

MLE and a little optimization

Rob McCulloch

1. Introduction
2. Finding a Minimum, one variable
3. Maximum Likelihood, the Bernoulli
4. Projecting onto a vector
5. Finding a Minimum, Several Variables
6. Maximum Likelihood, the normal
7. Simple Linear Regression
8. The Multinoulli MLE
9. Lagrange Multiplier
10. The Multinoulli MLE again
11. KKT

1. Introduction

When we did Naive Bayes we had to estimate

$$p(X_i = x_i | Y = y) \text{ (or } p(x_i | y) \text{)}.$$

How did we do it?

We simply used *the observed frequency*:

To estimate $p(X_i = x_i | Y = y)$:

in the training data, out of the times $Y = y$,
what fraction of observations have $X_i = x_i$.

If $X_i \sim \text{Bern}(p)$, we estimate p with the observed fraction of times $x_i = 1$.

We call p the *parameter* of the *statistical model* $X \sim \text{Bern}(p)$.

We consider a variety of statistical models and need to estimate the associated parameters.

For example, if we assume $Y_i \sim N(\mu, \sigma^2)$ then we have to estimate (μ, σ^2) .

While the observed conditional frequency seems very reasonable for estimating probabilities, we want a general approach to estimating the parameters of a statistical model.

Maximum likelihood is a very general approach which we will review.

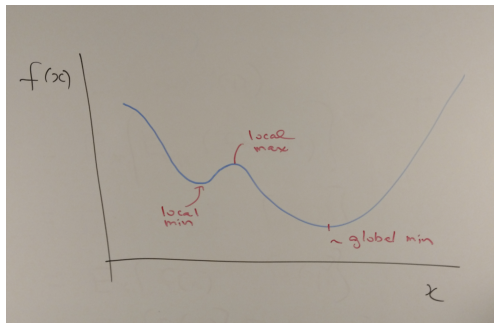
Along the way, we will also review some very basic ideas from optimization.

2. Finding a Minimum, one variable

Let f be a function of a single variable, so that $f(x)$ is a number for $x \in C \subset \mathbb{R}$.

x_0 is a local minimum if $f(x) \geq f(x_0)$ for all x close to x_0 .

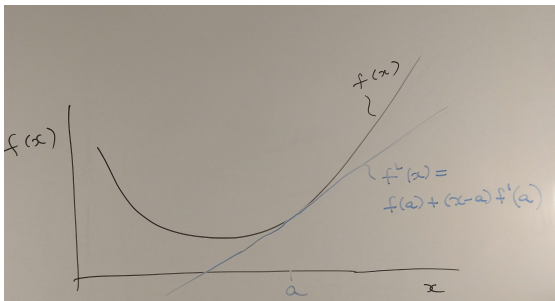
x_0 is a global minimum if $f(x) \geq f(x_0)$ for all $x \in C$.



Recall:

The derivative gives you a linear approximation to the function:

$$f(x) - f(a) \approx (x - a)f'(a).$$



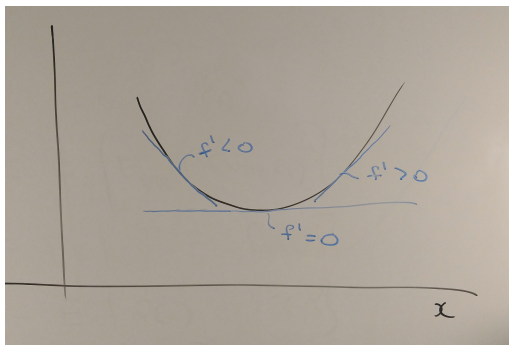
For x close to a , $f(x) \approx f^L(x)$.

Necessary Condition:

If x_0 is a local min (or max) then $f'(x_0) = 0$.

Sufficient Condition:

If $f'(x_0) = 0$ and $f''(x_0) > 0$, then x_0 is a local minimum.

