Maximum Likelihood Approaches

November 7, 2020

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Acknowledgements

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Maximum Likelihood

Parametric Models

Models

A **model** $\mathcal{P}$ is a set of probability distributions. We index each distribution with a parameter value $\theta \in \Theta$; we can then write the model as

$$\mathcal{P} = \{P_\theta \mid \theta \in \Theta\}$$

The set Θ is called the **parameter space** of the model.

Parametric model

The model is called **parametric** if the number of parameters (i.e. the vector θ) is (1) finite and (2) independent of the number of data points. Intuitively, the complexity of a parametric model does not increase with sample size.

Density representation

For parametric models, we can assume that $\Theta \subset \mathbb{R}^d$ for some fixed dimension d. We usually represent each P_θ via a density function $p(x \mid \theta)$.

Maximum Likelihood Estimation

Setting

- Given: Data $x_1, \ldots, x_n$, parametric model $\mathcal{P} = \{P_\theta \mid \theta \in \Theta\}$
- Objective: Find the distribution in $\mathcal{P}$ which best explain the data. That means we have to choose a "best" parameter value $\widehat{\theta}$.

Maximum Likelihood approach

Maximim Likelihood assumes that the data is best explained by the distribution in $\mathcal{P}$ under which it has the highest probability (or highest density value).

Hence, the **maximum likelihood estimator** is defined as

$$\widehat{\theta}_{\mathrm{ML}} := \operatorname*{argmax}_{\theta \in \Theta} p(x_1, \ldots, x_n \mid \theta)$$

the parameter which maximizes the joint density of the data.

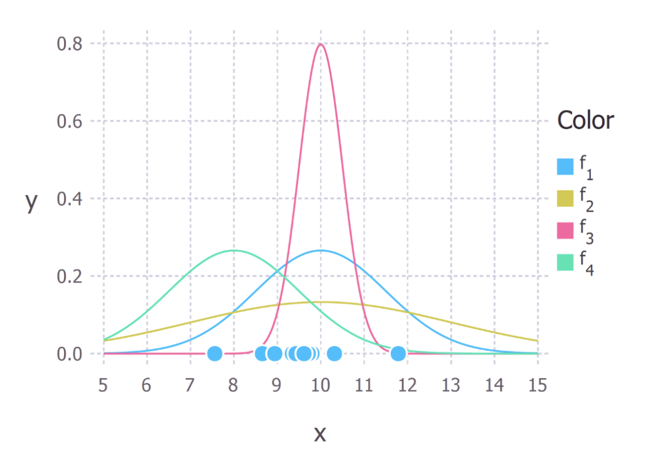
The i.i.d. assumption

The standard assumption of ML methods is that the data is **independent and identically distributed (i.i.d.)**, that is, generated by independently sampling repeatedly from the same distribution $\mathcal{P}$.

If the density of $\mathcal{P}$ is $p(x \mid \theta)$, that means the joint density decomposes as

$$p(x_1, ..., x_n) = \prod_{i=1}^{n} p(x_1 \mid \theta)$$

Illustration



Ten data points and four possible Gaussians from which they were drawn:
$f_1 \sim \mathcal{N}(10, 2.25)$, $f_2 \sim \mathcal{N}(10, 9)$, $f_3 \sim \mathcal{N}(10, 0.25)$, $f_4 \sim \mathcal{N}(8, 2.25)$.

Image Credit: Jonny Brooks-Bartlett

Maximum Likelihood in practice

Maximum Likelihood equation

In practice, the criterion for a maximum likelihood estimator (under the i.i.d assumption) is

$$\nabla_\theta \left(\prod_{i=1}^{n} p(x_i \mid \theta) \right) = 0$$

We use the “logarithm trick” to avoid a huge product rule computation.

