Lecture 5: Point Estimation

Method of Moments · Maximum Likelihood · Why MLE Works

Previously, on Lecture 4. . .

Likelihood: $L(\theta) = \prod f(X_i \mid \theta)$. How well does θ explain the data?

Score: $s(\theta) = \frac{\partial}{\partial\theta} \log f(X \mid \theta)$. How sensitive is the model to θ?

Fisher information: $I(\theta) = \mathrm{Var}[s(\theta)]$. How much info does one observation carry?

Cramér–Rao: $\mathrm{Var}(\hat{\theta}) \geq 1/(nI(\theta))$. The precision floor for unbiased estimators.

Admissibility & Stein: Biased estimators (shrinkage) can beat unbiased ones in $d \geq 3$.

Today: We know how to **judge** estimators. Now: how to **construct** them.

Two systematic recipes: **Method of Moments** and **Maximum Likelihood**.

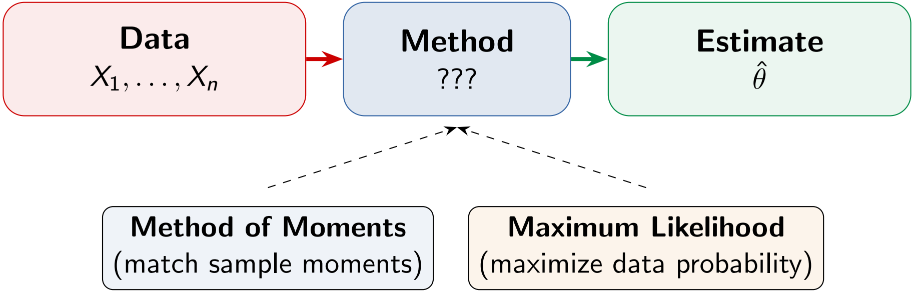
The Estimation Problem

A factory produces lightbulbs. You test 50 and find a mean lifetime of 1,200 hours.

What can you say about the **true** mean lifetime?

In Lectures 3–4 we learned how to **judge** estimators (bias, variance, MSE, efficiency).
Today: how to **construct** them systematically.

From Data to Parameters



Method of Moments (MoM)

Idea: Set population moments equal to sample moments, then solve for the parameters.

$$\begin{aligned} \mathbb{E}[X] &= g_1(\theta) \\ \mathbb{E}[X^2] &= g_2(\theta) \\ &\vdots \end{aligned} \quad \xrightarrow[\text{replace with}]{} \quad \begin{aligned} \bar{X} &= g_1(\hat{\theta}) \\ \tfrac{1}{n}\sum X_i^2 &= g_2(\hat{\theta}) \\ &\vdots \end{aligned}$$

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Pros:

- Simple, quick to compute
- No distributional assumption needed for computation

Cons:

- Can give impossible values (e.g., $\hat{\sigma}^2 < 0$)
- Generally less efficient than MLE
- Awkward with many parameters

MoM Example: Normal Distribution

Model: $X_1, \ldots, X_n \sim \mathcal{N}(\mu, \sigma^2)$. Two unknowns, need two equations.

1st moment: $\mathbb{E}[X] = \mu \quad \Rightarrow \quad \hat{\mu}_{\text{MoM}} = \bar{X}$

2nd moment: $\mathbb{E}[X^2] = \mu^2 + \sigma^2 \quad \Rightarrow \quad \hat{\sigma}^2_{\text{MoM}} = \frac{1}{n}\sum X_i^2 - \bar{X}^2 = \frac{1}{n}\sum (X_i - \bar{X})^2$

(Note: this divides by n, not $n-1$ — **biased!** Recall Bessel's correction from Lecture 3.)

MoM Example: Gamma Distribution

Model: $X_1, \ldots, X_n \sim \text{Gamma}(\alpha, \beta)$ (shape α, rate β). Two unknowns.