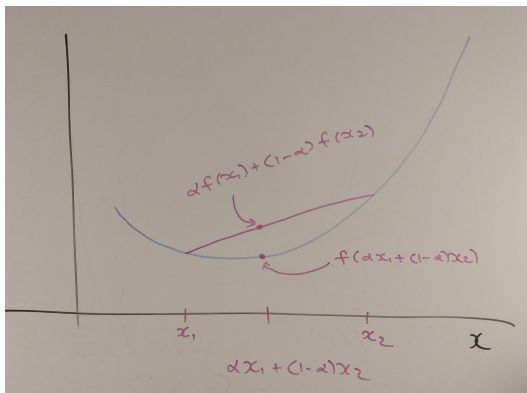


At a local minimum, the derivative is increasing.

Global Sufficient Condition

f is convex if

$$f(\alpha x_1 + (1 - \alpha)x_2) \leq \alpha f(x_1) + (1 - \alpha)f(x_2), \alpha \in [0, 1].$$



If f is convex and $f'(x_0) = 0$, then x_0 is a global minimum.

We use optimization *a lot* in Machine Learning.

In particular, learning on the training data is often done by some kind of optimization.

For example, in the model $y_i \approx \beta' x_i$ we learn (*estimate*) β by solving

$$\underset{\beta}{\text{minimize}} \sum_{i=1}^n (y_i - \beta' x_i)^2$$

We will spend a chunk of time on versions of this problem.

3. Maximum Likelihood, the Bernoulli

Suppose we have a statistical model

$$Y \sim f(y | \theta)$$

where θ is the parameter (possibly a vector).

Given data $Y = y$ how can we estimate θ ?

Maximum Likelihood:

Choose the θ that makes what you have seen most likely:

$$\hat{\theta} = \operatorname{argmax}_{\theta} f(y | \theta)$$

In the iid case, we have $Y = (Y_1, Y_2, \dots, Y_n)$ with

$$Y_i \sim f(y | \theta) \text{ iid},$$

so

$$f(y | \theta) = \prod_{i=1}^n f(y_i | \theta),$$

and the MLE is

$$\hat{\theta} = \operatorname{argmax}_{\theta} \prod_{i=1}^n f(y_i | \theta).$$

Note:

$f(y | \theta)$ viewed as a function of θ for a fixed y is called the likelihood function.

In practice we often maximize the log of the likelihood or minimize the negative of the log likelihood.

Bernoulli: MLE

$$Y_i \sim \text{Bern}(p) \quad Y_i \in \{0, 1\}$$

$$\begin{aligned} p(y_1, y_2, \dots, y_n | p) &= \prod_{i=1}^n p^{y_i} (1-p)^{1-y_i} \\ &= p^k (1-p)^{n-k} \quad k = \#(y_i = 1) \end{aligned}$$

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

$$\begin{aligned} \text{FOC: } \frac{k}{p} - \frac{(n-k)}{1-p} &= 0 \Rightarrow (n-k)p = k(1-p) \\ &\Rightarrow p = \frac{k}{n} \end{aligned}$$

FOC: "first order condition", $f' = 0$.

So, the observed sample frequency is the MLE!

4. Projecting onto a vector

Let x and $y \in R^n$.

So, for example, $x = (x_1, x_2, \dots, x_n)'$.

We will find the solution to the following problem very useful:

$$\min_{\beta \in R} \|y - \beta x\|^2$$

where $\|x\|^2 = \sum x_i^2$.

Recall:

$$x, y \in R^n,$$

The **inner product** is

$$\langle x, y \rangle = x'y = y'x = \sum x_i y_i.$$

The L^2 or Euclidean **norm** (squared) is

$$\|x\|^2 = \langle x, x \rangle = x'x = \sum x_i^2$$

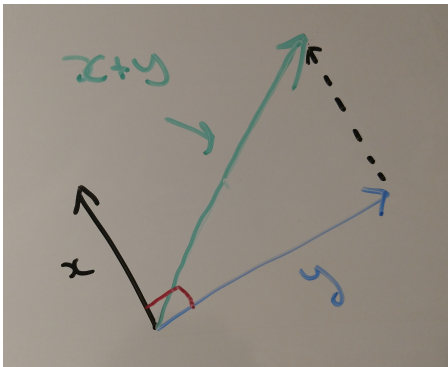
x and y are **orthogonal** if

$$\langle x, y \rangle = 0$$

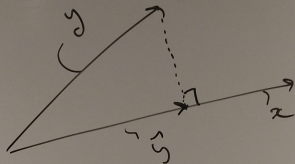
Note:

If x and y are orthogonal:

$$\begin{aligned}\|x + y\|^2 &= \langle x + y, x + y \rangle \\ &= \langle x, x \rangle + 2\langle x, y \rangle + \langle y, y \rangle \\ &= \|x\|^2 + \|y\|^2\end{aligned}$$



\hat{y} is the orthogonal projection of y onto x .



$$\hat{y} = \hat{\beta}x$$

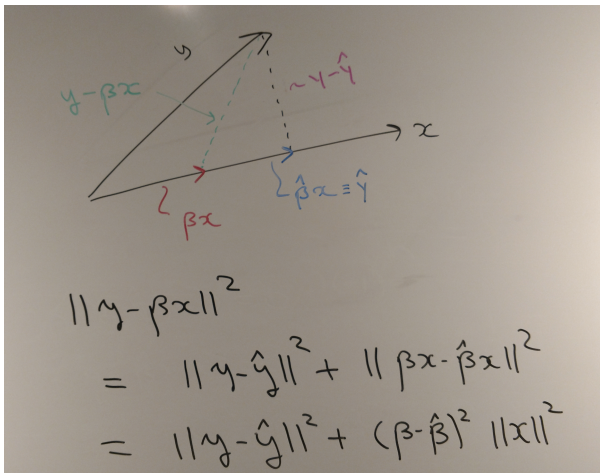
$$\langle y - \hat{y}, x \rangle = 0$$

$$\langle y - \hat{\beta}x, x \rangle = 0$$

$$\langle y, x \rangle = \hat{\beta} \langle x, x \rangle$$

$$\hat{\beta} = \frac{\langle y, x \rangle}{\langle x, x \rangle}$$

To solve our problem we have



So that obviously the min is obtained at $\beta^* = \hat{\beta}$.

5. Finding a Minimum, Several Variables

Now suppose $x = (x_1, x_2, \dots, x_p)'$

and $f(x) = f(x_1, x_2, \dots, x_p) \in R$.

How do we solve:

$$\min_x f(x)$$

The Gradient:

$$\nabla f(x) = \left[\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \dots, \frac{\partial f(x)}{\partial x_p} \right]$$

where

$$\frac{\partial f(x)}{\partial x_i}$$

is what you get by holding all the x_j , $j \neq i$ fixed, and then differentiating with respect to x_i .

The gradient is a multivariate derivative in that (skipping some technical details):

$$f(x) \approx f(a) + \nabla f(a)(x - a)$$

Note that $\nabla f(x)$ is a row vector so that the product above makes sense with x a column vector.

An alternative notation is:

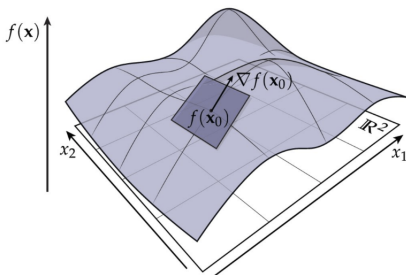
$$f(x) \approx f(a) + \langle \nabla f(a), (x - a) \rangle$$

Stolen off the web:

Gradient as Best Linear Approximation

Another way to think about it: at each point \mathbf{x}_0 , gradient is the vector $\nabla f(\mathbf{x}_0)$ that leads to the best possible approximation

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \langle \nabla f(\mathbf{x}_0), \mathbf{x} - \mathbf{x}_0 \rangle$$

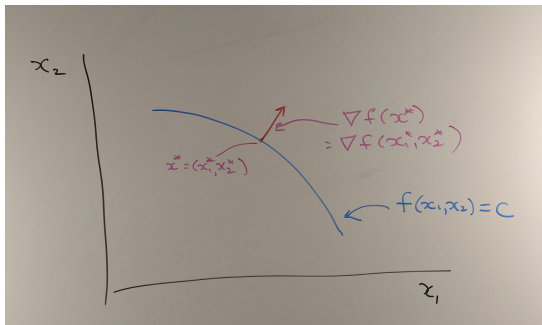


Starting at \mathbf{x}_0 , this term gets:

- bigger if we move in the direction of the gradient,
- smaller if we move in the opposite direction, and
- doesn't change if we move orthogonal to gradient.

