- More nuanced view: trade off bias and variance, through model selection, “regularization”, or Bayesian “priors”

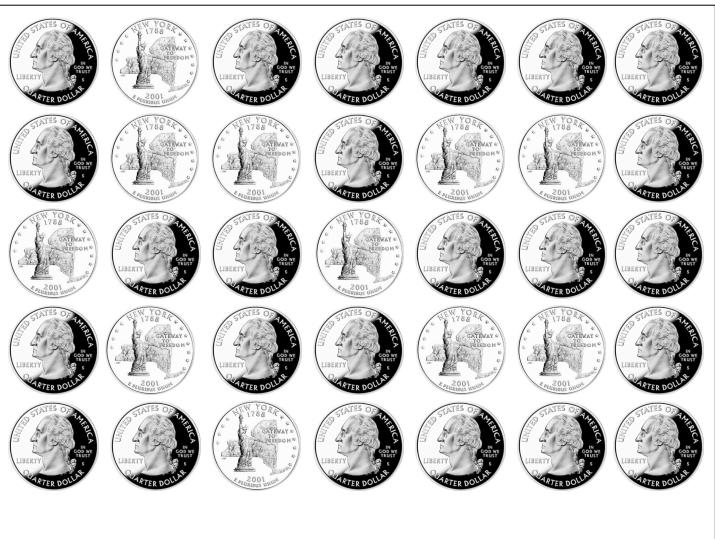
## The maximum likelihood (ML) estimator

Sample average is appropriate when one has direct measurements of the thing being estimated. But one may want to estimate something (e.g., a model parameter) that is *indirectly* related to the measurements...

Natural choice: assuming a probability model  $p(\vec{x} | \theta)$  find the value of  $\theta$  that maximizes this “likelihood” function

$$\begin{aligned}\hat{\theta}(\{\vec{x}_n\}) &= \arg \max_{\theta} \prod_n p(\vec{x}_n | \theta) \\ &= \arg \max_{\theta} \sum_n \log p(\vec{x}_n | \theta)\end{aligned}$$

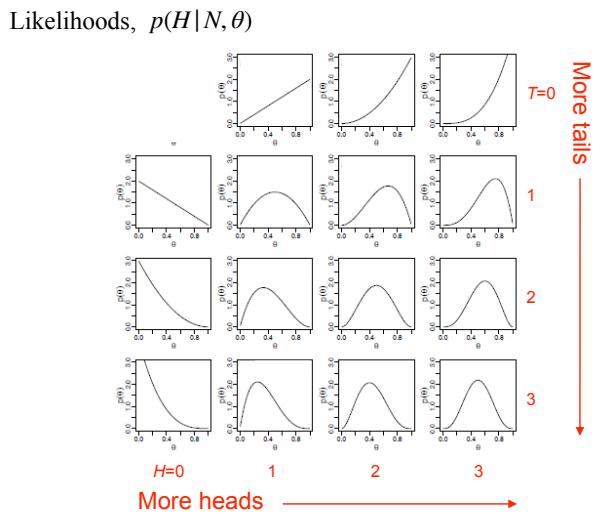
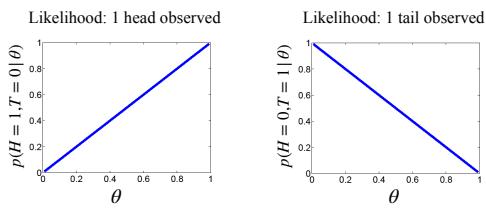
Example: Estimate the probability of a flipped coin landing “heads” up, by observing some samples



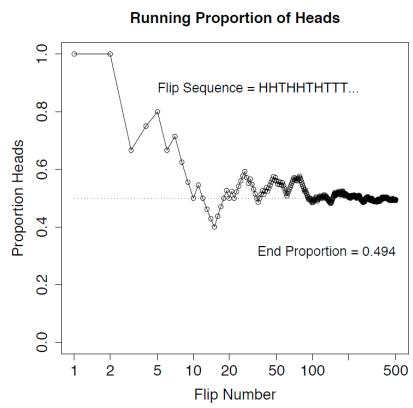
## Example ML Estimators - discrete

$$\text{Binomial: } p(H | N, \theta) = \binom{N}{H} \theta^H (1-\theta)^{N-H} \quad (\text{H = # heads observed, in N flips of a coin, with probability of heads } \theta)$$

