Point Estimation

Vibhav Gogate
The University of Texas at Dallas

Some slides courtesy of Carlos Guestrin, Chris Bishop, Dan Weld and Luke Zettlemoyer.

Basics: Expectation and Variance

Random variable x has domain $D(x)$.
Example: x has domain: $\{1, 2, 3, 4\}$
The distribution P is defined over $D(x)$.

$$\mathbb{E}_P[x] = \sum_{x \in D(x)} x P(x)$$

$$\mathrm{var}_P[x] = \sum_{x \in D(x)} (x - \mathbb{E}_P[x])^2 P(x)$$

Binary Variables (1)

- Coin flipping: heads=1, tails=0

$$p(x = 1|\mu) = \mu$$

- Bernoulli Distribution

$$\begin{aligned} \mathrm{Bern}(x|\mu) &= \mu^x (1-\mu)^{1-x} \\ \mathbb{E}[x] &= \mu \\ \mathrm{var}[x] &= \mu(1-\mu) \end{aligned}$$

Binary Variables (2)

- N coin flips:

$$p(m \text{ heads}|N, \mu)$$

- Binomial Distribution

$$\mathrm{Bin}(m|N,\mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}$$

$$\mathbb{E}[m] \equiv \sum_{m=0}^{N} m \mathrm{Bin}(m|N,\mu) = N\mu$$

$$\mathrm{var}[m] \equiv \sum_{m=0}^{N} (m - \mathbb{E}[m])^2 \, \mathrm{Bin}(m|N,\mu) = N\mu(1-\mu)$$

Your first consulting job

Billionaire in Dallas asks:

- He says: I have thumbtack, if I flip it, what's the probability it will fall with the nail up?
- You say: Please flip it a few times:





- You say: The probability is:
  - P(H) = 3/5
- **He says: Why???**
- You say: Because…

Thumbtack – Binomial Distribution

- P(Heads) = θ, P(Tails) = 1-θ

- Flips are *i.i.d.*:
  - Independent events
  - Identically distributed according to Binomial distribution
- Sequence *D* of α_H Heads and α_T Tails

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

Maximum Likelihood Estimation

- **Data:** Observed set D of α_H Heads and α_T Tails
- **Hypothesis:** Binomial distribution
- **Learning:** finding θ is an optimization problem
  - What's the objective function?

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- **MLE:** Choose θ to maximize probability of *D*

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} \; P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \; \ln P(\mathcal{D} \mid \theta)\end{aligned}$$

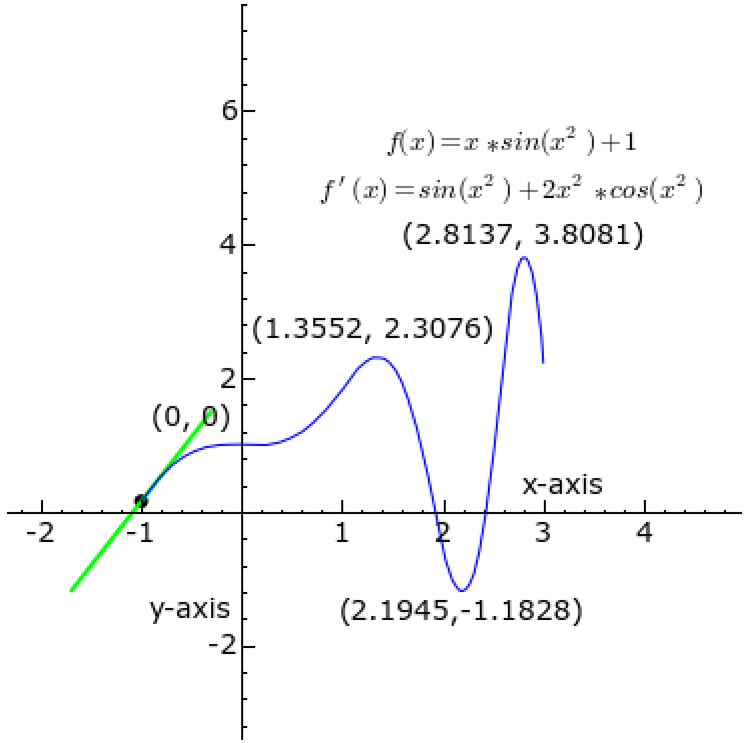
Your first parameter learning algorithm

$$\widehat{\theta} = \arg\max_{\theta} \ln P(\mathcal{D} \mid \theta)$$
$$= \arg\max_{\theta} \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- Set derivative to zero, and solve!

