lec06

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1 Lecture 6: Decision Theory — Loss, Risk, Admissibility, and Optimality

Data 145, Spring 2026: Evidence and Uncertainty
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Please run the setup cell below before reading.

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[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy import stats

plt.style.use('fivethirtyeight')
%matplotlib inline

# Color scheme for this lecture (colorblind-safe palette)
# Using IBM's colorblind-safe palette
COLOR_MLE = '#648FFF'        # Blue - MLE (unbiased)
COLOR_LAPLACE1 = '#785EF0'  # Purple - Laplace +1/+1
COLOR_LAPLACE2 = '#DC267F'  # Magenta - Laplace +2/+2
COLOR_BAD = '#FE6100'        # Orange - Inadmissible
COLOR_TRUE = '#000000'       # Black - True value
```

1.1 Introduction: A Coin Flip Experiment

In Lectures 3–5, we developed the theory of maximum likelihood estimation. We showed that the MLE is: - **Consistent**: $\hat{\theta}_n \xrightarrow{P} \theta_0$ - **Asymptotically normal**: $\sqrt{n}(\hat{\theta}_n - \theta_0) \xrightarrow{d} N(0, 1/I(\theta_0))$ - **Efficient**: Among unbiased estimators, it achieves the Cramér-Rao lower bound

This is a powerful result: if you want an unbiased estimator with small variance, the MLE is (asymptotically) the best you can do. But do we really need to be unbiased?

1.1.1 The Demo

In lecture, we flip a coin 16 times and count heads. Let's say we observe X heads.

If $X \neq 8$, the MLE $\hat{p} = X/16$ is different from 0.5. But most coins are pretty close to fair. If we suspect the true p is close to 0.5, should we *shrink* our estimate toward 0.5?

Could a biased estimator that shrinks toward 0.5 actually be *better* in some sense? To answer this, we need to be precise about what "better" means. As mathematicians, we want to do this at a higher level of abstraction — so we can say interesting things about many different estimation problems, not just this coin.

Today we'll see that: 1. Biased estimators can sometimes have *lower* mean squared error than the MLE 2. There's no single "best" estimator — different estimators are optimal under different criteria 3. This leads naturally to **Bayesian statistics** as one principled way to choose among estimators

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1.2 1. Decision Theory in Statistical Estimation

1.2.1 The Setup

Recall our standard setup: - **Data**: X (often $X_1, \ldots, X_n$ i.i.d.) - **Model**: f_θ indexed by parameter $\theta \in \Theta$ - **Estimand**: Some function $g(\theta)$ we want to estimate (often just θ itself) - **Estimator**: A function $T(X)$ that produces our estimate

When estimating θ itself, we typically write $\hat{\theta}(X)$ or just $\hat{\theta}$.

1.2.2 Loss Functions

