# Point Estimation

Vibhav Gogate
The University of Texas at Dallas

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

# 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:

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

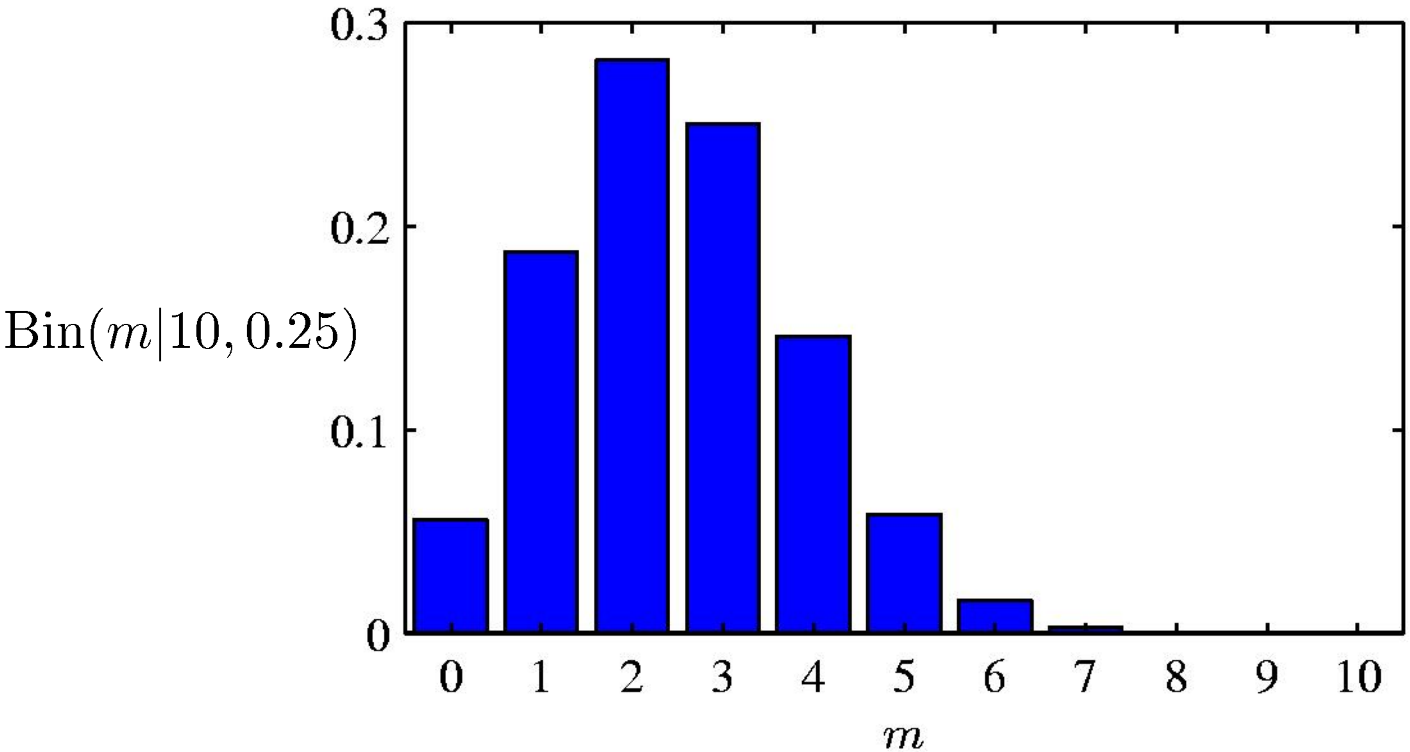
- Binomial Distribution

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

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

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

# Binomial Distribution



# 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) = $\theta$, P(Tails) = $1-\theta$

- Flips are *i.i.d.*:
  - Independent events
  - Identically distributed according to Binomial distribution
- Sequence $D$ of $\alpha_H$ Heads and $\alpha_T$ Tails

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

# Maximum Likelihood Estimation

- **Data:** Observed set $D$ of $\alpha_H$ Heads and $\alpha_T$ Tails
- **Hypothesis:** Binomial distribution
- **Learning:** finding $\theta$ is an optimization problem
  - What's the objective function?