CMU 15-462/662

We can visualize the gradient using the *contours* of f .
A *contour* is the set $\{x : f(x) = c\}$.



- ▶ If you want to increase f as fast as possible, go in the direction of the gradient ∇f .
- ▶ If you want to decrease f as fast as possible, go in the direction of the negative gradient $-\nabla f$.
- ▶ If you want to move without changing f to in a direction orthogonal to the gradient.

Necessary Condition for a local min/max:

If x^* is a local min (or max) then we must have

$$\nabla f(x^*) = 0$$

Again f is convex if,

$$f(\alpha x_1 + (1 - \alpha)x_2) \leq \alpha f(x_1) + (1 - \alpha)f(x_2), \alpha \in [0, 1].$$

exactly as before except that now x denotes a vector $\in R^p$.

As before, if f is convex, then a local minimum is a global minimum.

Let's defer multivariate conditions for convexity and the "second derivative".

6. Maximum Likelihood, the normal

Suppose

$$Y_i \sim N(\mu, \sigma^2), \text{ iid}$$

what is the MLE of $\theta = (\mu, \sigma^2)$?

$$\begin{aligned}
 f(y|\mu, \sigma^2) &= \prod f(y_i|\mu, \sigma^2) \\
 &= \prod \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} e^{-\frac{1}{2\sigma^2}(y_i-\mu)^2} \\
 &= (2\pi)^{-\frac{n}{2}} \sigma^{-n} e^{-\frac{1}{2\sigma^2} \sum (y_i-\mu)^2}
 \end{aligned}$$

$$-\log L(\mu, \sigma^2) = \frac{n}{2} \log(2\pi) + n \log \sigma + \frac{1}{2\sigma^2} \sum (y_i - \mu)^2$$

$$\text{Let } v = \sigma^2$$

$$= \frac{n}{2} \log(2\pi) + \frac{n}{2} \log(v) + \frac{1}{2v} \sum (y_i - \mu)^2$$

$$-2 \log L(\mu, v) = n \log(2\pi) + n \log(v) + \frac{1}{v} \sum (y_i - \mu)^2$$

$$\mathbf{1} = (1, 1, 1, \dots, 1)'$$

$$\sum (y_i - \mu)^2 = \|\mathbf{y} - \mu \mathbf{1}\|^2$$

$$\hat{\mu} = \frac{\langle \mathbf{y}, \mathbf{1} \rangle}{\langle \mathbf{1}, \mathbf{1} \rangle} = \frac{\sum y_i}{n} = \bar{y}$$

$$\begin{aligned} \sum (y_i - \mu)^2 &= \|\mathbf{y} - \bar{y} \mathbf{1}\|^2 + \|\mu \mathbf{1} - \bar{y} \mathbf{1}\|^2 \\ &= \sum (y_i - \bar{y})^2 + n(\bar{y} - \mu)^2 \end{aligned}$$

$$S = \sum (y_i - \bar{y})^2.$$

$$-2 \log L =$$

$$c + n \log(v) + \frac{1}{v} \left[S + n(\bar{y} - \mu)^2 \right]$$

$$\frac{\partial}{\partial \mu} = \frac{n}{v} \cdot 2(\bar{y} - \mu)(-1)$$

$$\Rightarrow \mu^* = \bar{y}$$

$$\frac{\partial}{\partial v} (\text{at } \mu^*) = \frac{n}{v} - \frac{S}{v^2}$$

$$v^* = \frac{S}{n} = \frac{\sum (y_i - \bar{y})^2}{n}$$

7. The Multinoulli MLE

The fundamental Bernoulli random variable considers the case where something is about to happen or not and we code one possibility up as a 1 and the other as a 0.