Population moments:

$$\mathbb{E}[X] = \alpha/\beta$$
$$\text{Var}(X) = \alpha/\beta^2$$

Set equal to sample moments and solve:

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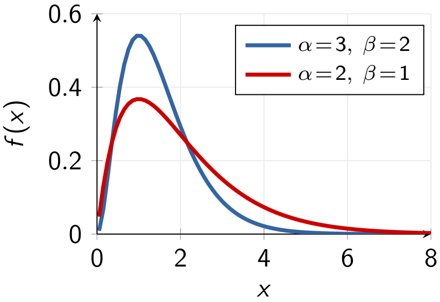
Set equal to sample moments and solve:

$$\boxed{\hat{\beta}_{\text{MoM}} = \frac{\bar{X}}{S^2}, \qquad \hat{\alpha}_{\text{MoM}} = \frac{\bar{X}^2}{S^2}}$$

Simple algebra — done! ✓

MLE for Gamma requires the digamma function $\psi(\alpha)$ — **no closed form**, numerical optimization only.



Gamma models waiting times, rainfall, income, insurance claims.

Lesson: MoM shines when MLE has no closed form. Quick, easy, often a good starting point.

When MoM Goes Wrong

MoM can give **impossible** parameter values because it doesn't "know" the constraints.

Example: Fit a Uniform$(0, \theta)$ distribution using MoM.

Population mean: $\mathbb{E}[X] = \theta/2 \quad \Rightarrow \quad \hat{\theta}_{\text{MoM}} = 2\bar{X}$

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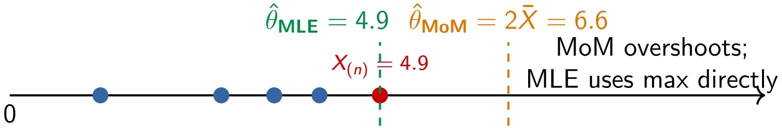
Problem: We need $\hat{\theta} \geq \max(X_i)$, but MoM doesn't enforce this!



MoM doesn't use the data efficiently here — it ignores the maximum, which is the sufficient statistic.

The Likelihood Function (Recap from Lecture 4)

Given the data I observed, how plausible is each parameter value?

$L(\theta) \;=\; \prod_{i=1}^{n} f(X_i \;\mid\; \theta) \qquad \ell(\theta) \;=\; \sum_{i=1}^{n} \log f(X_i \;\mid\; \theta)$

Data is fixed, θ varies. Log turns the product into a sum (same maximizer).

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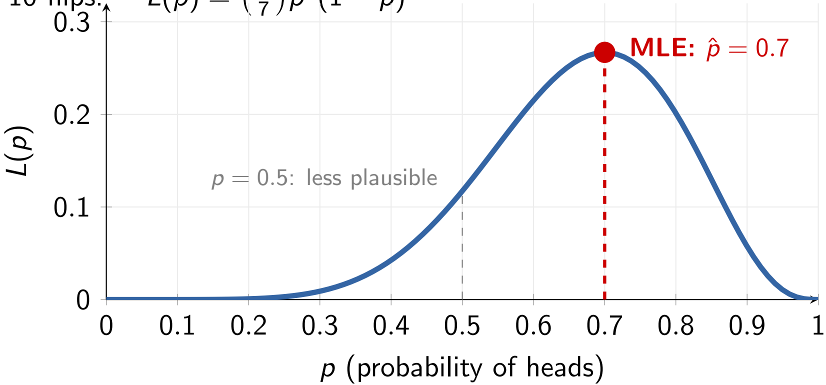
From Lecture 4, we already know:

- The **score** $s(\theta) = \ell'(\theta)$ measures sensitivity to θ; $\mathbb{E}[s] = 0$
- **Fisher information** $I(\theta) = \mathrm{Var}[s] = -\mathbb{E}[\ell'']$ measures the curvature
- **Cramér–Rao:** no unbiased estimator can have Var $< 1/(nI(\theta))$

Now: how to **use** the likelihood to actually **construct** estimators.