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

- **MLE:** Choose $\theta$ to maximize probability of *D*

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

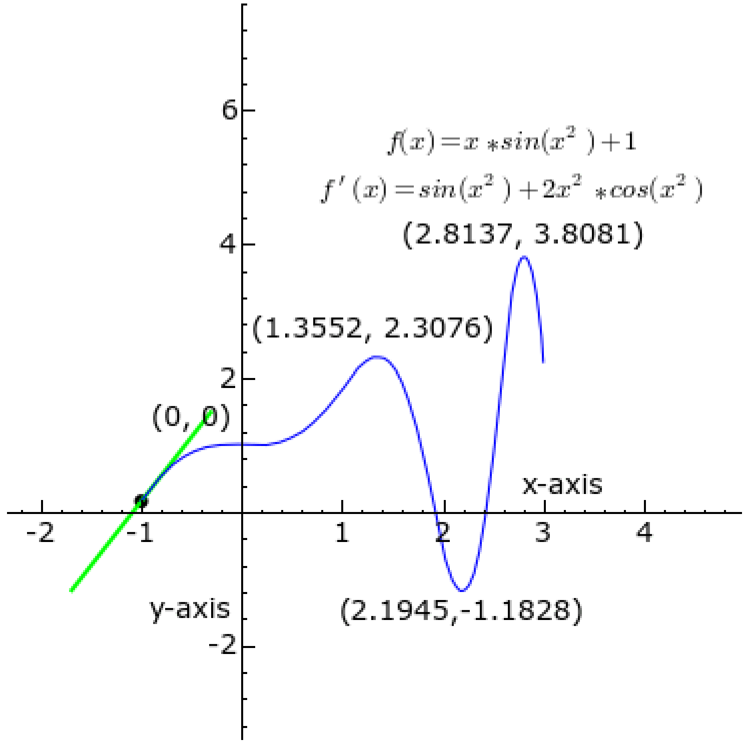
# Your first parameter learning algorithm

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

- Set derivative to zero, and solve!

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

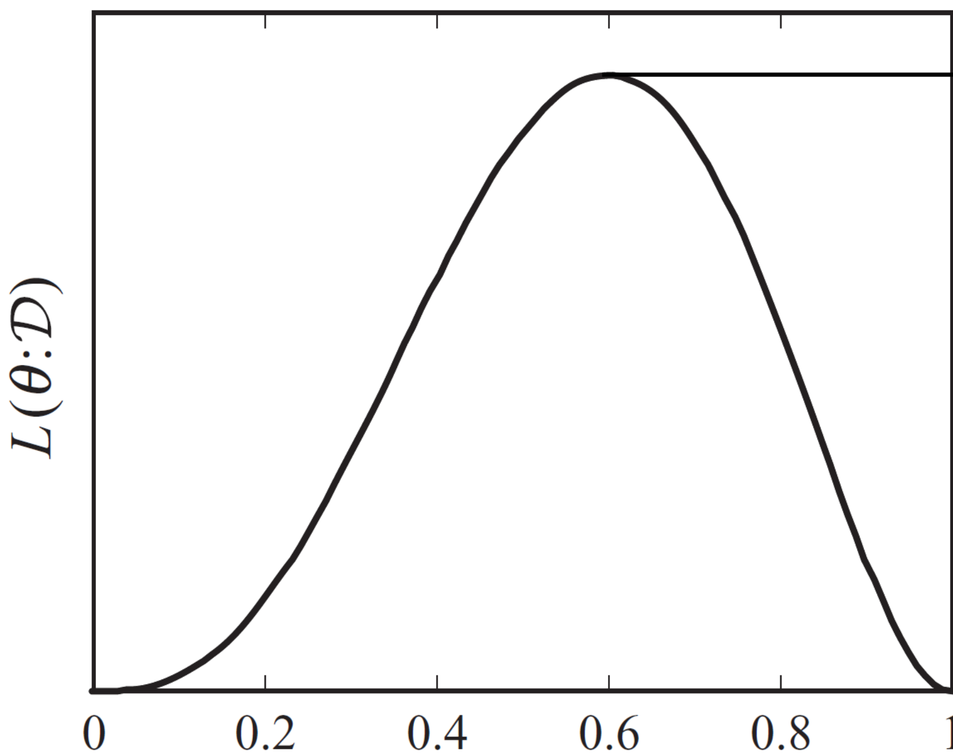
$$\boxed{\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}}$$