The Multinoulli distribution consider the more general case where there is a a set of k possible outcomes.

For example, if we survey a customer and ask them to rate our product on a 1-5 scale then there are 5 possible outcomes.

Let $\{1, 2, \dots, k\}$ denote the possible outcomes for Y .

Let

$$p = (p_1, p_2, \dots, p_k)$$

with

$$P(Y = j \mid p) = p_j$$

Then

$$Y \sim \text{Multinoulli}(p)$$

Given $Y_i \sim \text{Multinoulli}(p)$ we want to compute the MLE of p .

$$Y_{ij} = \begin{cases} 1 & \text{if } Y_i = j \\ 0 & \text{else} \end{cases} \quad \begin{array}{l} i=1,2,\dots,n \\ j=1,2,\dots,k \end{array}$$

$$\begin{aligned} p(y_1, y_2, \dots, y_n | p) &= \prod_i p_1^{y_{i1}} p_2^{y_{i2}} \dots p_k^{y_{ik}} \\ &= p_1^{m_1} p_2^{m_2} \dots p_k^{m_k} \end{aligned}$$

$$m_j = \sum_i Y_{ij} = \left[\# \text{ of times } Y_i = j \right]$$

How do we maximize this likelihood?

With just two possible outcomes we had one variable,
 $p = P(Y = 1)$.

Now we have $p_j, j = 1, 2, \dots, k$ with the constraint $\sum p_j = 1$.

We also have $0 \leq p_j \leq 1$, but we won't have to worry about this.

We could let $p_k = 1 - \sum_{j=1}^{k-1} p_j$ and then optimize over
 $(p_1, p_2, \dots, p_{k-1})$.

But, it is easier to use *lagrange multipliers*.

8. Lagrange Multiplier

Let $x \in R^p$.

We want to solve:

$$\min_x f(x), \quad \text{subject to } g(x) = 0$$

Let

$$\mathcal{L}(x, \lambda) = f(x) + \lambda g(x)$$

and then minimize \mathcal{L} unconstrained over (x, λ) .

Differentiating \mathcal{L} with respect to λ gives:

$$g(x) = 0$$

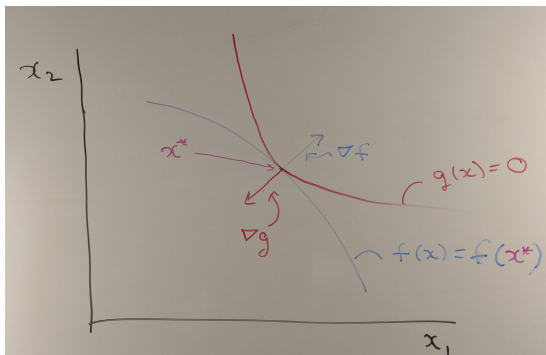
at the min/max.

Differentiating \mathcal{L} with respect to x give:

$$\nabla f(x) + \lambda \nabla g(x) = 0$$

at a local min (or max).

Because of the constraint $g(x) = 0$ you can only move orthogonal to ∇g .



But, $\nabla f \propto \nabla g$, tells you that “small” moves orthogonal to ∇g will not change f so it is a local minimum or maximum.

9. The Multinoulli MLE again

To obtain the Multinoulli MLE we will have

$$L(p) = \prod p_j^{m_j}$$

and we maximize this subject to

$$\sum p_j = 1.$$

We will max the log likelihood:

$$\mathcal{L}(p, \lambda) = \sum_j m_j \log(p_j) + \lambda(\sum_j p_j - 1)$$

$$L = \sum m_k \log p_k + \lambda (\sum p_k - 1)$$

$$\frac{\partial L}{\partial p_k} = \frac{m_k}{p_k} + \lambda$$

$$\Rightarrow p_k \propto m_k$$

$$\Rightarrow p_k^* = \frac{m_k}{\sum m_k} = \frac{m_k}{n}$$

The MLE is the observed sample frequency.

10. KKT

We will have occasion to consider constraint sets of the form

$$g(x) \leq 0$$

rather than just

$$g(x) = 0$$

The Karush-Kuhn-Tucker conditions cover both inequality and equality constraints.