$$\hat{\theta}_{\text{ML}} = \frac{H}{N}$$



## Convergence (“consistency”)



## Example ML Estimators - discrete

Binomial:  $p(H|N,\theta) = \binom{N}{H} \theta^H (1-\theta)^{N-H}$  ( $H = \# \text{ heads}$  observed, in  $N$  flips of a coin, with probability of heads  $\theta$ )

$$\hat{\theta}_{\text{ML}} = \frac{H}{N}$$

Poisson:  $p(\{k_n\}|\theta) = \prod_{n=1}^N \frac{\theta^{k_n} e^{-\theta}}{k_n!}$  ( $k_n$ 's are measured counts, with mean arrival rate of  $\theta$ )

$$\hat{\theta}_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N k_n$$

{on board}

## Example ML Estimators - Continuous

Uniform:  $p(x|\theta) = \begin{cases} \frac{1}{\theta} & 0 \leq x \leq \theta \\ 0 & \text{otherwise} \end{cases}$

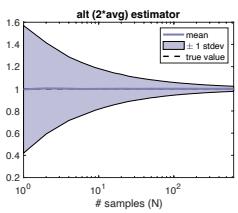
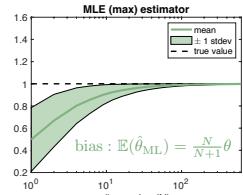
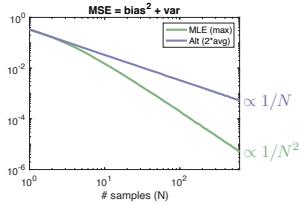
$$\hat{\theta}_{\text{ML}} = \max_n \{x_n\}$$
 (Note: this is biased!)

### Two estimators for range of a uniform distribution

Given  $N$  samples  $\{x_n\}$  from the uniform distribution over  $[0, \theta]$  consider two estimators of  $\theta$ :

$$\hat{\theta}_{\text{ML}}(\{x_n\}) = \max_n (x_n)$$

$$\hat{\theta}_{\text{alt}}(\{x_n\}) = \frac{2}{N} \sum_n x_n$$



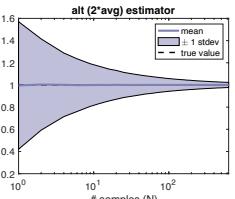
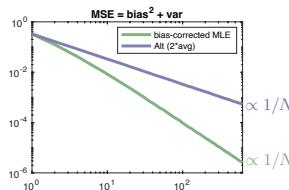
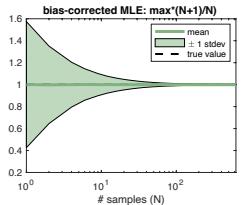
## Two estimators for range of a uniform distribution

Given  $N$  samples  $\{x_n\}$  from the uniform distribution over  $[0, \theta]$  consider two estimators of  $\theta$ :

$$\hat{\theta}_{cML}(\{x_n\}) = \frac{(N+1)}{N} \max(x_n)$$

$$\hat{\theta}_{alt}(\{x_n\}) = \frac{2}{N} \sum_n x_n$$

bias-corrected



## Example ML Estimators - Continuous

Uniform:  $p(x|\theta) = \begin{cases} \frac{1}{\theta} & 0 \leq x \leq \theta \\ 0 & \text{otherwise} \end{cases}$

$$\hat{\theta}_{ML} = \max_n \{x_n\}$$

(Note: this is biased!)

$$\hat{\theta}_{cML} = \frac{N+1}{N} \hat{\theta}_{ML}$$

Gaussian:  $p(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

$$\hat{\mu}_{ML} = \frac{\sum_n x_n}{N}$$

$$\hat{\sigma}_{ML}^2 = \frac{\sum_n (x_n - \hat{\mu})^2}{N}$$

(Note: this is biased!)

$$\hat{\sigma}_{cML}^2 = \frac{N}{N-1} \hat{\sigma}_{ML}^2$$

[on board]

## Properties of ML estimators

- Bias: the MLE is *asymptotically unbiased* and *Gaussian*, but can only rely on these if:
  - you have lots of data
  - the MLE can be computed
  - the likelihood model is correct
- Variance (confidence intervals / error bars):
  - S.E.M. (relevant for sample averages only)
  - second deriv of NLL (multi-D: "Hessian")
  - simulation (resample from  $p(x|\hat{\theta})$ )
  - bootstrapping (resample from *the data*, with replacement)