Likelihood: Coin Flip Example

Data: 7 heads in 10 flips. $L(p) = \binom{10}{7} p^7 (1-p)^3$



The MLE Idea: What Would the Data Choose?

Imagine you could ask the data: "Which parameter value explains you best?"

The **Maximum Likelihood Estimator** picks the θ that makes the observed data **most probable**:

$$\hat{\theta}_{\mathsf{MLE}} = \arg\max_\theta L(\theta) = \arg\max_\theta \ell(\theta)$$

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Intuition: If you flip a coin 10 times and get 7 heads...

- Is $p = 0.5$ plausible? Somewhat.
- Is $p = 0.7$ plausible? Very — it predicts exactly what you saw.
- Is $p = 0.99$ plausible? Not really — you'd expect more heads.

MLE picks $\hat{p} = 0.7$ because it maximizes the likelihood $L(p) = \binom{10}{7} p^7 (1-p)^3$.

At the MLE: $s(\hat{\theta}) = 0$ (score equals zero — first-order condition from Lecture 4).

MLE Recipe: Step by Step

In practice, finding the MLE is a calculus exercise:

Write $\ell(\theta)$ → Differentiate → Set $\frac{d\ell}{d\theta} = 0$ → Solve for $\hat{\theta}$ → Check $\ell'' < 0$

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When it's easy (closed form):

- Exponential families
- Normal, Bernoulli, Poisson, Exp
- Solve $s(\hat{\theta}) = 0$ by hand

When it's hard (numerical):

- Mixture models
- Logistic regression
- Use gradient ascent, Newton's method, or EM algorithm

Let's work through four closed-form examples.

MLE: Bernoulli (Coin Fairness)

Model: $X_i \sim \text{Bernoulli}(p), \quad$ observe k successes in n trials.

$$\ell(p) = k \log p + (n-k) \log(1-p)$$

$$\frac{\partial \ell}{\partial p} = \frac{k}{p} - \frac{n-k}{1-p} = 0$$

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$$\boxed{\hat{p}_{\text{MLE}} = \frac{k}{n} = \bar{X}}$$

The sample proportion — exactly what you'd guess intuitively.

MLE for Normal: Full Derivation

Model: $X_1, \ldots, X_n \overset{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$, both μ and σ^2 unknown.

Step 1. Write the likelihood (product of n Gaussian densities):

$$L(\mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(X_i - \mu)^2}{2\sigma^2}\right)$$

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Step 4. Set $\dfrac{\partial \ell}{\partial (\sigma^2)} = 0$: $\quad -\dfrac{n}{2\sigma^2} + \dfrac{\sum (X_i - \bar{X})^2}{2\sigma^4} = 0$

$$\Longrightarrow \quad \boxed{\hat{\sigma}^2_{\text{MLE}} = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^2}$$

How Good Is the Normal MLE?

For $\hat{\mu} = \bar{X}$:

- Bias $= 0$ (unbiased)
- Var $= \sigma^2/n$
- MSE $= \sigma^2/n$

✓ $=$ CR bound — **efficient!**

For $\hat{\sigma}^2 = \frac{1}{n}\sum(X_i - \bar{X})^2$:

- Bias $= -\sigma^2/n$ (biased!)
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- MSE $= (2n-1)\sigma^4/n^2$

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Compare with Bessel's $S^2 = \frac{1}{n-1}\sum(X_i - \bar{X})^2$ (unbiased):

	$\hat{\sigma}^2_{\text{MLE}}$ (divide by n)	S^2 (divide by $n-1$)
Bias	$-\sigma^2/n$	0
MSE	$(2n-1)\sigma^4/n^2$	$2\sigma^4/(n-1)$

$\text{MSE}(\hat{\sigma}^2_{\text{MLE}}) < \text{MSE}(S^2)$ **always!** The biased MLE wins on MSE (Lecture 3 tradeoff).