$$\frac{d}{d\theta} \ln P(\mathcal{D} \mid \theta) = \frac{d}{d\theta}\left[\ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\right]$$
$$= \frac{d}{d\theta}\left[\alpha_H \ln \theta + \alpha_T \ln(1-\theta)\right]$$
$$= \alpha_H \frac{d}{d\theta} \ln \theta + \alpha_T \frac{d}{d\theta} \ln(1-\theta)$$
$$= \frac{\alpha_H}{\theta} - \frac{\alpha_T}{1-\theta} = 0$$

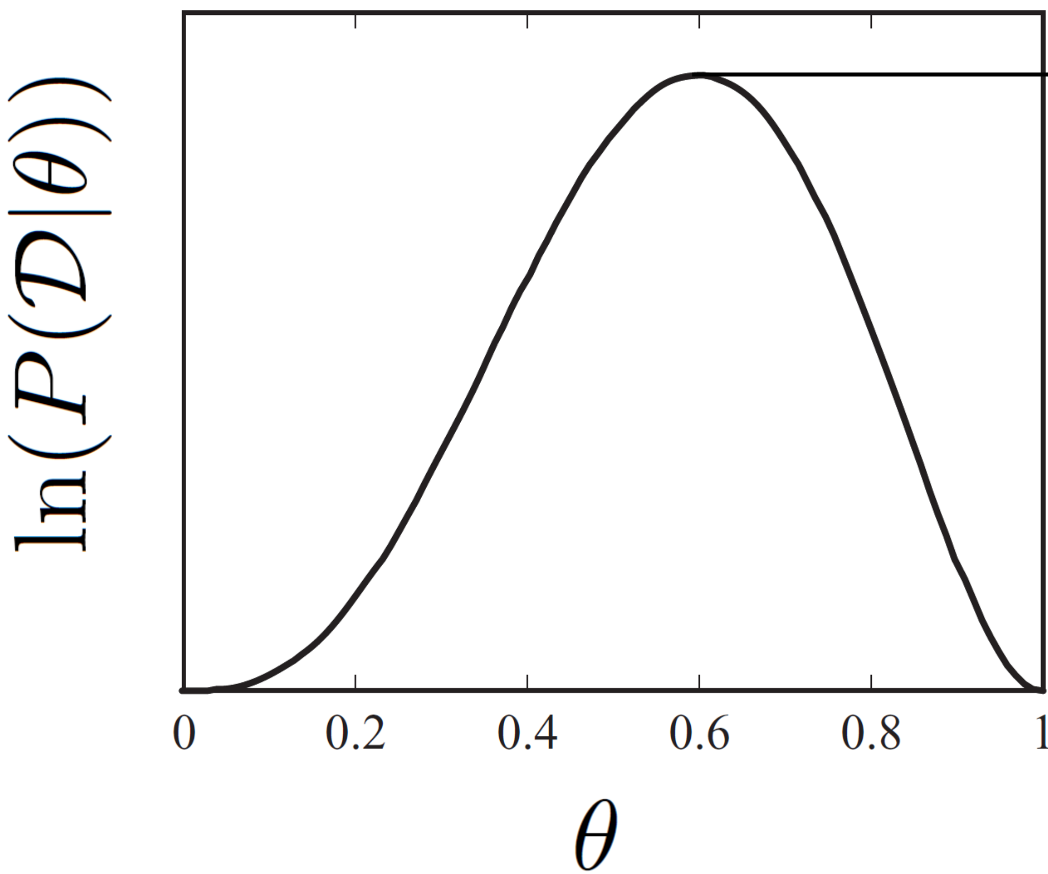
$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$



At each point, the derivative is the slope of a line that is tangent to the curve. Note: derivative is **positive where green**, **negative where red**, and **zero where black**.

Source: Wikipedia.com

Data



$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

But, how many flips do I need?