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

**Source: Wikipedia.com**

# Data




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

# Parameter Estimation: Summary

- ML for Bernoulli

Given: $\mathcal{D} = \{x_1, \ldots, x_N\}$, $m$ heads (1), $N-m$ tails (0)

$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \prod_{n=1}^{N} \mu^{x_n}(1-\mu)^{1-x_n}$$

$$\ln p(\mathcal{D}|\mu) = \sum_{n=1}^{N} \ln p(x_n|\mu) = \sum_{n=1}^{N} \{x_n \ln \mu + (1-x_n)\ln(1-\mu)\}$$

$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n = \frac{m}{N}$$

# But, how many flips do I need?

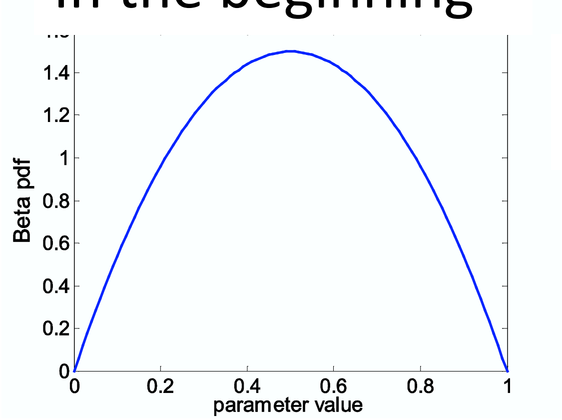
$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

- Billionaire says: I flipped 3 heads and 2 tails.
- You say: $\theta$ = 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.

# What if I have prior beliefs?

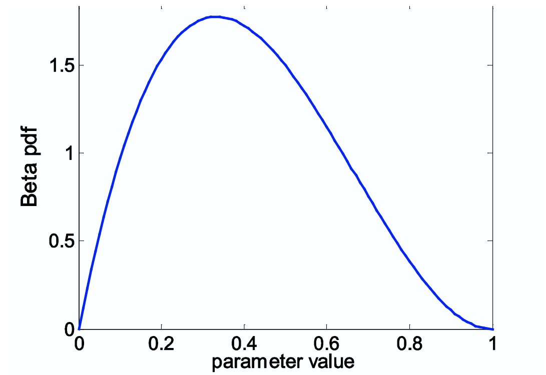
- Billionaire says: Wait, I know that the thumbtack is "close" to 50-50. What can you do for me now?
- **You say: I can learn it the Bayesian way…**
- Rather than estimating a single θ, we obtain a distribution over possible values of θ

In the beginning




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

After observations

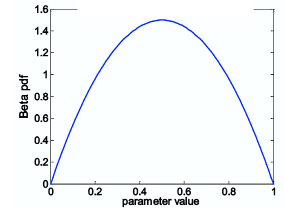


# Bayesian Learning

Use Bayes rule:

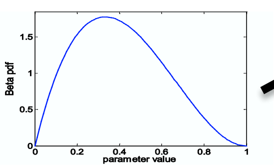
Data Likelihood

Prior




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

Posterior




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 $\mu \in [0, 1]$.