From MLE to Machine Learning

In ML, we model: $y_i = f(\mathbf{x}_i;\, \mathbf{w}) + \varepsilon_i, \quad \varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$

So $y_i \mid \mathbf{x}_i \sim \mathcal{N}\big(f(\mathbf{x}_i; \mathbf{w}),\ \sigma^2\big)$. The log-likelihood of $\mathbf{w}$:

$$\ell(\mathbf{w}) = \underbrace{-\tfrac{n}{2}\log(2\pi\sigma^2)}_{\text{const w.r.t. } \mathbf{w}} - \frac{1}{2\sigma^2}\sum_{i=1}^{n}\big(y_i - f(\mathbf{x}_i; \mathbf{w})\big)^2$$

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$$\max_{\mathbf{w}}\ \ell(\mathbf{w}) \quad \Longleftrightarrow \quad \min_{\mathbf{w}} \sum_{i=1}^{n}\big(y_i - f(\mathbf{x}_i; \mathbf{w})\big)^2 \quad = \quad \textbf{MSE loss!}$$

Gaussian noise + MLE = Least Squares

The MSE loss in machine learning is not arbitrary —
it is exactly **maximum likelihood under Gaussian noise**.

Linear regression, neural nets with MSE loss, OLS — all are doing MLE.

Not just Gaussian — every noise model gives a different loss function...

MLE and Cross-Entropy

Now: $y_i \in \{0, 1\}$ (spam/not spam, click/no click, disease/healthy).

Model: $P(y_i = 1 \mid \mathbf{x}_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$ where $\sigma(z) = \frac{1}{1+e^{-z}}$ (logistic function)

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The log-likelihood:

$$\ell(\mathbf{w}) = \sum_{i=1}^{n} \left[y_i \log \hat{p}_i + (1-y_i) \log(1-\hat{p}_i) \right] \qquad \hat{p}_i = \sigma(\mathbf{w}^\top \mathbf{x}_i)$$

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$$\max_{\mathbf{w}} \ \ell(\mathbf{w}) \quad \Longleftrightarrow \quad \min_{\mathbf{w}} \ \underbrace{-\sum \left[\, y_i \log \hat{p}_i + (1-y_i) \log(1-\hat{p}_i) \,\right]}_{\textbf{binary cross-entropy loss}}$$

Bernoulli outcome + MLE = Cross-Entropy Loss

Logistic regression, neural nets with sigmoid output — all doing MLE.

Gaussian → MSE — **Bernoulli** → Cross-Entropy — **Laplace** → MAE

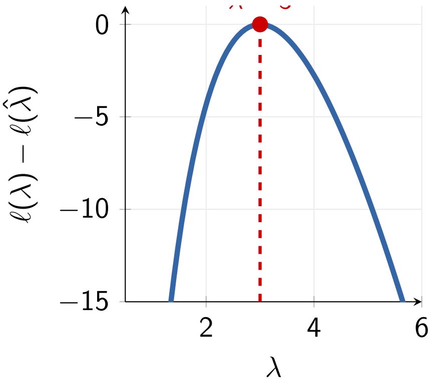
MLE: Poisson (Rare Events)

Model: $X_i \sim \text{Pois}(\lambda)$

(goals/match, earthquakes/yr, typos/pg)

$\ell(\lambda) = (\sum X_i) \log \lambda - n\lambda + \text{c}$

$\frac{\partial \ell}{\partial \lambda} = \frac{\sum X_i}{\lambda} - n = 0$



Example: $n = 20$, $\sum X_i = 60$

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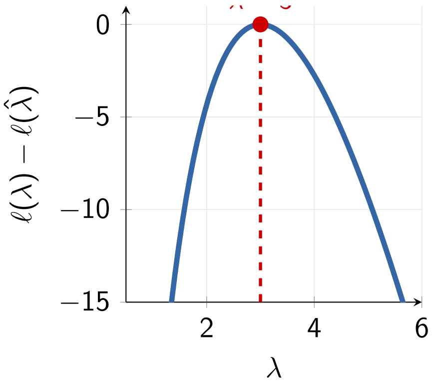
$\frac{\partial \ell}{\partial \lambda} = \frac{\sum X_i}{\lambda} - n = 0$

$$\boxed{\hat{\lambda}_{\text{MLE}} = \bar{X}}$$

Sample mean estimates the *rate*.