A **loss function** $L(\theta, a)$ measures how bad it is to report the estimate a when the true parameter is θ.

Squared error loss is the most common choice:

$$L(\theta, a) = (\theta - a)^2$$

Other loss functions exist (absolute error, 0-1 loss, etc.), but we'll focus on squared error.

1.2.3 Risk Functions

The loss for a single dataset doesn't tell us much — one estimator might beat another by luck. We want to average over the sampling distribution.

The **risk function** is the expected loss:

$$R(\theta; T) = E_\theta[L(\theta, T(X))]$$

We write $R(\theta; T)$ with a semicolon because the risk is primarily a function of θ; the estimator T is fixed.

For squared error loss, this is the **mean squared error (MSE)**:

$$R(\theta; T) = \mathrm{MSE}_\theta(T) = E_\theta[(T(X) - \theta)^2]$$

1.2.4 The Fundamental Problem

The risk function depends on θ, which we don't know! Different estimators may be better for different values of θ.

This creates a fundamental tension: **how do we compare estimators when their relative performance depends on the unknown parameter?**

1.3 2. The Binomial Example

1.3.1 Setup

Let's work with a concrete example where we can visualize everything.

Example (Coin flipping): Flip a coin n times. Let X = number of heads. We want to estimate the probability p of heads.

The coin flipping example is a nice warm-up, **but this isn't just about coins!** The same mathematics applies to: - **Clinical trials**: n patients receive treatment, X respond positively, estimate the success rate p. - **Surveys/polls**: n respondents, X support a candidate, estimate the proportion p.

In these applications, we have no strong prior belief that $p \approx 0.5$. We care about doing well across the entire parameter space $p \in [0, 1]$.

Mathematically: $X \sim \text{Binomial}(n, p)$, and we want to estimate $p \in [0, 1]$.

This example is nice because: - The parameter space $[0, 1]$ is bounded, so we can plot risk functions over the entire space - X is the sum of n i.i.d. Bernoulli(p) random variables, so results from Lectures 4–5 apply

We'll use $n = 16$ throughout (connecting to our coin flip demo, and making calculations nice).

1.3.2 The MLE

The MLE for p is the sample proportion:

$$\hat{p} = \frac{X}{n}$$

From Lectures 4–5 (applied to Bernoulli observations), we know: - **Unbiased**: $E_p[\hat{p}] = p$ - **Variance**: $\text{Var}_p(\hat{p}) = \frac{p(1-p)}{n}$ - **Fisher information** (per observation): $I(p) = \frac{1}{p(1-p)}$ - **Efficient**: $\text{Var}_p(\hat{p}) = \frac{1}{nI(p)}$ achieves the Cramér-Rao bound

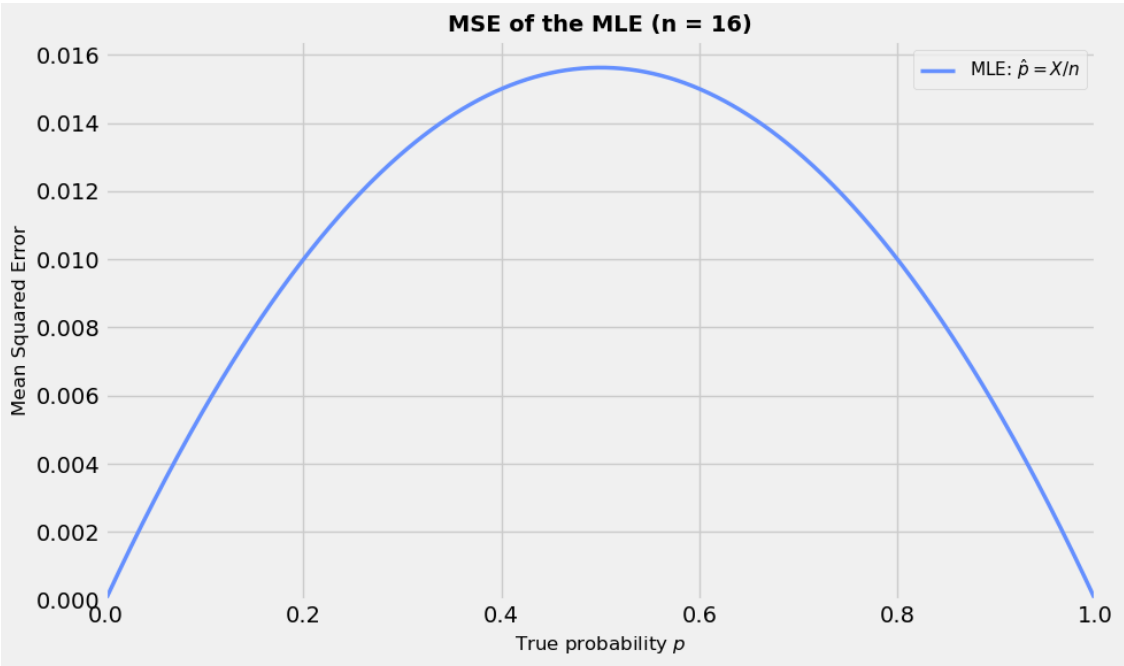
Since the MLE is unbiased, its MSE equals its variance:

$$\text{MSE}_p(\hat{p}) = \frac{p(1-p)}{n}$$

Key observation: The MSE depends on p, which we don't know. We care about doing well across the whole parameter space, not just at one point.

[2]:

```python
# Plot the MSE of the MLE
n = 16
p_grid = np.linspace(0.001, 0.999, 500)

# MSE of MLE
mse_mle = p_grid * (1 - p_grid) / n

fig, ax = plt.subplots(figsize=(10, 6))
ax.plot(p_grid, mse_mle, color=COLOR_MLE, linewidth=2.5, label=r'MLE: $\hat{p}␣
↪= X/n$')

ax.set_xlabel('True probability $p$', fontsize=12)
ax.set_ylabel('Mean Squared Error', fontsize=12)
ax.set_title(f'MSE of the MLE (n = {n})', fontsize=14, fontweight='bold')
ax.set_xlim(0, 1)
ax.set_ylim(0, None)
ax.legend(fontsize=11)

plt.tight_layout()
plt.show()

print(f"Maximum MSE occurs at p = 0.5: MSE = {0.5 * 0.5 / n:.4f}")
```




```
Maximum MSE occurs at p = 0.5: MSE = 0.0156
```

1.3.3 Returning to the Coin Flip

For the coin example specifically, consider $n = 16$ flips. If we observe $X = 12$ heads, the MLE says $\hat{p} = 12/16 = 0.75$.

Do we really believe the coin has a 75% chance of heads? Most real coins are close to fair. If we had some prior belief that p is likely near 0.5, we might want to **shrink** our estimate toward 0.5.

The MLE is the best *unbiased* estimator. **But who said we have to be unbiased?**

1.4 3. Shrinkage Estimators

1.4.1 Laplace's Estimator: Adding Pseudodata

Intuition: If we think extreme values of p (near 0 or 1) are unlikely, maybe we should shrink our estimate toward 1/2.

Laplace's idea (1774): Pretend we observed two extra flips before seeing the data — one head and one tail. This gives:

$$\tilde{p}_1 = \frac{X+1}{n+2}$$

For our example with $n = 16$, $X = 12$: - MLE: $\hat{p} = 12/16 = 0.75$ - Laplace: $\tilde{p}_1 = 13/18 \approx 0.722$

The Laplace estimator shrinks toward 0.5.

1.4.2 More Aggressive Shrinkage

What if we add *two* heads and *two* tails of pseudodata?

$$\tilde{p}_2 = \frac{X+2}{n+4}$$

For $n = 16$, $X = 12$: - Laplace +2/+2: $\tilde{p}_2 = 14/20 = 0.70$

This shrinks even more toward 0.5.

1.4.3 A Bootstrap Estimator

Here's another idea: what if we use the bootstrap to improve our estimate?

Bootstrap procedure: 1. From the original n Bernoulli observations, draw B bootstrap samples (each of size n, with replacement) 2. Compute the MLE $\hat{p}^{(b)} = X^{(b)}/n$ for each bootstrap sample 3. Average them: $\hat{p}_{\text{boot}} = \frac{1}{B}\sum_{b=1}^{B}\hat{p}^{(b)}$

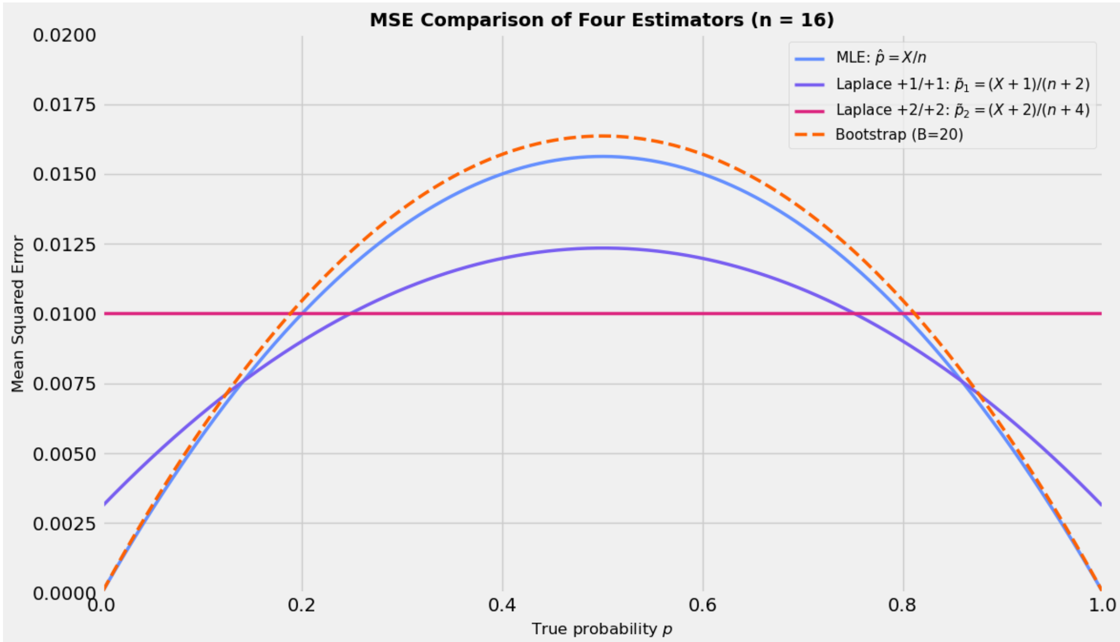
This might seem like a clever way to reduce variance — after all, the bootstrap is useful for quantifying uncertainty. But does averaging bootstrap estimates actually improve the original estimate?

Spoiler: It doesn't! The bootstrap estimator has the same bias as the MLE (zero) but *higher* variance. We'll see why.

Let's see how all four estimators compare.

[3]:
```
# Define MSE functions for all four estimators
def mse_mle(p, n):
    """MSE of MLE: X/n"""
    return p * (1 - p) / n

def mse_laplace1(p, n):
    """MSE of Laplace +1/+1: (X+1)/(n+2)"""
    # E[(X+1)/(n+2)] = (np + 1)/(n+2)
    # Bias = (np + 1)/(n+2) - p = (1 - 2p)/(n+2)
    # Var = n * p(1-p) / (n+2)^2
    bias = (1 - 2*p) / (n + 2)
    var = n * p * (1 - p) / (n + 2)**2
    return bias**2 + var

def mse_laplace2(p, n):
    """MSE of Laplace +2/+2: (X+2)/(n+4)"""
    # E[(X+2)/(n+4)] = (np + 2)/(n+4)
    # Bias = (np + 2)/(n+4) - p = (2 - 4p)/(n+4) = 2(1 - 2p)/(n+4)
    # Var = n * p(1-p) / (n+4)^2
    bias = 2 * (1 - 2*p) / (n + 4)
    var = n * p * (1 - p) / (n + 4)**2
    return bias**2 + var

def mse_bootstrap(p, n, B=20):
    """MSE of bootstrap estimator: average of B bootstrap MLEs

    Each bootstrap sample draws n observations with replacement from the
    original n Bernoullis. If X = sum of originals, then each bootstrap
    sample has X* ~ Binomial(n, X/n) conditional on X, where X ~ Binomial(n, p).

    The bootstrap estimator averages B such bootstrap MLEs.
    Unconditionally: E[X*/n] = E[E[X*/n | X]] = E[X/n] = p (unbiased)

    Variance is HIGHER than MLE due to added resampling variability.
    Var(X*/n | X) = (X/n)(1 - X/n)/n
    Var(bootstrap mean | X) = (X/n)(1 - X/n)/(nB)

    By law of total variance:
    Var(bootstrap mean) = E[Var(mean | X)] + Var(E[mean | X])
                        = E[p_hat(1 - p_hat)/(nB)] + Var(p_hat)
                        = E[p_hat(1 - p_hat)]/(nB) + p(1-p)/n

    E[p_hat(1 - p_hat)] = E[p_hat] - E[p_hat^2] = p - (Var(p_hat) + p^2)
                        = p - p(1-p)/n - p^2 = p(1-p)(1 - 1/n)
```