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

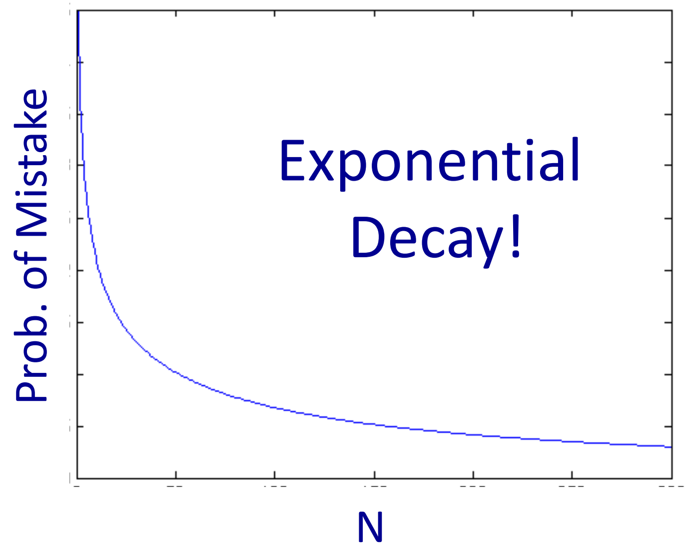
- Billionaire says: I flipped 3 heads and 2 tails.
- You say: θ = 3/5, I can prove it!
- He says: What if I flipped 30 heads and 20 tails?
- You say: Same answer, I can prove it!
- **He says: What's better?**
- You say: Umm… The more the merrier???
- He says: Is this why I am paying you the big bucks???
- You say: I will give you a theoretical bound.

A bound (from Hoeffding's inequality)

For $N = \alpha_H + \alpha_T$, and $\quad \widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$

Let θ^* be the true parameter, for any $\varepsilon > 0$:

$$P(|\,\widehat{\theta} - \theta^*\,| \geq \epsilon) \;\leq\; 2e^{-2N\epsilon^2}$$



PAC Learning

- PAC: Probably Approximate Correct
- Billionaire says: I want to know the thumbtack θ, within ε = 0.1, with probability of mistake, δ <= 0.05.
- How many flips? Or, how big do I set N?

$$P(|\widehat{\theta} - \theta^*| \geq \epsilon) \leq 2e^{-2N\epsilon^2}$$

$$P(\text{mistake}) \text{ is less than or equal to } 2e^{-2N\epsilon^2} \leq \delta$$

$$\ln \delta \geq \ln 2 - 2N\epsilon^2$$

$$N \geq \frac{\ln(2/\delta)}{2\epsilon^2}$$

Interesting! Lets look at some numbers!

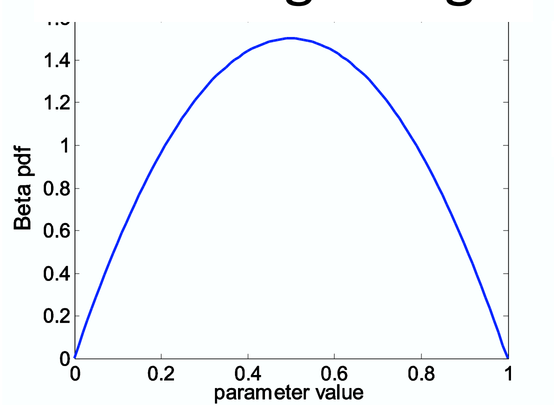
ε = 0.1, δ=0.05

$$N \geq \frac{\ln(2/0.05)}{2 \times 0.1^2} \approx \frac{3.8}{0.02} = 190$$

What if I have prior beliefs?

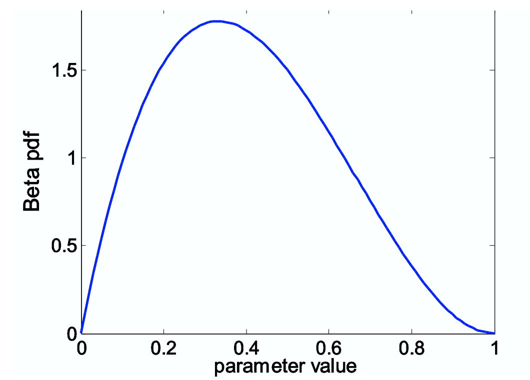
- **Billionaire says:** Wait, I know that the thumbtack is "close" to 50-50. What can you do for me now?
- **You say: I can learn it the Bayesian way…**
- Rather than estimating a single θ, we obtain a distribution over possible values of θ