Recall: Logarithms turn products into sums

$$\log\left(\prod_i f_i\right) = \sum_i \log(f_i)$$

Logarithms and maxima

The logarithm is monotonically increasing on $\mathbb{R}_+$.
Consequence: Application of log does not change the *location* of a maximum or minimum:

$$\max_y \log(g(y)) \neq \max_y g(y) \qquad \text{The } \textit{value} \text{ changes.}$$

$$\operatorname*{argmax}_y \log(g(y)) = \operatorname*{argmax}_y g(y) \qquad \text{The } \textit{location} \text{ does not change.}$$

Maximum Likelihood in practice

Likelihood and logarithm trick

$$\widehat{\theta}_{\mathrm{ML}} = \operatorname*{argmax}_{\theta} \prod_{i=1}^{n} p(x_i|\theta) = \operatorname*{argmax}_{\theta} \log\left(\prod_{i=1}^{n} p(x_i|\theta)\right) = \operatorname*{argmax}_{\theta} \sum_{i=1}^{n} \log p(x_i|\theta)$$

Maximum Likelihood in practice (revisited)

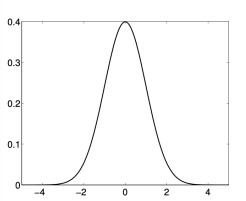
$$0 = \sum_{i=1}^{n} \nabla_{\theta} \log p(x_i|\theta) = \sum_{i=1}^{n} \frac{\nabla_{\theta} p(x_i|\theta)}{p(x_i|\theta)}$$

Whether or not we can solve this analytically depends on the choice of model!

Maximum Likelihood Example

Gaussian density in one dimension

$$g(x;\mu,\sigma) := \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



- μ = expected value of x, σ^2 = variance, σ = standard deviation
- The quotient $\frac{x-\mu}{\sigma}$ measures deviation of x from its expected value in units of σ (i.e., σ defines the length scale).

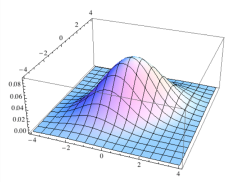
Gaussian density in d dimensions

The quadratic function

$$-\frac{(x-\mu)^2}{2\sigma^2} = -\frac{1}{2}(x-\mu)(\sigma^1)^{-1}(x-\mu)$$

is replaced by a quadratic form:

$$g(\boldsymbol{x};\boldsymbol{\mu},\Sigma) := \frac{1}{\sqrt{2\pi|\Sigma|}}\exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$$



Example: Gaussian Mean MLE

Model: Multivariate Gausians

The model $\mathcal{P}$ is the set of all Gaussian densities on $\mathbb{R}^d$ with *fixed* covariance matrix Σ

$$\mathcal{P} = \{g(\cdot \mid \mu, \Sigma) \mid \mu \in \mathbb{R}^d\}$$

where g is the Gaussian density function. The parameter space is $\Theta = \mathbb{R}^d$.

MLE equation

We have to solve the maximum likelihood equation

$$\sum_{i=1}^{n} \nabla_\mu \log g(x_i \mid \mu, \Sigma) = 0$$

for μ.

Example: Gaussian Mean MLE

$$
\begin{aligned}
0 &= \sum_{i=1}^{n} \nabla_\mu \log \left[\frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right) \right] \\
&= \sum_{i=1}^{n} \nabla_\mu \left[\log \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \right] + \nabla_\mu \left[\log \left(\exp\left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right) \right) \right] \\
&= \sum_{i=1}^{n} \nabla_\mu \left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right) = -\sum_{i=1}^{n} \Sigma^{-1} (x_i - \boldsymbol{\mu})
\end{aligned}
$$

Multiplication by $(-\Sigma)$ gives

$$
0 = \sum_{i=1}^{n} (x_i - \boldsymbol{\mu}) \implies \boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i
$$

Conclusion

The maximum likelihood estimator of the Gaussian expectation parameter for fixed covariance is

$$
\widehat{\boldsymbol{\mu}}_{\mathrm{ML}} := \frac{1}{n} \sum_{i=1}^{n} x_i
$$

Example: Gaussian with Unknown Mean, Covariance

Model: Multivariate Gaussians

The model $\mathcal{P}$ is now

$$\mathcal{P} = \{g(\cdot \mid \mu, \Sigma) \mid \mu \in \mathbb{R}^d, \Sigma \in \Delta_d\}$$

where Δ_d is the set of postive definite $d \times d$-matrices. The parameter space is $\Theta = \mathbb{R}^d \times \Delta_d$.