```
    So: Var(bootstrap) = p(1-p)(1 - 1/n)/(nB) + p(1-p)/n
                       = p(1-p)/n * [1 + (1 - 1/n)/B]
                       = p(1-p)/n * (1 + (n-1)/(nB))
    """
    # Unbiased, so MSE = Variance
    return p * (1 - p) / n * (1 + (n - 1) / (n * B))

# Compute MSE for all estimators
n = 16
B = 20  # Number of bootstrap samples
p_grid = np.linspace(0.001, 0.999, 500)

mse_vals = {
    'MLE': mse_mle(p_grid, n),
    'Laplace +1/+1': mse_laplace1(p_grid, n),
    'Laplace +2/+2': mse_laplace2(p_grid, n),
    'Bootstrap': mse_bootstrap(p_grid, n, B)
}

# Plot all MSE curves
fig, ax = plt.subplots(figsize=(12, 7))

ax.plot(p_grid, mse_vals['MLE'], color=COLOR_MLE, linewidth=2.5,
        label=r'MLE: $\hat{p} = X/n$')
ax.plot(p_grid, mse_vals['Laplace +1/+1'], color=COLOR_LAPLACE1, linewidth=2.5,
        label=r'Laplace +1/+1: $\tilde{p}_1 = (X+1)/(n+2)$')
ax.plot(p_grid, mse_vals['Laplace +2/+2'], color=COLOR_LAPLACE2, linewidth=2.5,
        label=r'Laplace +2/+2: $\tilde{p}_2 = (X+2)/(n+4)$')
ax.plot(p_grid, mse_vals['Bootstrap'], color=COLOR_BAD, linewidth=2.5,
 ↪linestyle='--',
        label=f'Bootstrap (B={B})')

ax.set_xlabel('True probability $p$', fontsize=12)
ax.set_ylabel('Mean Squared Error', fontsize=12)
ax.set_title(f'MSE Comparison of Four Estimators (n = {n})', fontsize=14,
 ↪fontweight='bold')
ax.set_xlim(0, 1)
ax.set_ylim(0, 0.02)
ax.legend(fontsize=11, loc='upper right')

plt.tight_layout()
plt.show()
```



1.4.4 Observations from the Plot

1. **The bootstrap estimator is strictly worse than the MLE everywhere!** Its MSE curve lies entirely above the MLE curve.
2. **The other curves cross.** No single estimator (among MLE, Laplace +1/+1, Laplace +2/+2) is best for all values of p.
3. **Near** $p = 0.5$, the Laplace estimators beat the MLE. Their shrinkage toward 0.5 helps when p really is near 0.5.
4. **Near** $p = 0$ **or** $p = 1$, the MLE beats the Laplace estimators. Shrinking toward 0.5 hurts when the truth is extreme.

To understand *why* these patterns occur, we need to examine the bias-variance tradeoff.

1.5 4. Bias-Variance Calculations and Admissibility

1.5.1 The Bias-Variance Decomposition

For any estimator T of θ, let $\mu = E_\theta[T]$ be its mean. Then:

$$E_\theta[(T-\theta)^2] = E_\theta[(T-\mu+\mu-\theta)^2] = E_\theta[(T-\mu)^2] + (\mu-\theta)^2$$

The cross term vanishes because $E_\theta[T-\mu] = 0$. So:

$$\text{MSE}_\theta(T) = \text{Var}_\theta(T) + \text{Bias}_\theta(T)^2$$

where $\text{Bias}_\theta(T) = E_\theta[T] - \theta$.

1.5.2 MLE: $\hat{p} = X/n$

The MLE is unbiased, so its MSE equals its variance:

$$\text{MSE}_p(\hat{p}) = \text{Var}_p(\hat{p}) = \frac{p(1-p)}{n}$$

1.5.3 General Laplace Estimator: $\tilde{p}_k = (X+k)/(n+2k)$

Consider adding $2k$ pseudoflips: k heads and k tails. This gives the estimator:

$$\tilde{p}_k = \frac{X+k}{n+2k}$$

Bias:

$$E_p[\tilde{p}_k] = \frac{np+k}{n+2k}, \qquad \text{Bias}_p(\tilde{p}_k) = \frac{np+k}{n+2k} - p = \frac{k(1-2p)}{n+2k}$$

The bias is positive when $p < 0.5$ and negative when $p > 0.5$: the estimator **shrinks toward 0.5**.

Variance:

$$\text{Var}_p(\tilde{p}_k) = \frac{np(1-p)}{(n+2k)^2}$$

Note that the variance is **smaller** than the MLE's variance because the denominator is larger.

MSE:

$$\text{MSE}_p(\tilde{p}_k) = \frac{k^2(1-2p)^2 + np(1-p)}{(n+2k)^2}$$

For $k = 1$: Laplace +1/+1. For $k = 2$: Laplace +2/+2.

1.5.4 Bootstrap Estimator

The bootstrap estimator averages B bootstrap MLEs, where each bootstrap sample resamples the original n Bernoulli observations with replacement.

Key insight: Conditional on the original data (with MLE $\hat{p} = X/n$), each bootstrap sample has $X^* \sim \text{Binomial}(n, \hat{p})$.

Bias: The bootstrap estimator is unbiased!

$$E[\hat{p}_{\text{boot}}] = E[E[\hat{p}_{\text{boot}}|X]] = E[\hat{p}] = p$$

Variance: By the law of total variance:

$$\text{Var}(\hat{p}_{\text{boot}}) = E[\text{Var}(\hat{p}_{\text{boot}}|X)] + \text{Var}(E[\hat{p}_{\text{boot}}|X])$$

The second term is just $\text{Var}(\hat{p}) = p(1-p)/n$. The first term adds extra variance from resampling:

$$\text{Var}(\hat{p}_{\text{boot}}) = \frac{p(1-p)}{n} \cdot \left(1 + \frac{n-1}{nB}\right) > \frac{p(1-p)}{n}$$

The bootstrap estimator has **the same bias** as the MLE (zero) but **higher variance**. Its MSE is strictly larger than the MLE's for all $p \neq 0, 1$.

[4]:
```
# Summary table of bias, variance, MSE formulas
print("Summary of Estimator Properties")
print("=" * 85)
print(f"{'Estimator':<25} {'Bias':^20} {'Variance':^25} {'MSE':^20}")
print("-" * 85)
print(f"{'MLE: X/n':<25} {'0':^20} {'p(1-p)/n':^25} {'p(1-p)/n':^20}")
print(f"{'Laplace +1: (X+1)/(n+2)':<25} {'(1-2p)/(n+2)':^20} {'np(1-p)/(n+2)²':
↪^25} {'[formula]':^20}")
print(f"{'Laplace +2: (X+2)/(n+4)':<25} {'2(1-2p)/(n+4)':^20} {'np(1-p)/(n+4)²':
↪^25} {'[formula]':^20}")
print(f"{'Bootstrap (B samples)':<25} {'0':^20} {'> p(1-p)/n':^25} {'> p(1-p)/
↪n':^20}")
print("=" * 85)
```