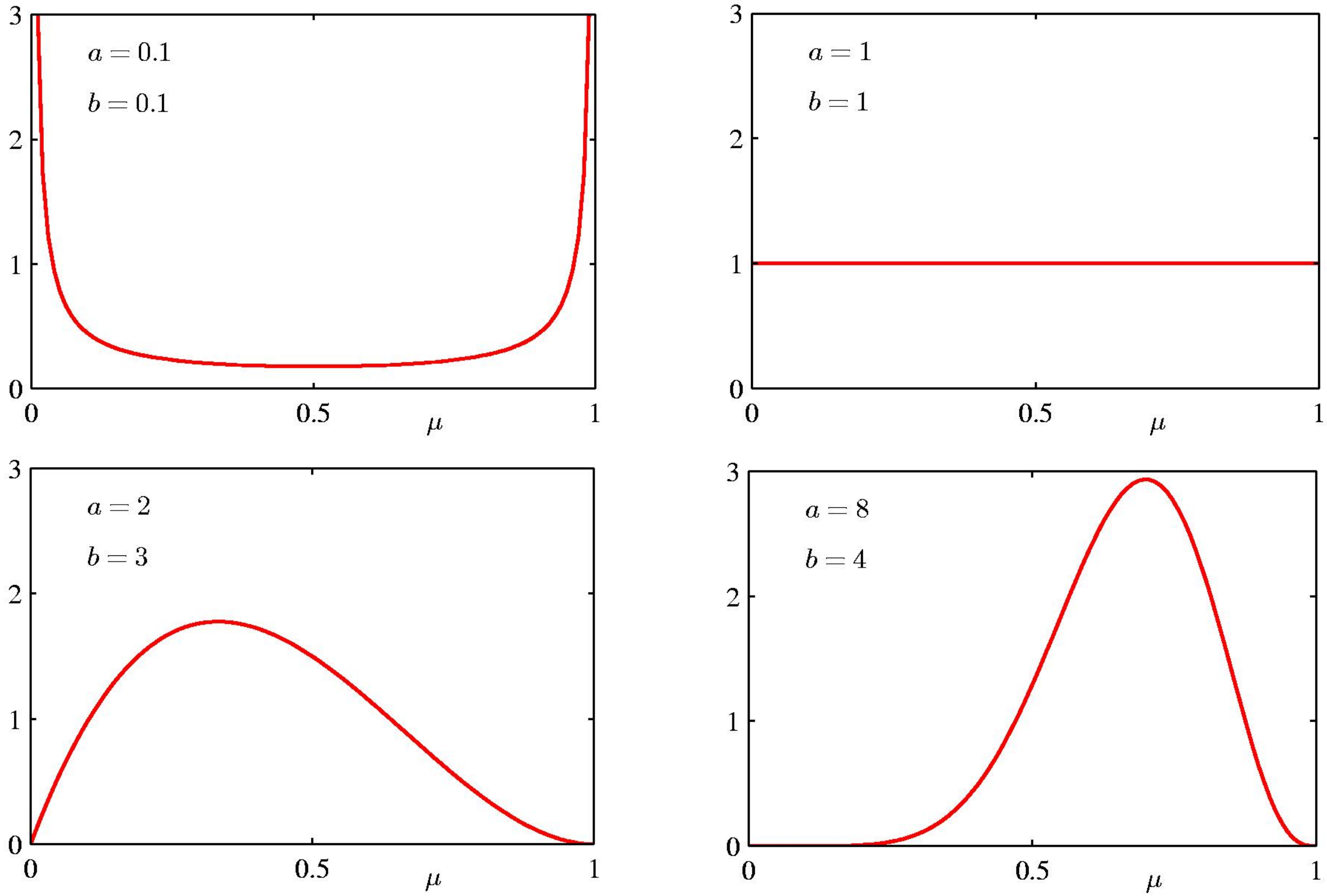
$$B(a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}$$

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

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

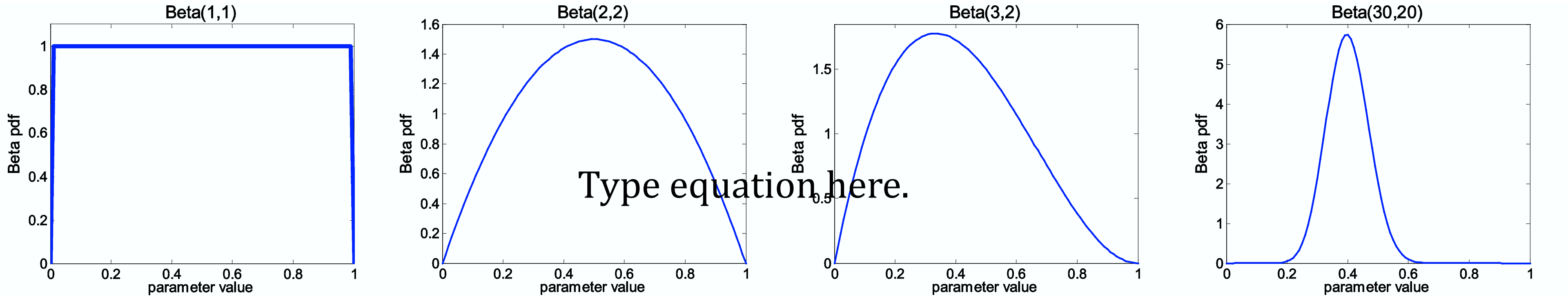
$$\Gamma(a) = \int_0^{\infty} u^{a-1}e^{-a}du$$