ML approach

Since we have just seen that the ML estimator of μ does not depend on Σ, we can compute $\widehat{\boldsymbol{\mu}}_{\mathrm{ML}}$ first. We then estimate Σ using the criterion

$$\sum_{i=1}^{n} \nabla_\Sigma \log g(x_i \mid \widehat{\boldsymbol{\mu}}_{\mathrm{ML}}, \Sigma) = 0$$

for μ.

Solution

The ML estimator of Σ is

$$\widehat{\Sigma}_{\mathrm{ML}} = \frac{1}{n} \sum^{n} (x_i - \widehat{\mu}_{\mathrm{ML}})(x_i - \widehat{\mu}_{\mathrm{ML}})^T$$

Anomaly Detection

Anomaly Detection with Multivariate Gaussians

Given a fitted Gaussian model, how can we assess the anomalousness of test data?

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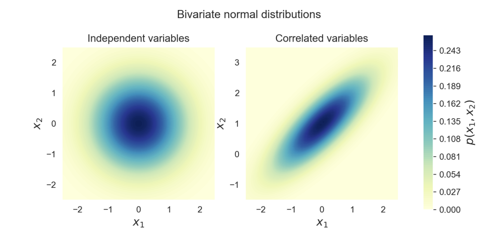

Image Credit: Peter Roelants

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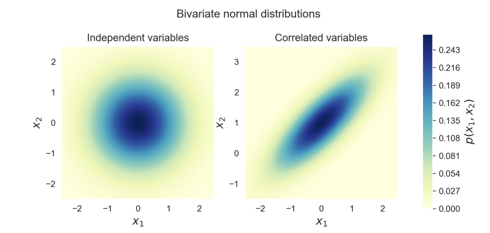


Image Credit: Peter Roelants

Mahalanobis Distance

For a Gaussian random variable $X \sim N(\boldsymbol{\mu}, \Sigma)$, the quadratic form (or *squared Mahalanobis distance*) has known distribution

$$\Delta^2 = (\boldsymbol{X} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{X} - \boldsymbol{\mu}) \sim \chi^2(d)$$

This can be used to assess the anomalousness of test data.

Optimization

Optimization problem

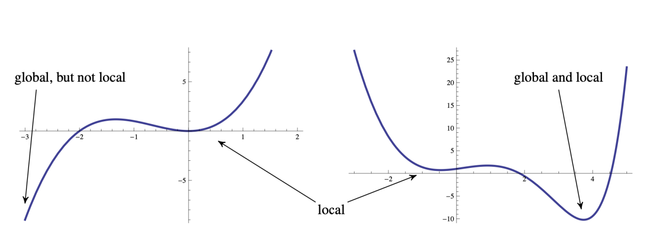
An *optimization problem* for a given function $f : \mathbb{R}^d \to \mathbb{R}$ is a problem of the form

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

which we read as "find $\boldsymbol{x}_0 = \arg\min_{\boldsymbol{x}} f(\boldsymbol{x})$"'.

Note that finding the maximum likelihood requires minimizing the cost function that is the negative log likelihood.

Local and global modes



Local and global minima

A minimum of a function f at x is called

- **Global** if f assumes no smaller value on its domain.
- **Local** if there is some open neighborhood U of x such that $f(x)$ is a global minimum of f restricted to U.

Image Credit: Peter Orbanz

Analytic criteria for local minima

Recall that $\boldsymbol{x}$ is a local minimum of f if

$$f'(\boldsymbol{x}) = 0 \quad \text{and} \quad f''(\boldsymbol{x}) > 0$$

In $\mathbb{R}^d$,

$$\nabla f(\boldsymbol{x}) = 0 \text{ and } H_f(\boldsymbol{x}) = \left(\frac{\delta f}{\delta x_i \delta x_j}(\boldsymbol{x})\right)_{i,j=1,\dots,n} \text{ positive definite}$$

The $d \times d$-matrix $H_f(\boldsymbol{x})$ is called the **Hessian matrix** of f at $\boldsymbol{x}$.