```
Summary of Estimator Properties
================================================================================
=====
Estimator                          Bias                  Variance
MSE
--------------------------------------------------------------------------------
-----
MLE: X/n                            0                    p(1-p)/n
p(1-p)/n
Laplace +1: (X+1)/(n+2)        (1-2p)/(n+2)           np(1-p)/(n+2)²
[formula]
Laplace +2: (X+2)/(n+4)       2(1-2p)/(n+4)           np(1-p)/(n+4)²
[formula]
Bootstrap (B samples)               0                   > p(1-p)/n             >
p(1-p)/n
================================================================================
=====
```

1.5.5 What Went Wrong with the Bootstrap Estimator?

The bootstrap estimator has: - **Same bias** as the MLE (zero) - **Higher variance** — the resampling process adds variability

It adds variance without any compensating bias reduction toward a likely value. That's a bad trade!

The lesson: Bootstrap is great for *quantifying* uncertainty (e.g., computing confidence intervals), but averaging bootstrap estimates doesn't *reduce* uncertainty. The bootstrap can only simulate the sampling distribution; it can't improve on the original estimator.

The Laplace estimators, by contrast, make a **smart trade**: - They add bias (toward 0.5) - But they reduce variance (by inflating the denominator) - When p is near 0.5, the bias is small and the variance reduction helps - When p is near 0 or 1, the bias penalty outweighs the variance benefit

1.5.6 Admissibility

Definition: An estimator T_1 is **inadmissible** if there exists another estimator T_2 such that: - $R(\theta; T_2) \leq R(\theta; T_1)$ for all $\theta \in \Theta$ - $R(\theta; T_2) < R(\theta; T_1)$ for at least one θ

In this case, we say T_2 **dominates** T_1. An estimator that is not inadmissible is called **admissible**.

Our estimators: - The **bootstrap estimator is inadmissible** — it is dominated by the MLE - The **MLE, Laplace +1/+1, and Laplace +2/+2 are all admissible** — none dominates another

Admissibility is a minimal requirement: we should never use an inadmissible estimator. But among admissible estimators, we still need a way to choose.

1.6 5. Optimality Criteria

1.6.1 The Fundamental Problem

We have multiple admissible estimators. How do we choose among them?

Question: Is it possible to find an estimator that's best for *all* values of p?

Answer: No! (At least not for MSE.)

Why not? Think about it: if $p = 0.75$ is really the truth, then the constant estimator $T(X) \equiv 0.75$ has MSE = 0 at that point. No other estimator can beat it there. But that constant estimator would be terrible if $p = 0.25$.

No estimator can beat every other estimator at every p.

1.6.2 Two Approaches to Choosing Among Admissible Estimators

Approach 1: Restrict to a class of estimators

For example, among **unbiased** estimators, the MLE is optimal.

Why? For unbiased estimators, MSE = Variance. So minimizing MSE is the same as minimizing variance. By the Cramér-Rao bound, the MLE achieves the minimum variance among unbiased estimators.

Another example: among **equivariant** estimators (you'll see these in Worksheet 3, Problem 5), there's often a unique best choice.

Note: We won't pursue optimality among restricted classes further in this course. Instead, we'll focus on the second approach.

Approach 2: Summarize the risk function by a single number

Instead of comparing entire risk curves, we can reduce each estimator to a single number and compare those.

1.6.3 Worst-Case Risk (Minimax)

Define the **worst-case risk**:

$$R_{\max}(T) = \max_{p \in [0,1]} \text{MSE}_p(T)$$

A **minimax estimator** minimizes the worst-case risk.

This is a conservative approach: we guard against the worst possible scenario.

[5]:
```python
# Calculate worst-case risk for each estimator
n = 16
B = 20
p_grid = np.linspace(0.001, 0.999, 1000)

worst_case = {
    'MLE': np.max(mse_mle(p_grid, n)),
    'Laplace +1/+1': np.max(mse_laplace1(p_grid, n)),
    'Laplace +2/+2': np.max(mse_laplace2(p_grid, n)),
    'Bootstrap': np.max(mse_bootstrap(p_grid, n, B))
}

print("Worst-Case Risk (Maximum MSE over all p)")
print("=" * 50)
for name, wc in worst_case.items():
    print(f"{name:<20}: {wc:.6f}")
print("=" * 50)
print(f"\nMinimax estimator: Laplace +2/+2 (smallest worst-case risk)")
```