In the beginning



Observe flips
e.g.: {tails, tails}

After observations

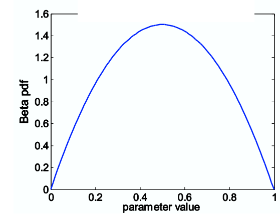


Bayesian Learning

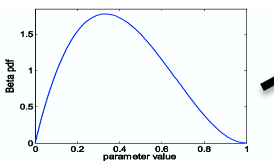
Use Bayes rule:

Data Likelihood

Prior



Posterior



$$P(\theta \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid \theta) P(\theta)}{P(\mathcal{D})}$$

Normalization

Or equivalently: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$

Also, for uniform priors:

→ reduces to MLE objective

$$P(\theta) \propto 1 \qquad P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta)$$

Bayesian Learning for Thumbtacks

$$P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$$

Likelihood function is Binomial:

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H} (1 - \theta)^{\alpha_T}$$

- What about prior?
  - Represent expert knowledge
  - Simple posterior form
- Conjugate priors:
  - Closed-form representation of posterior
  - **For Binomial, conjugate prior is Beta distribution**

Beta Distribution

- Distribution over $\mu \in [0, 1]$.

$$B(a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}$$

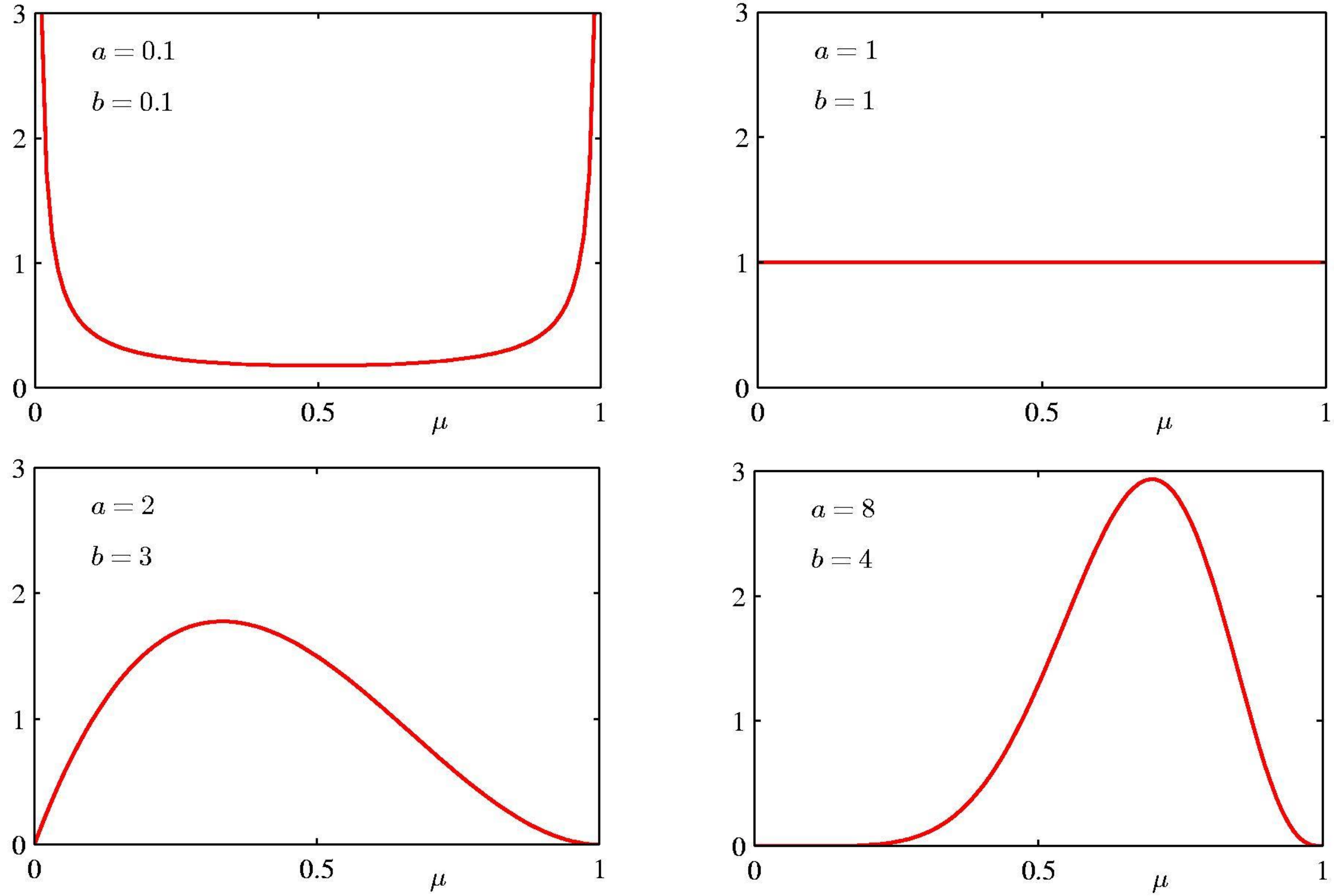
$$\begin{aligned} \mathrm{Beta}(\mu|a,b) &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1} \\ \mathbb{E}[\mu] &= \frac{a}{a+b} \\ \mathrm{var}[\mu] &= \frac{ab}{(a+b)^2(a+b+1)} \end{aligned}$$