The MLE and Global Maximizers

You may have noticed that the maximum likelihood equation is only tracking a *local* maximality criterion. In fact, it also ignored the second-order condition. What gives?

- Many well-known distributions[1] have strictly concave likelihoods, in which case the MLE equation is sufficient to verify a global maximum.
- For many other distributions, it can be hard to find the global maximizer of the likelihood. Thus a local maximizer is often used and is called an MLE. The local optimizer is typically found by an optimization procedure, from which the second order condition generally follows.

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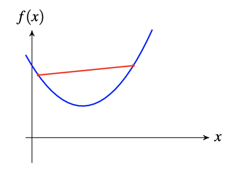
[1] In particular, those in the exponential family. We will cover this in the next slide deck.

Convex Functions

Definition

A function f is **convex** if every line segment between function values lies above the graph of f



Analytic criterion

A twice differentiable function is convex if $f''(\boldsymbol{x}) \geq 0$ (or $H_f(\boldsymbol{x})$ positive semidefinite) for all $\boldsymbol{x}$.

Implications for optimization

If f is convex, then:

- $f'(\boldsymbol{x}) = 0$ is a sufficient criterion for a minimum.
- Local minima are global.
- If f is strictly convex ($f'' > 0$ or H_f positive definite), there is only one minimum (which is both global and local).

Exponential Family

Exponential Family Models

Definition

We consider a model $\mathcal{P}$ for data in a sample space $\mathcal{X}$ with parameter space $\Theta \subset \mathbb{R}^m$. Each distribution in $\mathcal{P}$ has density $p(x \mid \theta)$ for some $\theta \in \Theta$.

The model is called an **exponential family model** (EFM) if p can be written as

$$p(x \mid \theta) = h(x) \exp\{\eta(\theta)^T s(x) - a(\theta)\}$$

where we refer to

- h as the base measure
- η as the natural parameter
- s as the sufficient statistics
- a as the log normalizer.

Exponential families are important because

- The special form of p gives them many nice properties.[2]
- Many important parametric models (Gaussian, Poisson, beta, gamma, etc.) are EFM's.
- Many algorithms and methods can be formulated generically for all EFM's.

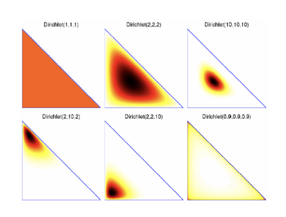
An observation

The data and the parameter interact only through the linear term $\eta(\theta)^T s(x)$ in the exponent.

[2] Indeed, we have already seen one. More will come up in this workshop.

Example: The Dirichlet Distribution

We can write the density of the Dirichlet distribution in exponential form:



$$
\begin{aligned}
p(\pi \mid \alpha) &= \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \pi_1^{\alpha_1 - 1} \cdots \pi_K^{\alpha_K - 1} \\
&= \exp\left\{ \sum_{k=1}^{K} (\alpha_k - 1) \log \pi_k - \left[\sum_k \log \Gamma(\alpha_k) - \log \Gamma\left(\sum \alpha_k\right) \right] \right\}
\end{aligned}
$$

with natural parameter $\eta(\alpha) = [\alpha_1 - 1, ..., \alpha_K - 1]^T$, sufficient statistics $s(\pi) = \log \pi = [\log \pi_1, ..., \log \pi_K]^T$, base measure $h(\pi) = 1$, and log normalizer $a(\alpha) = \sum_k \log \Gamma(\alpha_k) - \log \Gamma(\sum_k \alpha_k)$. $\square$

Exercise: The Bernoulli distribution

As an example, let's put the Bernoulli (in its usual form) into exponential family form. The Bernoulli you are used to seeing is:

$$p(x \mid \pi) = \pi^x \, (1 - \pi)^{1-x} \quad x \in \{0, 1\}$$

Exercise: The Bernoulli distribution

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$$p(x \mid \pi) = \pi^x \, (1-\pi)^{1-x} \quad x \in \{0, 1\}$$