```
Worst-Case Risk (Maximum MSE over all p)
==================================================
MLE                 : 0.015625
Laplace +1/+1       : 0.012346
Laplace +2/+2       : 0.010000
Bootstrap           : 0.016357
==================================================

Minimax estimator: Laplace +2/+2 (smallest worst-case risk)
```

For $n = 16$, the **Laplace +2/+2 estimator** $\tilde{p}_2 = (X + 2)/(n + 4)$ is the minimax estimator!

Its MSE curve is relatively flat, with its maximum at $p = 0.5$. By shrinking toward the center, it avoids extremely bad performance anywhere.

1.6.4 Average-Case Risk

Instead of worst-case, we could consider **average-case** risk:

$$R_{\text{avg}}(T) = \int_0^1 \text{MSE}_p(T)\, dp$$

This averages the MSE uniformly over all possible values of p.

Question: We've considered worst-case and average-case risk. Why not **best-case** risk?

Answer: Every estimator can achieve arbitrarily small best-case risk — just find some p where it happens to do well (e.g., the constant estimator $T \equiv c$ has MSE $= 0$ at $p = c$). Best-case risk doesn't discriminate between estimators, so it's not useful.

Which estimator minimizes average-case risk? Let's find out.

1.7 6. Minimizing Average-Case Risk: A Surprising Answer

1.7.1 The Problem

We want to find the estimator $T(X)$ that minimizes:

$$R_{\text{avg}}(T) = \int_0^1 \text{MSE}_p(T)\, dp = \int_0^1 E_p[(T(X) - p)^2]\, dp$$

1.7.2 Rewriting the Objective

Let's rewrite the integral as an expectation:

$$R_{\text{avg}}(T) = \int_0^1 E_p[(T(X) - p)^2]\, dp = E\left[(T(X) - p)^2\right]$$

where the expectation is over the **joint distribution** of (X, p) with: - $p \sim \text{Uniform}(0, 1)$ - $X \mid p \sim \text{Binomial}(n, p)$

1.7.3 Finding the Optimal $T(X)$

For any fixed value of $X = x$, what choice of $T(x)$ minimizes $E[(T(x) - p)^2 \mid X = x]$?

By the same argument we used for the bias-variance decomposition (with p playing the role of the target and $E[p \mid X]$ playing the role of the mean), we have:

$$E[(T(X) - p)^2 \mid X] = \text{Var}(p \mid X) + (E[p \mid X] - T(X))^2$$

The first term doesn't depend on T. The second term is minimized (to zero) when $T(X) = E[p \mid X]$.

So the optimal estimator is the **conditional mean**: $T^*(X) = E[p \mid X]$.

1.7.4 Computing $E[p \mid X]$

We need the conditional distribution of p given X.

Click to expand: Full derivation of the conditional distribution

We compute the conditional distribution using Bayes' rule.

Joint distribution:

For $p \in [0,1]$ and $x \in \{0, 1, \dots, n\}$:

$$f(x,p) = P(X = x \mid p) \cdot f(p) = \binom{n}{x} p^x (1-p)^{n-x} \cdot 1$$

Marginal distribution of X:

$$P(X = x) = \int_0^1 \binom{n}{x} p^x (1-p)^{n-x} dp$$

This integral involves the **Beta function**. Recall that:

$$B(a,b) = \int_0^1 p^{a-1}(1-p)^{b-1} dp = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} = \frac{(a-1)!(b-1)!}{(a+b-1)!}$$

for positive integers a, b.

So:

$$P(X = x) = \binom{n}{x} \int_0^1 p^x (1-p)^{n-x} dp = \binom{n}{x} B(x+1, n-x+1)$$

$$= \binom{n}{x} \frac{x!(n-x)!}{(n+1)!} = \frac{n!}{x!(n-x)!} \cdot \frac{x!(n-x)!}{(n+1)!} = \frac{1}{n+1}$$

Interesting! Under a uniform prior on p, the marginal distribution of X is uniform on $\{0, 1, \dots, n\}$.

Conditional distribution of p given X:

$$f(p \mid x) = \frac{f(x,p)}{P(X = x)} = \frac{\binom{n}{x} p^x (1-p)^{n-x}}{1/(n+1)} = (n+1)\binom{n}{x} p^x (1-p)^{n-x}$$

This is proportional to $p^x(1-p)^{n-x}$, which is the kernel of a **Beta distribution**:

$$p \mid X = x \sim \text{Beta}(x+1, n-x+1)$$

Conditional mean:

The mean of a $\text{Beta}(\alpha, \beta)$ distribution is $\frac{\alpha}{\alpha+\beta}$.

So:

$$E[p \mid X] = \frac{X+1}{(X+1) + (n-X+1)} = \frac{X+1}{n+2}$$

1.7.5 The Punchline

The estimator that minimizes average-case risk $\int_0^1 \text{MSE}_p(T)\, dp$ is:

$$T^*(X) = E[p \mid X] = \frac{X+1}{n+2}$$

This is exactly Laplace's estimator $\tilde{p}_1$!

Laplace's "add one head and one tail" rule, which seemed like an intuitive hack, is actually the *optimal* estimator if we measure quality by average MSE over $p \in [0,1]$.

1.7.6 The Bayesian Interpretation

What we just computed has a name: it's the **posterior mean** of p given X.

- The distribution $p \sim \text{Uniform}(0, 1)$ is called the **prior distribution** — it represents our beliefs about p before seeing data
- The distribution $p \mid X \sim \text{Beta}(X + 1, n - X + 1)$ is called the **posterior distribution** — it represents our updated beliefs after seeing data
- The posterior mean $E[p \mid X]$ is the **Bayes estimator** for squared error loss

You've already seen Beta-Binomial conjugacy in your probability class — this is the same calculation! The uniform distribution $\text{Uniform}(0, 1)$ is the same as $\text{Beta}(1, 1)$, and after observing X successes in n trials, the posterior is $\text{Beta}(1 + X, 1 + n - X) = \text{Beta}(X + 1, n - X + 1)$.

An estimator that minimizes average risk (with respect to some prior distribution) is called a Bayes estimator.

1.7.7 What About $\tilde{p}_2$?

The Laplace +2/+2 estimator $\tilde{p}_2 = (X + 2)/(n + 4)$ is also a Bayes estimator — for the **Beta(2, 2) prior** instead of the uniform prior.

The Beta(2,2) prior puts more weight near $p = 0.5$ and less weight near the extremes. If we believe p is likely to be moderate, this prior (and its corresponding Bayes estimator) makes sense.

Different priors lead to different Bayes estimators, each optimal for its own average-case criterion.

[6]:
```python
# Calculate average-case risk for each estimator
from scipy import integrate