Example: $n = 20$, $\sum X_i = 60$

MLE: Exponential (Waiting Times)

Model: $X_i \sim \text{Exp}(\lambda)$ (time between arrivals, device lifetimes)

$f(x \mid \lambda) = \lambda e^{-\lambda x}$ for $x \geq 0$

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

$\frac{\partial \ell}{\partial \lambda} = \frac{n}{\lambda} - \sum X_i = 0$

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$$\boxed{\hat{\lambda}_{\text{MLE}} = \frac{1}{\bar{X}}}$$

The reciprocal of the sample mean — intuitive since $\mathbb{E}[X] = 1/\lambda$.

MLE: Summary of Examples

Distribution	Parameter	MLE	Real-world use
Bernoulli(p)	p	$\bar{X}$	Coin fairness, conversion rates
Normal(μ, σ^2)	μ, σ^2	$\bar{X},\ \frac{1}{n}\sum(X_i - \bar{X})^2$	Measurement error
Poisson(λ)	λ	$\bar{X}$	Count data, rare events
Exponential(λ)	λ	$1/\bar{X}$	Waiting times, lifetimes

Notice: for exponential families, MLE often equals MoM! We'll see why shortly.

MoM vs MLE: When to Use Which?

	Method of Moments	**Maximum Likelihood**
Idea	Match sample moments	Maximize data probability
Computation	Usually algebraic	May need optimization
Efficiency	Generally less efficient	Asymptotically optimal
Impossible values?	Can happen ($\hat{\sigma}^2 < 0$)	Respects constraints
Invariance	No	Yes ($g(\hat{\theta})$ is MLE of $g(\theta)$)
Exp. family	Often same as MLE	Always uses suff. stat

Rule of thumb: Use MLE when you can (it's optimal).
Use MoM as a quick starting point, or when MLE has no closed form.

Invariance Property

If $\hat{\theta}_{\text{MLE}}$ is the MLE of θ, then for any function g:

$$\widehat{g(\theta)}_{\text{MLE}} \quad = \quad g(\hat{\theta}_{\text{MLE}})$$

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Example:

- MLE of λ for Exp is $\hat{\lambda} = 1/\bar{X}$
- Want MLE of mean $\mu = 1/\lambda$?
- Apply $g(\lambda) = 1/\lambda$: $\hat{\mu} = \bar{X}$ ✓

This doesn't hold for MoM or other estimators in general.

$$\begin{tikzcd}
\theta \arrow[r, "g"] \arrow[d, "\text{MLE}"'] \arrow[dr, phantom, "="] & g(\theta) \arrow[d, "\text{MLE}"] \\
\hat{\theta}_{\text{MLE}} \arrow[r, "g"'] & g(\hat{\theta}_{\text{MLE}})
\end{tikzcd}$$

Identifiability

Can we even hope to recover θ?