We'll see how things change with one inequality constraint and then state the general result.

KKT:

To minimize $f(x)$ subject to $g(x) \leq 0$, form

$$L(x, \alpha) = f(x) + \alpha g(x)$$

and then solve

$$\min_x \max_{\alpha, \alpha \geq 0} L(x, \alpha).$$

With $\alpha \geq 0$ we must have $g(x) \leq 0$, since otherwise we could get a max of infinity.

Also note that at the solution:

$$\alpha^* g(x^*) = 0.$$

This captures the fact that there are two possibilities:

- ▶ If the constraint is *binding* then $g(x^*) = 0$ and we can have $\alpha^* > 0$.
- ▶ If the constraint is not binding so that $g(x^*) < 0$ then the max over non-negative α is clearly obtained at $\alpha^* = 0$.

If $g(x) < 0$ ($\alpha = 0$) at the optimal value then the constraint is not binding and we can just use our usual solve $\nabla f = 0$ approach.

If $g(x) = 0$ ($\alpha > 0$) then the KKT result says we can solve the unconstrained problem of minimizing:

$$\min f(x) + \alpha g(x).$$

As before, the term

$$\min f(x) + \alpha g(x)$$

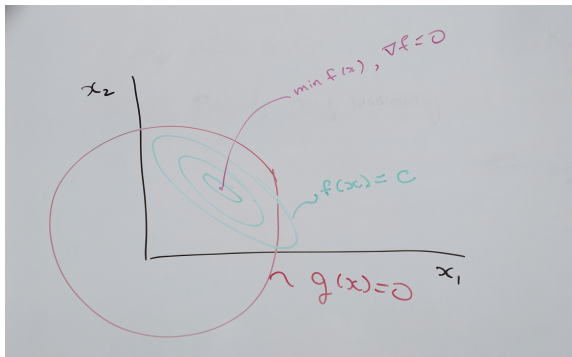
is called the “lagrangian” and α is the lagrange multiplier.

The FOC (first order condition) associate with the lagrangian is:

$$\nabla f(x) + \alpha \nabla g(x) = 0.$$

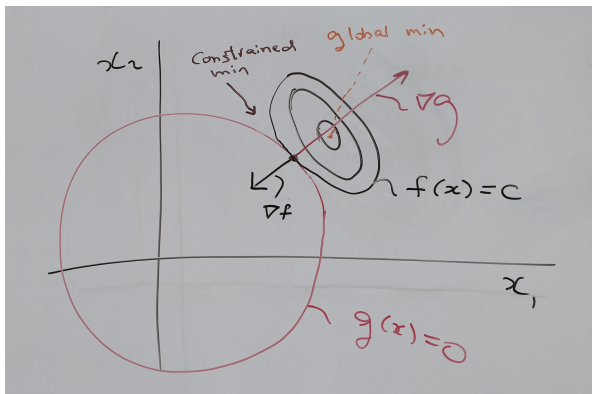
Here is the case where the constraint is not binding.

The global min is in the interior of the set $g(x) \leq 0$.



Here is the key picture for the case where the constraint is binding.

Remember, ∇f is the direction in which f goes up the fastest!!
 ∇f points perpendicularly to the contour of f .



It is intuitive that $\nabla f + \alpha \nabla g = 0$ with $\alpha > 0$.

The general form of the KKT theorem.

Just notice that with equality constraints you don't know the sign of the constraint coefficient.

$$\min f(x)$$

$$\text{s.t. : } \begin{cases} h_i(x) = 0 \\ g_j(x) \leq 0 \end{cases}$$

$$L(x, \lambda, \alpha) = f(x) + \sum \lambda_i h_i(x) + \sum \alpha_j g_j(x)$$

$$\min_x \max_{\lambda} \max_{\alpha, \alpha_j \geq 0} L(x, \lambda, \alpha)$$

Example:

What happens when we do

$$\min_{x: \|x\| < c} a'x$$

What happens when we do

$$\max_{x: \|x\| < c} a'x$$