$B(a,b) = \int_0^1 u^{a-1}(1-u)^{b-1}du,$ a>0, b>0

$$\Gamma(a) = \int_0^\infty u^{a-1}e^{-a}du$$

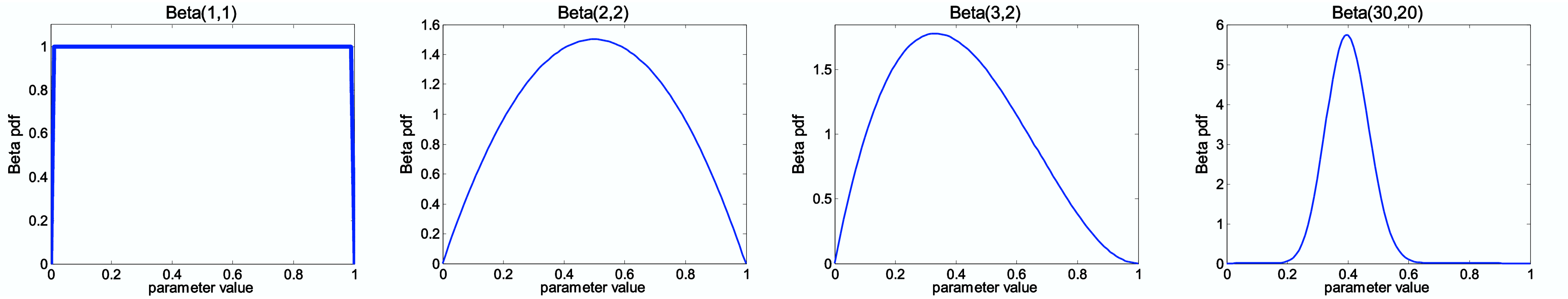
Beta Distribution

$$\mathrm{Beta}(\mu|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}$$



Beta prior distribution – P(θ)

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$



- Likelihood function: $P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$
- Posterior: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$

$$P(\theta \mid \mathcal{D}) \propto \theta^{\alpha_H}(1-\theta)^{\alpha_T}\ \theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}$$

$$= \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_T - 1}$$

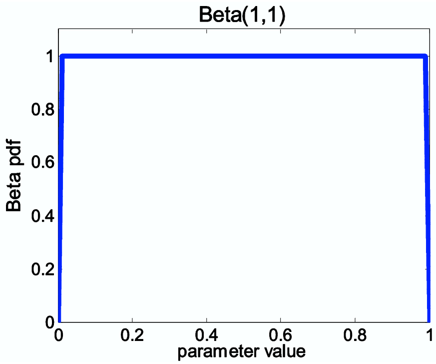
$$= Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

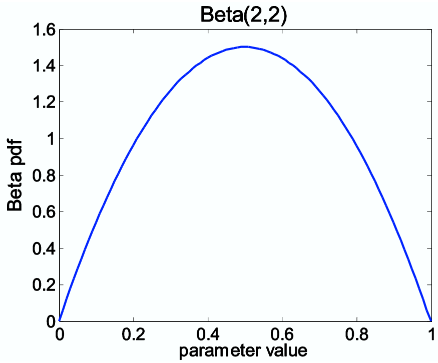
Posterior Distribution

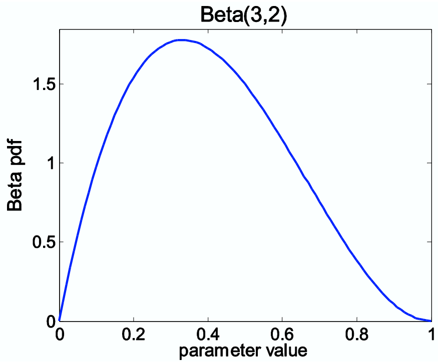
- Prior: $Beta(\beta_H, \beta_T)$
- Data: α_H heads and α_T tails