n = 16
B = 20

# Average risk = integral of MSE over p from 0 to 1
avg_risk_mle, _ = integrate.quad(lambda p: mse_mle(p, n), 0, 1)
avg_risk_lap1, _ = integrate.quad(lambda p: mse_laplace1(p, n), 0, 1)
avg_risk_lap2, _ = integrate.quad(lambda p: mse_laplace2(p, n), 0, 1)
avg_risk_boot, _ = integrate.quad(lambda p: mse_bootstrap(p, n, B), 0, 1)

print("Average-Case Risk (Mean MSE over uniform p)")
print("=" * 50)
print(f"{'MLE':<20}: {avg_risk_mle:.6f}")
print(f"{'Laplace +1/+1':<20}: {avg_risk_lap1:.6f}  <-- Minimum!")
print(f"{'Laplace +2/+2':<20}: {avg_risk_lap2:.6f}")
print(f"{'Bootstrap':<20}: {avg_risk_boot:.6f}")
print("=" * 50)
print(f"\nLaplace +1/+1 minimizes average-case risk (it's the Bayes estimator␣
↪for uniform prior)")
```

```
Average-Case Risk (Mean MSE over uniform p)
```

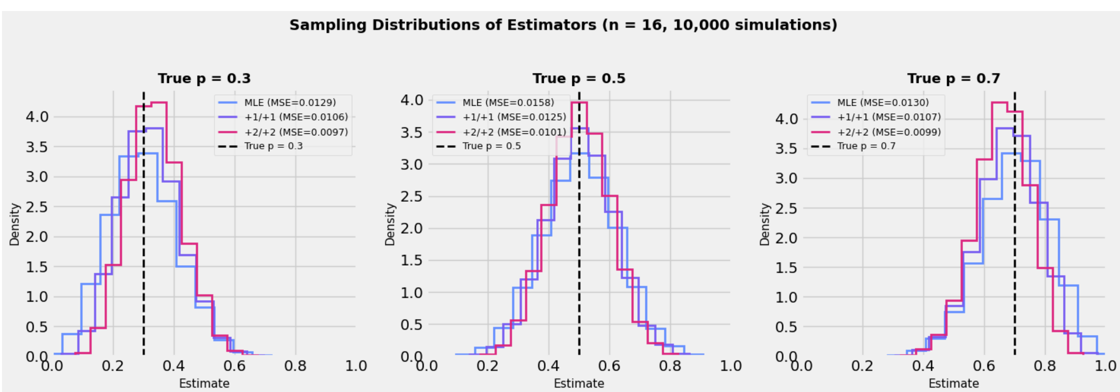
```
==================================================
MLE                   : 0.010417
Laplace +1/+1         : 0.009259  <-- Minimum!
Laplace +2/+2         : 0.010000
Bootstrap             : 0.010905
==================================================

Laplace +1/+1 minimizes average-case risk (it's the Bayes estimator for uniform
prior)
```

1.8 Simulation: Sampling Distributions of the Estimators

Let's visualize how the different estimators behave by simulating their sampling distributions for a specific true value of p.

[7]:
```python
# Simulate sampling distributions for different true values of p
np.random.seed(42)

n = 16
n_sims = 10000
true_p_values = [0.3, 0.5, 0.7]

fig, axes = plt.subplots(1, 3, figsize=(15, 5))

for ax, true_p in zip(axes, true_p_values):
    # Simulate X ~ Binomial(n, true_p)
    X = np.random.binomial(n, true_p, size=n_sims)