# Beta Distribution



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

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

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

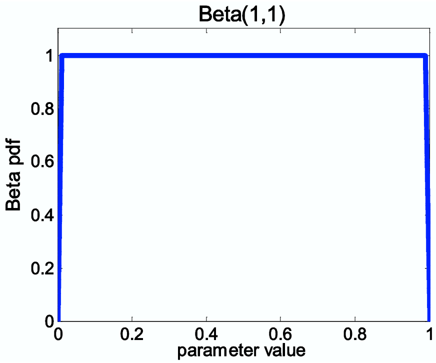
$$= Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

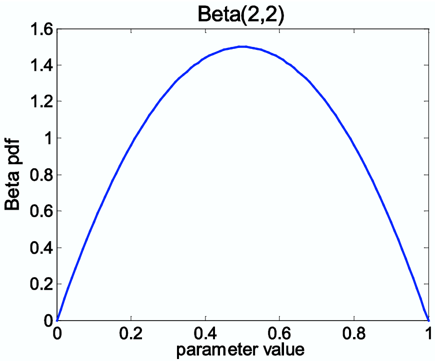
# Posterior Distribution

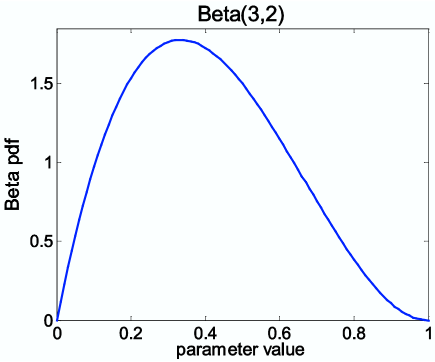
- Prior: $Beta(\beta_H, \beta_T)$
- Data: $\alpha_H$ heads and $\alpha_T$ tails

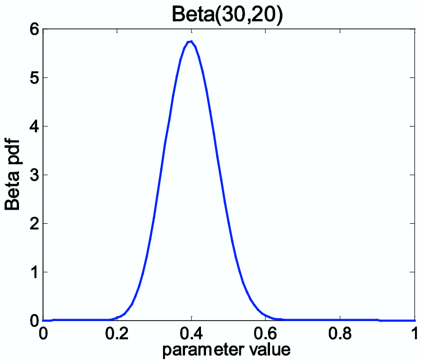
- Posterior distribution:

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

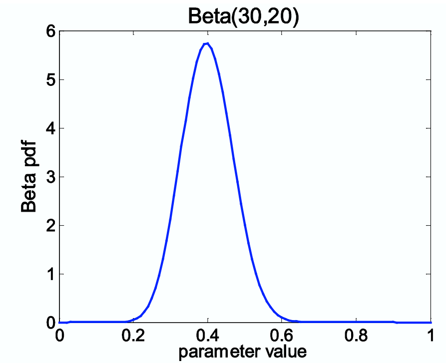








# Bayesian Posterior Inference




- Posterior distribution:

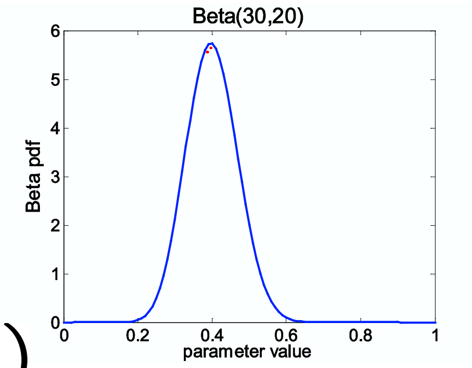
$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

- 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




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

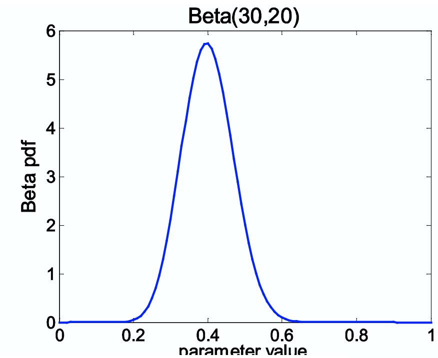
$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

- 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:

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

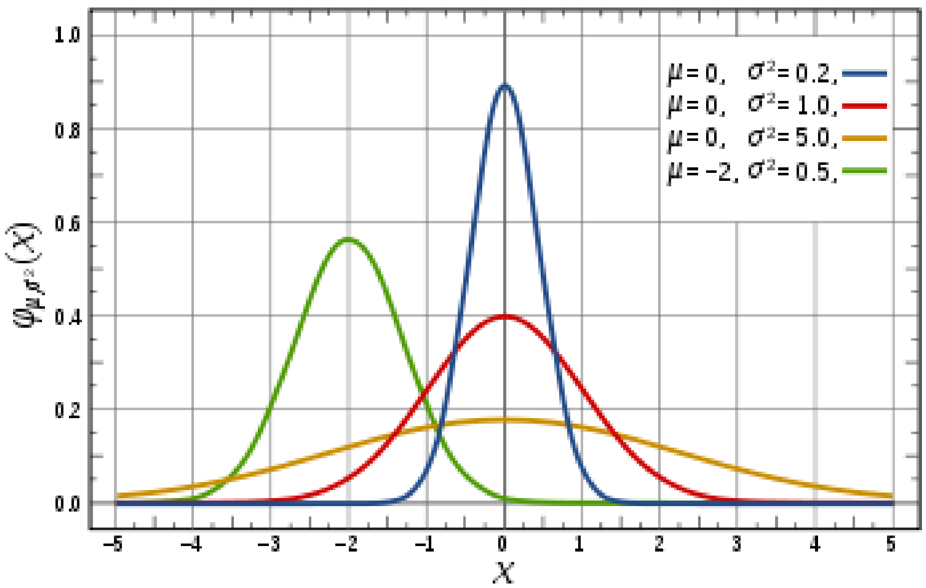
Beta prior equivalent to extra thumbtack flips

As $N \rightarrow \infty$, prior is “forgotten”

**But, for small sample size, prior is important!**

# What about continuous variables?

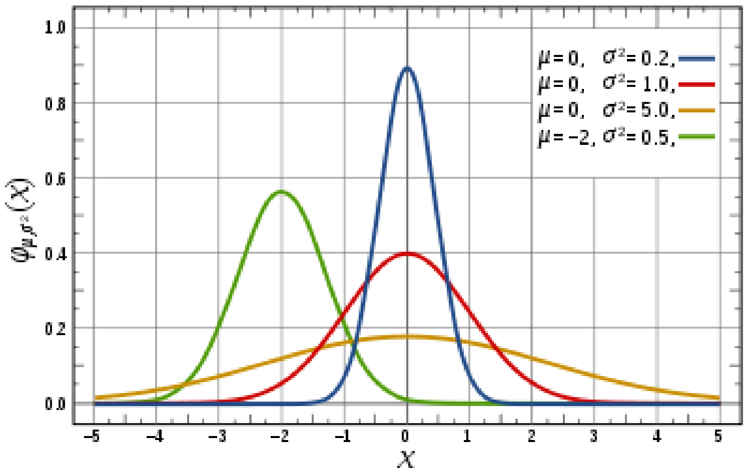
- **Billionaire says:** If I am measuring a continuous variable, what can you do for me?
- **You say: Let me tell you about Gaussians…**




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

# Some properties of Gaussians

- Affine transformation (multiplying by scalar and adding a constant) are Gaussian
  - $X \sim N(\mu, \sigma^2)$
  - $Y = aX + b \rightarrow Y \sim N(a\mu + b, a^2\sigma^2)$




- Sum of Gaussians is Gaussian
  - $X \sim N(\mu_X, \sigma^2_X)$
  - $Y \sim N(\mu_Y, \sigma^2_Y)$
  - $Z = X+Y \rightarrow Z \sim N(\mu_X+\mu_Y, \sigma^2_X+\sigma^2_Y)$

- Easy to differentiate, as we will see soon!

# Learning a Gaussian

- Collect a bunch of data
  - Hopefully, i.i.d. samples
  - e.g., exam scores
- Learn parameters
  - Mean: $\mu$
  - Variance: $\sigma$

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

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

# 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$_1$,…,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?

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

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

# MLE for variance

- Again, set derivative to zero:

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

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

# 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:

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

# Bayesian learning of Gaussian parameters

- Conjugate priors
  - Mean: Gaussian prior
  - Variance: Wishart Distribution

- Prior for mean:

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