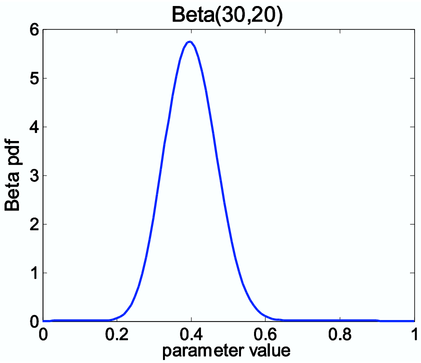
- Posterior distribution:

$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

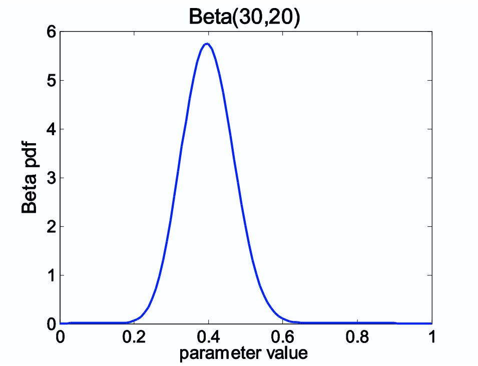








Bayesian Posterior Inference



- Posterior distribution:

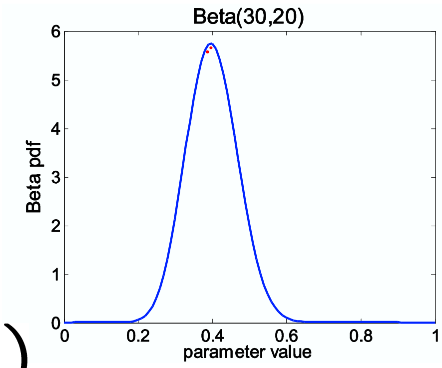
$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

- Bayesian inference:
  - No longer single parameter
  - For any specific *f*, the function of interest
  - Compute the expected value of *f*

$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

  - Integral is often hard to compute

MAP: Maximum a Posteriori Approximation



$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

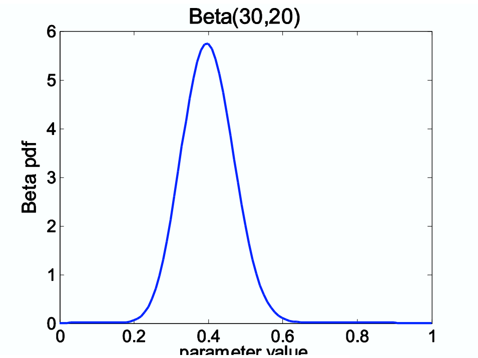
$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

- As more data is observed, Beta is more certain
- MAP: use most likely parameter to approximate the expectation

$$\widehat{\theta} = \arg\max_{\theta} P(\theta \mid \mathcal{D})$$

$$E[f(\theta)] \approx f(\widehat{\theta})$$

MAP for Beta distribution



$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H+\alpha_H-1}(1-\theta)^{\beta_T+\alpha_T-1}}{B(\beta_H+\alpha_H, \beta_T+\alpha_T)} \sim Beta(\beta_H+\alpha_H, \beta_T+\alpha_T)$$

MAP: use most likely parameter:

$$\widehat{\theta} = \arg\max_{\theta} P(\theta \mid \mathcal{D}) = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