    # Compute estimates
    est_mle = X / n
    est_lap1 = (X + 1) / (n + 2)
    est_lap2 = (X + 2) / (n + 4)

    # Create bins centered at the actual discrete values each estimator can take
    # MLE takes values k/16 for k=0,...,16
    # Laplace +1/+1 takes values k/18 for k=1,...,17
    # Laplace +2/+2 takes values k/20 for k=2,...,18

    # For MLE: bins centered at k/16, so edges at (k-0.5)/16 and (k+0.5)/16
    mle_bins = (np.arange(n + 2) - 0.5) / n

    # For Laplace +1/+1: bins centered at k/18
    lap1_bins = (np.arange(n + 4) - 0.5) / (n + 2)

    # For Laplace +2/+2: bins centered at k/20
    lap2_bins = (np.arange(n + 6) - 0.5) / (n + 4)
```

```python
    # Compute histogram counts
    counts_mle, _ = np.histogram(est_mle, bins=mle_bins, density=True)
    counts_lap1, _ = np.histogram(est_lap1, bins=lap1_bins, density=True)
    counts_lap2, _ = np.histogram(est_lap2, bins=lap2_bins, density=True)

    # Plot using stairs
    ax.stairs(counts_mle, mle_bins, color=COLOR_MLE, linewidth=2,
              label=f'MLE (MSE={np.mean((est_mle - true_p)**2):.4f})')
    ax.stairs(counts_lap1, lap1_bins, color=COLOR_LAPLACE1, linewidth=2,
              label=f'+1/+1 (MSE={np.mean((est_lap1 - true_p)**2):.4f})')
    ax.stairs(counts_lap2, lap2_bins, color=COLOR_LAPLACE2, linewidth=2,
              label=f'+2/+2 (MSE={np.mean((est_lap2 - true_p)**2):.4f})')

    # Mark true value
    ax.axvline(true_p, color=COLOR_TRUE, linestyle='--', linewidth=2, label=f'True p = {true_p}')

    ax.set_xlabel('Estimate', fontsize=11)
    ax.set_ylabel('Density', fontsize=11)
    ax.set_title(f'True p = {true_p}', fontsize=13, fontweight='bold')
    ax.legend(fontsize=9)
    ax.set_xlim(0, 1)

plt.suptitle(f'Sampling Distributions of Estimators (n = {n}, {n_sims:,} simulations)',
             fontsize=14, fontweight='bold', y=1.02)
plt.tight_layout()
plt.show()
```



1.8.1 Observations from the Simulation

- **At** $p = 0.5$: The Laplace estimators have lower MSE than the MLE. Their shrinkage toward 0.5 helps because 0.5 is the truth!
- **At** $p = 0.3$ **and** $p = 0.7$: The MLE and Laplace estimators are more comparable. The Laplace estimators are biased toward 0.5, which slightly hurts them here.
- **All three admissible estimators** concentrate around the true value, but with different bias-variance tradeoffs.

1.9 7. Summary

1.9.1 Key Concepts

Concept	Definition
Loss function	$L(\theta, a)$ — measures how bad estimate a is when truth is θ
Risk function	$R(\theta; T) = E_\theta[L(\theta, T(X))]$ — expected loss
MSE	$E_\theta[(T(X) - \theta)^2] = \text{Bias}^2 + \text{Variance}$
Admissible	Not dominated by any other estimator
Minimax	Minimizes worst-case risk $\max_\theta R(\theta; T)$
Bayes estimator	Minimizes average risk $\int R(\theta; T)\pi(\theta)d\theta$

1.9.2 What We Learned

1. **The MLE is not always the best estimator.** It's the best *unbiased* estimator, but biased estimators can have lower MSE.
2. **Shrinkage can help.** The Laplace estimators shrink toward 0.5, trading bias for reduced variance. This helps when the true p is near 0.5.
3. **Admissibility is a minimal requirement.** The bootstrap estimator is inadmissible — strictly dominated by the MLE. But many admissible estimators exist.
4. **Bootstrap doesn't reduce uncertainty.** Averaging bootstrap estimates only adds variance. Bootstrap is useful for *quantifying* uncertainty, not *reducing* it.
5. **No uniformly best estimator exists.** Different estimators win for different values of p.
6. **Optimality criteria help us choose:**
   - **Minimax**: Laplace +2/+2 minimizes worst-case risk
   - **Bayes (uniform prior)**: Laplace +1/+1 minimizes average-case risk
7. **The Bayes estimator is the posterior mean.** This is our first glimpse of Bayesian statistics — arrived at through a purely frequentist argument!

1.9.3 Next Time

In Lecture 7, we'll develop the **Bayesian perspective** more fully: - Treat θ as a random variable with a **prior distribution** - Update to a **posterior distribution** after seeing data - Understand why the **likelihood** is all that matters (given the prior) - Explore the asymptotic behavior of the posterior

1.9.4 Worksheet 3 Preview

Problem 5 explores **scale-equivariant estimation** and proves that unbiased equivariant estimators are always inadmissible — you can always improve by shrinking! This complements today's theme: unbiasedness is not always a virtue.