A model is **identifiable** if different parameter values give different distributions:

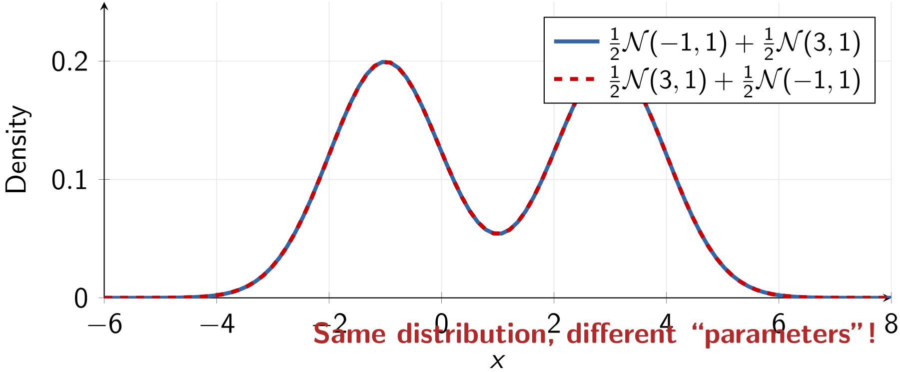
$$\theta_1 \neq \theta_2 \quad \Rightarrow \quad f(\cdot \mid \theta_1) \neq f(\cdot \mid \theta_2)$$

When it fails:

- **Mixture models:** swapping component labels gives the same distribution
- **Overparameterized models:** more parameters than the data can distinguish
- **Symmetric likelihoods:** multiple maxima, MLE is not unique

If the model isn't identifiable, no amount of data will help.

Visualizing Non-Identifiability



Same distribution, different "parameters"!

MLE and Sufficient Statistics

In Lecture 3 we learned: a **sufficient statistic** $T(\mathbf{X})$ captures everything about θ.

Key fact: The MLE depends on the data **only through** the sufficient statistic.
If $T(\mathbf{X})$ is sufficient for θ, then the MLE $\hat{\theta}$ is a function of T.

Check our examples:

Model	**Suff. stat T**	**MLE**	**Function of T?**
Bern(p)	$\sum X_i$	$\bar{X} = T/n$	✓
$N(\mu, \sigma_0^2)$	$\sum X_i$	$\bar{X} = T/n$	✓
Pois(λ)	$\sum X_i$	$\bar{X} = T/n$	✓
Exp(λ)	$\sum X_i$	$1/\bar{X} = n/T$	✓

No coincidence — MLE **always** uses sufficient statistics. No information is wasted.

MLE in Exponential Families

Recall the **exponential family** form from Lecture 3: $f(x \mid \theta) = h(x) \exp\big(\eta(\theta)\, T(x) - A(\theta)\big)$

For n i.i.d. observations, the log-likelihood is:

$$\ell(\theta) = \eta(\theta) \sum_{i=1}^{n} T(X_i) - nA(\theta) + \text{const}$$

Setting the derivative to zero:

$$\eta'(\theta) \sum_{i=1}^{n} T(X_i) = nA'(\theta)$$

For natural exponential families ($\eta = \theta$):

$A'(\hat{\theta}_{\text{MLE}}) = \frac{1}{n} \sum_{i=1}^{n} T(X_i)$ (match population mean to sample mean)

The MLE is **always** a function of the sufficient statistic $\sum T(X_i)$, and it **equals the MoM estimator** in natural form!

Why MLE Works: The Big Theoretical Guarantees

Under regularity conditions (Lecture 4), MLE has remarkable properties:

1. Consistent: $\hat{\theta}_{\text{MLE}} \xrightarrow{P} \theta_0$ as $n \to \infty$ (gets the right answer eventually)

2. Asymptotically Normal: $\sqrt{n}(\hat{\theta}_{\text{MLE}} - \theta_0) \xrightarrow{d} N\left(0, \frac{1}{I(\theta_0)}\right)$

3. Asymptotically Efficient: achieves the **Cramér–Rao bound** as $n \to \infty$

4. Invariant: MLE of $g(\theta)$ is $g(\hat{\theta}_{\text{MLE}})$ for any function g

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1. Consistent: $\hat{\theta}_{\text{MLE}} \xrightarrow{P} \theta_0$ as $n \to \infty$ (gets the right answer eventually)

2. Asymptotically Normal: $\sqrt{n}(\hat{\theta}_{\text{MLE}} - \theta_0) \xrightarrow{d} N\left(0, \frac{1}{I(\theta_0)}\right)$