# Bootstrapping

- “The Baron had fallen to the bottom of a deep lake. Just when it looked like all was lost, he thought to pick himself up by his own bootstraps”  
[Adventures of Baron von Munchausen, by Rudolph Erich Raspe]
- A (re)sampling method for computing estimator dispersion (incl. stdev error bars or confidence intervals)
- Idea: instead of looking at distribution of estimates across repeated experiments, look across repeated resampling (with replacement) from the *existing* data (“bootstrapped” data sets)

HEART ATTACK RISK  
FOUND TO BE CUT  
BY TAKING ASPIRIN  
  
LIVESAVING EFFECTS SEEN  
  
Study Finds Benefit of Tablet  
Every Other Day Is Much  
Greater Than Expected

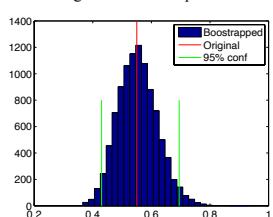
[New York Times, 27 Jan 1987]

The summary statistics in the newspaper article are very simple:

	heart attacks (fatal plus non-fatal)	subjects
aspirin group:	104	11037
placebo group:	189	11034

$$\hat{\theta} = \frac{104/11037}{189/11034} = .55. \quad (1.1)$$

Histogram of bootstrap estimates:



=> with 95% confidence,

$$0.43 < \theta < 0.7$$

If this study can be believed, and its solid design makes it very believable, the aspirin-takers only have 55% as many heart attacks as placebo-takers.

Of course we are not really interested in  $\hat{\theta}$ , the estimated ratio. What we would like to know is  $\theta$ , the true ratio

[Efron & Tibshirani '98]

	strokes	subjects	.
aspirin group:	119	11037	.
placebo group:	98	11034	(1.3)

For strokes, the ratio of rates is

$$\hat{\theta} = \frac{119/11037}{98/11034} = 1.21. \quad (1.4)$$

It now looks like taking aspirin is actually harmful. However the interval for the true stroke ratio  $\theta$  turns out to be

$$.93 < \theta < 1.59 \quad (1.5)$$

with 95% confidence. This includes the neutral value  $\theta = 1$ , at which aspirin would be no better or worse than placebo vis-à-vis strokes. In the language of statistical hypothesis testing, aspirin was found to be significantly beneficial for preventing heart attacks, but not significantly harmful for causing strokes.

[Efron & Tibshirani '98]

## Bayesian Inference

$$p(\theta | \text{data}) = \frac{p(\text{data} | \theta)p(\theta)}{p(\text{data})}$$

"Posterior"

"Likelihood"

"Prior"

Normalization factor

### Example: Posterior for coin

infer whether a coin is fair by flipping it repeatedly  
here,  $x$  is the probability of heads (50% is fair)  
 $y_{1\dots n}$  are the outcomes of flips

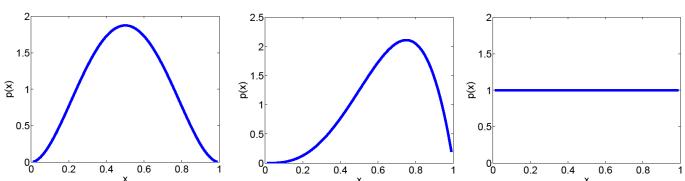


Consider three different priors:

suspect fair

suspect biased

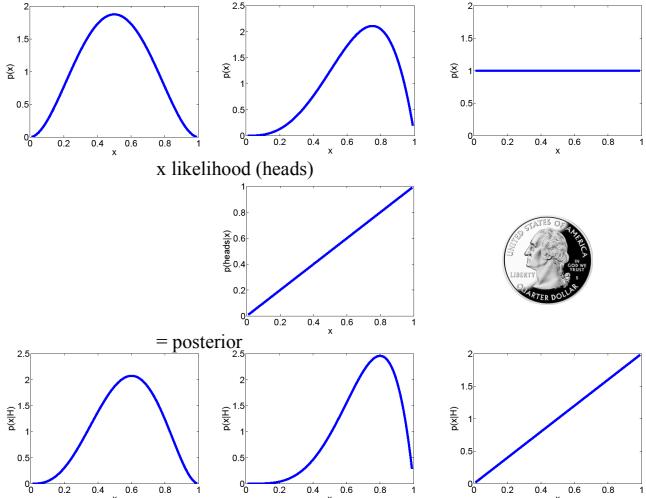
no idea

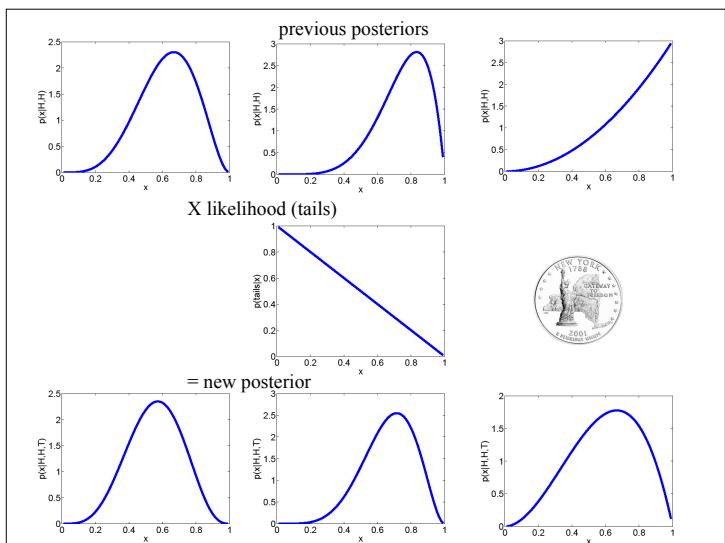
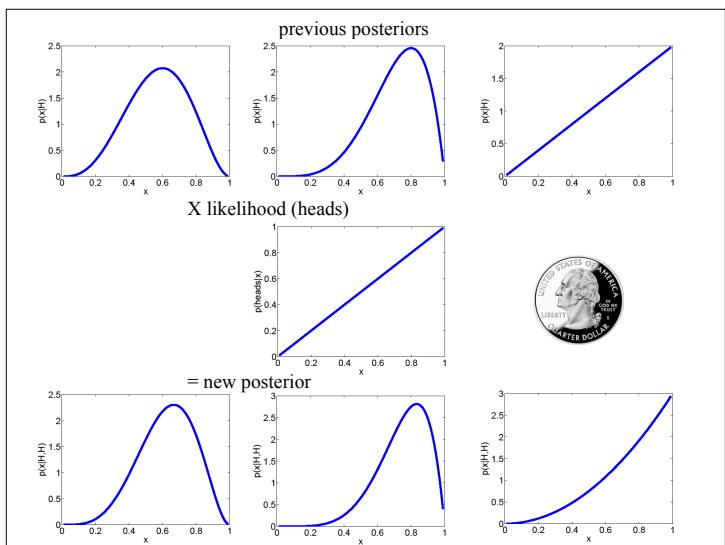


prior fair

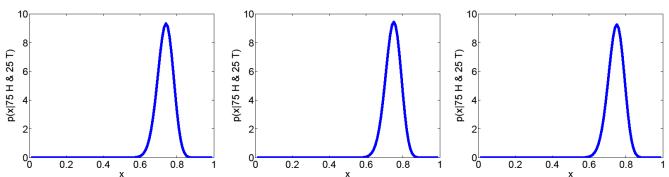
prior biased

prior uncertain





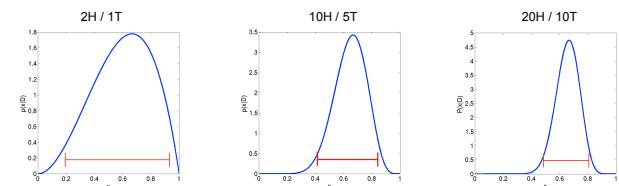
Posteriors after observing 75 heads, 25 tails



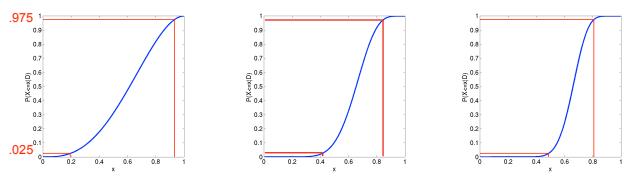
→ prior differences are ultimately overwhelmed by data