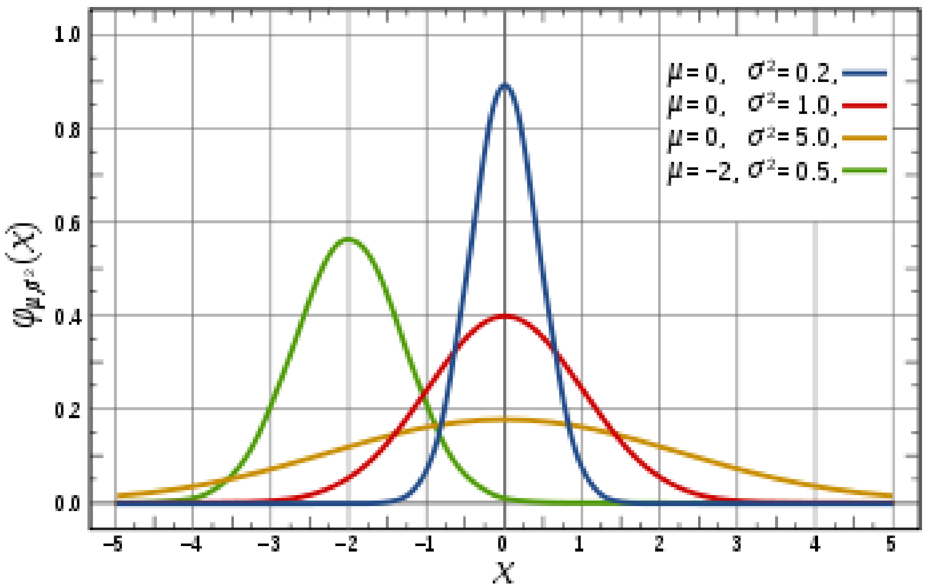
Beta prior equivalent to extra thumbtack flips

As $N \rightarrow \infty$, prior is "forgotten"

But, for small sample size, prior is important!

What about continuous variables?

- Billionaire says: If I am measuring a continuous variable, what can you do for me?
- **You say: Let me tell you about Gaussians…**



$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Learning a Gaussian

$X_i = i$	**Exam Score**
0	85
1	95
2	100
3	12
…	…
99	89

- Collect a bunch of data
  - Hopefully, i.i.d. samples
  - e.g., exam scores
- Learn parameters
  - Mean: μ
  - Variance: σ

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

MLE for Gaussian: $P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$

- Prob. of i.i.d. samples $D=\{x_1,\ldots,x_N\}$:

$$P(\mathcal{D} \mid \mu, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}$$

$$\mu_{MLE}, \sigma_{MLE} = \arg\max_{\mu,\sigma} P(\mathcal{D} \mid \mu, \sigma)$$

- Log-likelihood of data:

$$\begin{aligned} \ln P(\mathcal{D} \mid \mu, \sigma) &= \ln\left[\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}\right] \\ &= -N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{2\sigma^2} \end{aligned}$$

Your second learning algorithm: MLE for mean of a Gaussian

- What's MLE for mean?

$$\frac{d}{d\mu}\ln P(\mathcal{D} \mid \mu, \sigma) = \frac{d}{d\mu}\left[-N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N}\frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= \frac{d}{d\mu}\left[-N \ln \sigma\sqrt{2\pi}\right] - \sum_{i=1}^{N}\frac{d}{d\mu}\left[\frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= -\sum_{i=1}^{N}\frac{(x_i-\mu)}{\sigma^2} = 0$$

$$= -\sum_{i=1}^{N} x_i + N\mu = 0$$

$$\widehat{\mu}_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

MLE for variance

- Again, set derivative to zero:

$$\begin{aligned}
\frac{d}{d\sigma} \ln P(\mathcal{D} \mid \mu, \sigma) &= \frac{d}{d\sigma}\left[-N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{2\sigma^2}\right] \\
&= \frac{d}{d\sigma}\left[-N \ln \sigma\sqrt{2\pi}\right] - \sum_{i=1}^{N} \frac{d}{d\sigma}\left[\frac{(x_i-\mu)^2}{2\sigma^2}\right] \\
&= -\frac{N}{\sigma} + \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{\sigma^3} \qquad = 0
\end{aligned}$$

$$\widehat{\sigma}^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \widehat{\mu})^2$$

Learning Gaussian parameters

- MLE:

$$\widehat{\mu}_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\widehat{\sigma}^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N} (x_i - \widehat{\mu})^2$$

- BTW. MLE for the variance of a Gaussian is **biased**
  - Expected result of estimation is **not** true parameter!
  - Unbiased variance estimator:

$$\widehat{\sigma}^2_{unbiased} = \frac{1}{N-1}\sum_{i=1}^{N} (x_i - \widehat{\mu})^2$$