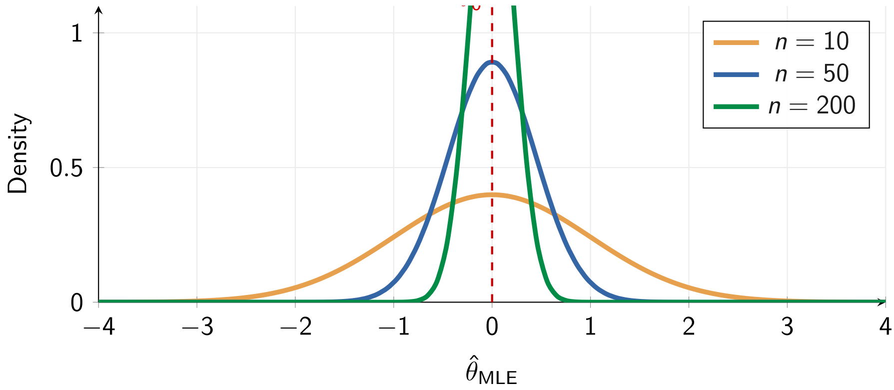
3. Asymptotically Efficient: achieves the **Cramér–Rao bound** as $n \to \infty$

4. Invariant: MLE of $g(\theta)$ is $g(\hat{\theta}_{\text{MLE}})$ for any function g

Translation: With enough data, MLE is approximately unbiased, approximately normal, and **no other estimator can do better**.
This is why MLE is the default method in statistics and machine learning.

Asymptotic Normality: Seeing It

As n grows, the sampling distribution of the MLE converges to a Normal centered at the truth:



Variance shrinks as $\frac{1}{n\,I(\theta_0)}$: more data $\Rightarrow$ tighter bell $\Rightarrow$ more precise estimate.
With $n = 200$ observations, MLE is practically pinpointed at the truth.

From MLE to Standard Errors

Asymptotic normality says: $\hat{\theta}_{\text{MLE}} \dot\sim N\left(\theta_0,\ \frac{1}{n\, I(\theta_0)}\right)$

Problem: We don't know θ_0 — that's what we're estimating!

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Solution: Plug in $\hat{\theta}$ to get the **standard error**:

$$\boxed{\text{SE}(\hat{\theta}) = \frac{1}{\sqrt{n\,I(\hat{\theta})}}} \qquad \text{or equivalently:} \qquad \boxed{\text{SE}(\hat{\theta}) = \frac{1}{\sqrt{J_n(\hat{\theta})}}}$$

where $J_n(\hat{\theta}) = -\ell_n''(\hat{\theta})$ is the **observed** Fisher information (the actual curvature at the MLE).

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Example: Bernoulli, $\hat{p} = 0.3$, $n = 100$.

$$I(p) = \frac{1}{p(1-p)} \;\Rightarrow\; \text{SE} = \sqrt{\frac{\hat{p}(1-\hat{p})}{n}} = \sqrt{\frac{0.3\cdot 0.7}{100}} = 0.046$$

This is how statistical software reports standard errors.

Every time you see $\hat{\theta} \pm \text{SE}$ in R, Python, or a paper,
it's using Fisher information under the hood. More in Lecture 9.

MLE Achieves the Cramér–Rao Bound

From Lecture 4, the **CR bound**: $\mathrm{Var}(\hat{\theta}) \geq \frac{1}{n\,I(\theta)}$ for unbiased estimators.

Does MLE hit this bound?