## Bayesian confidence intervals

PDFs



CDFs, and 95% confidence intervals



## Bayesian inference: Gaussian case

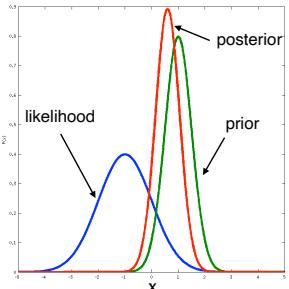
For measurements with Gaussian noise, and assuming a Gaussian prior:

- posterior is Gaussian, allowing sequential updating
- precision is sum of measurement and prior precisions
- mean is precision-weighted average of prior mean and measurement
- explains “regression to the mean”, as

## Bayesian inference: Gaussian case

$$y = x + n, \quad x \sim N(\mu_x, \sigma_x^2), \quad n \sim N(0, \sigma_n^2)$$

$$\begin{aligned} p(x|y) &\propto p(y|x)p(x) \\ &\propto e^{-\frac{1}{2}\left[\frac{1}{\sigma_n^2}(x-y)^2\right]} e^{-\frac{1}{2}\left[\frac{1}{\sigma_x^2}(x-\mu_x)^2\right]} \\ &= e^{-\frac{1}{2}\left[\left(\frac{1}{\sigma_n^2} + \frac{1}{\sigma_x^2}\right)x^2 - 2\left(\frac{y}{\sigma_n^2} + \frac{\mu_x}{\sigma_x^2}\right)x + \dots\right]} \end{aligned}$$



Completing the square shows that this posterior is also Gaussian, with

$$\begin{aligned} \frac{1}{\sigma^2} &= \frac{1}{\sigma_n^2} + \frac{1}{\sigma_x^2} \\ \mu &= \left(\frac{y}{\sigma_n^2} + \frac{\mu_x}{\sigma_x^2}\right) \Big/ \left(\frac{1}{\sigma_n^2} + \frac{1}{\sigma_x^2}\right) \end{aligned}$$

The average of  $y$  and  $\mu_x$ , weighted by inverse variances (a.k.a. “precisions”)!

## Regression to the mean

“Depressed children treated with an energy drink improve significantly over a three-month period. I made up this newspaper headline, but the fact it reports is true: if you treated a group of depressed children for some time with an energy drink, they would show a clinically significant improvement....”

“It is also the case that depressed children who spend some time standing on their head or hug a cat for twenty minutes a day will also show improvement.”

- D. Kahneman

Two noisy measurements of the same variable:

$$y_1 = x + n_1 \quad x \sim N(0, \sigma_x)$$

$$y_2 = x + n_2 \quad n_k \sim N(0, \sigma_n), \text{ independent}$$

Joint measurement distribution:  $\vec{y} \sim N(\vec{0}, \sigma_x^2 \vec{1}\vec{1}^T + \sigma_n^2 I)$

LS Regression:

$$\hat{\beta} = \arg \min_{\beta} \|y_2 - \beta y_1\|^2$$

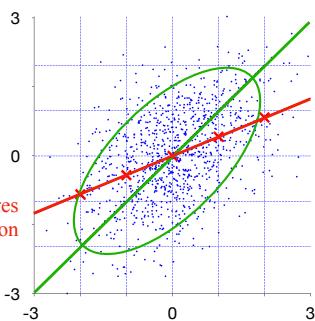
$$= \frac{\sigma_x^2}{\sigma_x^2 + \sigma_n^2}$$

$$\mathbb{E}(y_2|y_1) = \hat{\beta} y_1$$

Least-squares regression

“regression to the mean”

TLS regression  
(largest eigenvector)



## The hierarchy of statistical estimators

- Maximum likelihood (ML):  $\hat{x}(\vec{d}) = \arg \max_x p(\vec{d}|x)$
- Maximum a posteriori (MAP):  $\hat{x}(\vec{d}) = \arg \max_x p(x|\vec{d})$   
(requires prior,  $p(x)$ )
- Bayes estimator (general):  $\hat{x}(\vec{d}) = \arg \min_{\hat{x}} \mathbb{E} \left( L(x, \hat{x}) \mid \vec{d} \right)$   
(requires loss,  $L(x, \hat{x})$ )
- Bayes least squares (BLS):  $\hat{x}(\vec{d}) = \arg \min_{\hat{x}} \mathbb{E} \left( (x - \hat{x})^2 \mid \vec{d} \right)$   
(special case, squared loss)  

$$= \mathbb{E} \left( x \mid \vec{d} \right)$$