In exponential family form:

$$\begin{aligned} p(x \mid \pi) &= \exp\left(\log\left[\pi^x \, (1-\pi)^{1-x}\right]\right) \\ &= \exp\Big(x \log \pi + (1-x)\log(1-\pi)\Big) \\ &= \exp\Big(x \log \pi - x \log(1-\pi) + \log(1-\pi)\Big) \\ &= \exp\Big(x \log(\pi/(1-\pi)) + \log(1-\pi)\Big) \end{aligned}$$

which reveals the exponential family where

$$\begin{aligned} \eta &= \log(\pi/(1-\pi)) \\ s(x) &= x \\ a(\eta) &= -\log(1-\pi) = \log(1+e^{\eta}) \\ h(x) &= 1 \end{aligned}$$

Note that the relationship between π and η is invertible

$$\pi = 1/(1 + e^{-\eta})$$

This it the *logistic function*.

Exercise: The Gaussian distribution

The familiar form of the univariate Gaussian is

$$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \, \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$

Exercise: The Gaussian distribution

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$$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \; \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$

We put it in exponential family form by expanding the square

$$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}x^2 - \frac{1}{2\sigma^2}\mu^2 - \log\sigma\right)$$

which reveals the exponential family where

$$\begin{aligned} \eta &= [\mu/\sigma^2, -1/2\sigma^2] \\ s(x) &= [x, x^2] \\ a(\eta) &= \mu^2/2\sigma^2 + \log\sigma \\ h(x) &= 1/\sqrt{2\pi} \end{aligned}$$

Examples of Exponential Families

Model	Sample space	Sufficient statistic
Gaussian	$\mathbb{R}^d$	$S(\mathbf{x}) = (\mathbf{x}\mathbf{x}^t, \mathbf{x})$
Gamma	$\mathbb{R}_+$	$S(x) = (\ln(x), x)$
Poisson	$\mathbb{N}_0$	$S(x) = x$
Multinomial	$\{1, \ldots, K\}$	$S(x) = x$
Wishart	Positive definite matrices	(requires more details)
Mallows	Rankings (permutations)	(requires more details)
Beta	$[0, 1]$	$S(x) = (\ln(x), \ln(1 - x))$
Dirichlet	Probability distributions on d events	$S(\mathbf{x}) = (\ln x_1, \ldots, \ln x_d)$
Bernoulli	$\{0, 1\}$	$S(x) = x$
...	...	...

The Exponential Family and Maximum Likelihood

i.i.d samples from an exponential family distribution

If $\boldsymbol{x} = (x_1, ..., x_n)$ are n independent samples from the same exponential family distribution, then

$$p(\boldsymbol{x} \mid \theta) = \prod_{i=1}^{n} h(x_i) \exp\left\{\eta(\theta)^T \sum_{i=1}^{n} s(x_i) - n\, a(\eta(\theta))\right\}$$

Maximum likelihood with exponential families

The goal for maximum likelihood is to determine parameter

$$\theta_{ML} = \underset{\theta}{\operatorname{argmax}} \log p(\boldsymbol{x} \mid \theta)$$

Let us assume that $\boldsymbol{x} = (x_1, ..., x_n)$ are i.i.d observations from a fixed exponential family, so that the likelihood has form above.

The Exponential Family and Maximum Likelihood

Let us compute the gradient with respect to the natural parameter η of $\ell(\eta) := \log p(\boldsymbol{x} \mid \eta)$

$$\nabla_\eta \ell(\eta) = \sum_{i=1}^{n} s(x_i) - n \, \nabla_\eta a(\eta)$$

Setting the gradient to zero, we obtain

$$\nabla_\eta a(\eta) = \frac{1}{n} \sum_{i=1}^{n} s(x_i)$$

But[3] $\nabla_\eta a(\eta) = \mathbb{E}[s(X)]$. Thus, we should set θ_{ML} such that

$$\mu(\theta_{ML}) = \frac{1}{n} \sum_{i=1}^{n} s(x_i)$$

where $\mu := \mathbb{E}[s(x)]$ refers to the mean parametrization of the likelihood.

[3] A useful fact about exponential families. The proof is straightforward.