Model	**MLE**	$\mathrm{Var}(\hat{\theta}_{\mathrm{MLE}})$	**CR bound**	**Efficient?**
Bern(p)	$\bar{X}$	$\frac{p(1-p)}{n}$	$\frac{p(1-p)}{n}$	**Yes**
$N(\mu, \sigma_0^2)$	$\bar{X}$	$\frac{\sigma_0^2}{n}$	$\frac{\sigma_0^2}{n}$	**Yes**
Pois(λ)	$\bar{X}$	$\frac{\lambda}{n}$	$\frac{\lambda}{n}$	**Yes**

For **exponential families**, the MLE of the natural parameter is efficient (hits the CR bound exactly). For other models, MLE is **asymptotically** efficient — it approaches the bound as $n \to \infty$.

When MLE Goes Wrong

MLE has great asymptotic theory, but several things can go wrong:

- **Small samples:** MLE is asymptotic — can be poor for small n.
  Example: 0 heads in 3 flips $\Rightarrow \hat{p}_{\text{MLE}} = 0$. Surely too extreme!

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  n groups with 2 obs each, own mean μ_i: MLE of σ^2 converges to $\sigma^2/2$!

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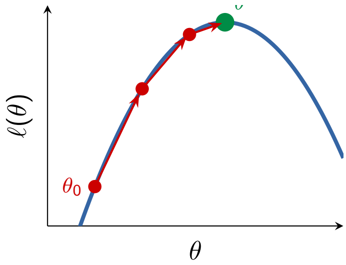
  n groups with 2 obs each, own mean μ_i: MLE of σ^2 converges to $\sigma^2/2$!
- **Overfitting:** Flexible models memorize noise.
  Degree-20 polynomial through 25 points $\Rightarrow$ wild oscillations.

Common cure: Add a prior $\rightarrow$ MAP estimation (Lecture 6).
Prior = regularization = controlled bias toward simpler models.

When There's No Closed Form

Many models (logistic regression, mixtures, neural nets) require **numerical** optimization.



Gradient ascent:

$$\theta_{t+1} = \theta_t + \alpha \cdot \ell'(\theta_t)$$

Follow the slope uphill. The default in deep learning.

Newton–Raphson:

$$\theta_{t+1} = \theta_t - \frac{\ell'(\theta_t)}{\ell''(\theta_t)}$$

Uses curvature ($\ell'' \leftrightarrow$ Fisher info) for smarter steps.

In Python: `scipy.optimize.minimize`

For latent variables: **EM algorithm** (Lecture 7)

Practical: Implement MLE

1. Implement MLE for a Gaussian **from scratch**:
   - Write the log-likelihood function
   - Optimize numerically (`scipy.optimize`) and compare with closed form
2. Compare $\hat{\sigma}^2_{\text{MLE}}$ (divides by n) with S^2 (divides by $n-1$). Verify the bias from Lecture 3 empirically with simulation.
3. Fit a Poisson to real count data. Check: is the MLE efficient? Compute the CR bound and compare with the observed variance.
4. Plot the log-likelihood surface — observe the peak at the MLE and relate its **curvature** to Fisher information.

Homework

1. Derive the MLE for Geometric(p): $f(x \mid p) = (1-p)^{x-1}p, \;\; x = 1, 2, \dots$
   Is this MLE unbiased? Is it efficient (check against the CR bound)?
2. For $X_1, \dots, X_n \sim N(\mu, \sigma^2)$, show that $\hat{\sigma}^2_{\text{MLE}} = \frac{1}{n}\sum(X_i - \bar{X})^2$
   equals the MoM estimator. Why is this not a coincidence? (Hint: exponential family.)
3. Show that the MLE for Uniform$(0, \theta)$ is $\hat{\theta} = X_{(n)} = \max(X_1, \dots, X_n)$.
   Is this unbiased? Is it consistent? (Note: this is **not** an exponential family!)
4. Simulate $n = 50$ samples from Poisson$(\lambda = 3)$ and compute the MLE.
   Repeat 10,000 times. Verify: (a) $\hat{\lambda}$ is approximately unbiased, (b) Var$(\hat{\lambda}) \approx \lambda/n$.

Questions?

Next: Lecture 6 — MAP estimation, priors, and the Bayesian perspective