MLE and a little optimization

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1. Introduction

When we did Naive Bayes we had to estimate

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

How did we do it?

We simply used *the observed frequency*:

To estimate $p(X_i = x_i \mid Y = y)$:
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 estimated 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 esitmating probabilities, we want a general approach to estimating the parameters of a statisical model.

Maximimum likelihood is a very general appproach 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 an number for $x \in C \subset R$.

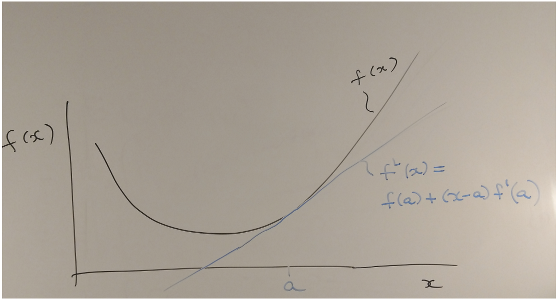
x_0 is a local minimum if $f(x) \geq f(x_0)$ for all x close to x_0.

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:

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



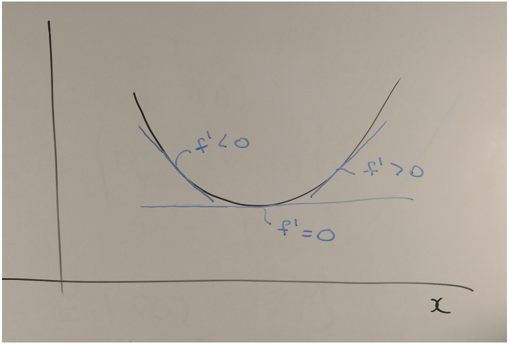
For x close to a, $f(x) \approx f^L(x)$.

Neccessary Condition:

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

Sufficient Condition:

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

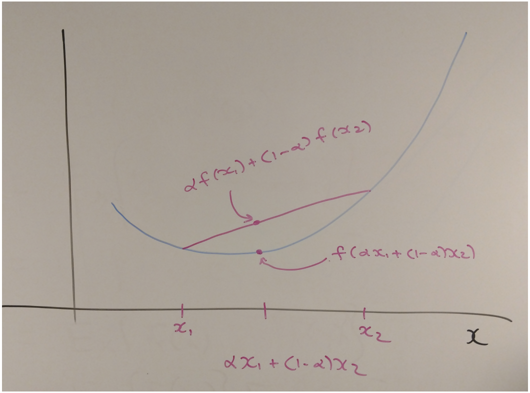


At a local minimum, the derivative is increasing.

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 us 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

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

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:

$$\hat{\theta} = \underset{\theta}{\text{argmax}}\, f(y \mid \theta)$$

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

$$Y_i \sim f(y \mid \theta) \;\; iid,$$

so

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

and the MLE is

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

Note:

$f(y \mid \theta)$ 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

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

$$p(y_1, y_2, \dots y_n | p) = \prod_{i=1}^{n} p^{y_i} (1-p)^{1-y_i}$$

$$= p^k (1-p)^{n-k} \qquad k = \#(y_i = 1)$$

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

FOC: $$\frac{k}{p} - \frac{(n-k)}{1-p} = 0 \Rightarrow (n-k)p = k(1-p)$$

$$\Rightarrow p = \frac{k}{n}$$

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, $x = (x_1, x_2, \ldots, x_n)'$.

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

$$< x, y >= x'y = y'x = \sum x_i y_i.$$

The L^2 or Euclidean norm (squared) is

$$||x||^2 =< x, x >= x'x = \sum x_i^2$$

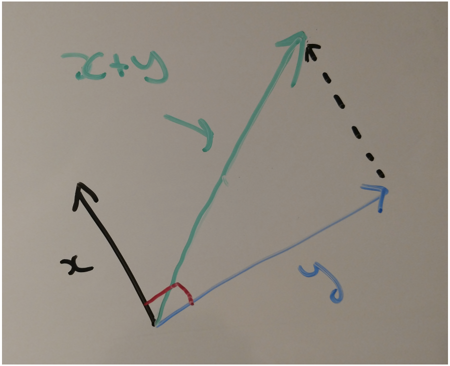
x and y are orthogonal if

$$< x, y >= 0$$

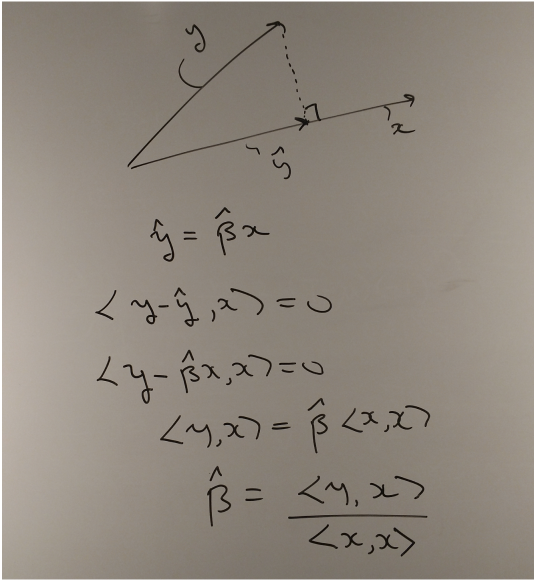
Note:

If x and y are orthogonal:

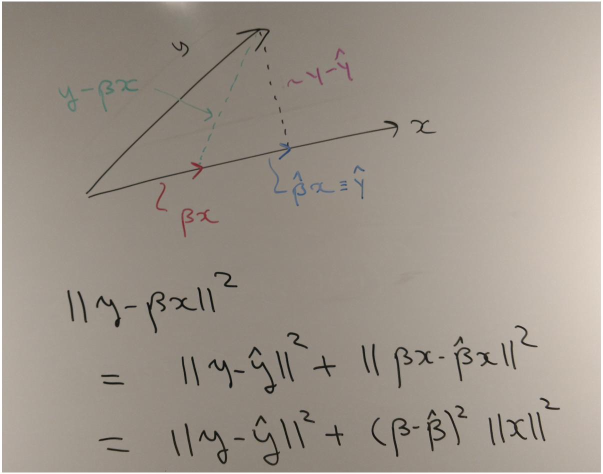
$$\begin{aligned} ||x+y||^2 &= <x+y, x+y> \\ &= <x,x> + 2<x,y> + <y,y> \\ &= ||x||^2 + ||y||^2 \end{aligned}$$



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



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 $x = (x_1, x_2, \ldots, x_p)'$

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

How do we solve:

$$\min_x f(x)$$

The Gradient:

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

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):

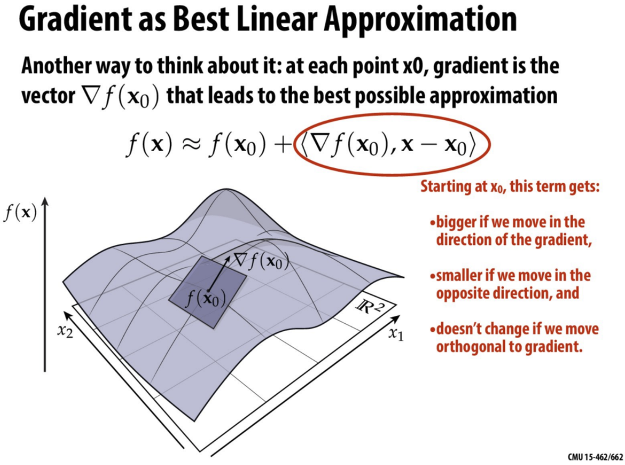
$$f(x) \approx f(a) + \nabla f(a)(x - a)$$

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

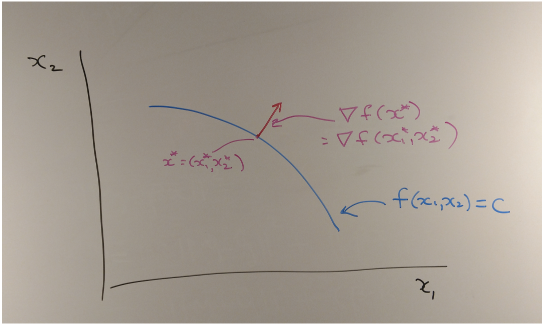
An alternative notation is:

$$f(x) \approx f(a) + < \nabla f(a), (x - a) >$$

Stolen off the web:



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 go in a direction orthogonal to the gradient.

Neccessary 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.

6. Maximum Likelihood, the normal

Suppose

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

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

$$f(y|\mu,\sigma^2) = \prod f(y_i|\mu,\sigma^2)$$

$$= \prod \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} e^{-\frac{1}{2\sigma^2}(y_i-\mu)^2}$$

$$= (2\pi)^{-\frac{n}{2}} \sigma^{-n} e^{-\frac{1}{2\sigma^2}\Sigma(y_i-\mu)^2}$$

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

Let $v = \sigma^2$

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

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

We want to simplify $\sum(y_i - \mu)^2$.

$$\sum_{i=1}^{n}(y_i - \bar{y}) = \Sigma y_i - \Sigma \bar{y} = n\frac{\Sigma y_i}{n} - n\bar{y} = 0$$

$$\sum_{i=1}^{n}(y_i - \mu)^2 = \Sigma\left((y_i - \bar{y}) + (\bar{y} - \mu)\right)^2$$

$$= \Sigma(y_i - \bar{y})^2 + 2\,\Sigma(y_i - \bar{y})(\bar{y} - \mu) + \Sigma(\bar{y} - \mu)^2$$

$$= \Sigma(y_i - \bar{y})^2 + 2(\bar{y} - \mu)\Sigma(y_i - \bar{y}) + n(\bar{y} - \mu)^2$$

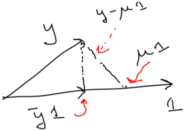
$$= \Sigma(y_i - \bar{y})^2 + n(\bar{y} - \mu)^2$$

Here is another way.

$$\sum_{i=1}^{n} (y_i-\mu)^2 = \|y-\mu\underline{1}\|^2$$

$$y = (y_1, y_2, \cdots y_n)' \qquad \mu\underline{1} = \begin{bmatrix} \mu \\ \mu \\ \vdots \\ \mu \end{bmatrix}$$

$$\underline{1} = (1, 1, \cdots 1)'$$



$$\|y-\mu\underline{1}\|^2 = \|y-\bar{y}\underline{1}\|^2 + \|\bar{y}\underline{1}-\mu\underline{1}\|^2$$

$$= \Sigma(y_i-\bar{y})^2 + n(\bar{y}-\mu)^2$$

$$\bar{y} = \frac{\langle y, \underline{1}\rangle}{\langle \underline{1}, \underline{1}\rangle} = \frac{\Sigma y_i}{n}$$

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

$$-2 \log L =$$

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

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

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

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

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

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

Let

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

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.

$$y_{ij} = \begin{cases} 1 & \text{if } y_i = j \\ 0 & \text{else} \end{cases} \qquad \begin{matrix} i = 1, 2, \cdots n \\ j = 1, 2, \cdots k \end{matrix}$$

$$p(y_1, y_2, \cdots y_n | p) = \prod_i p_1^{y_{i1}} \, p_2^{y_{i2}} \cdots p_k^{y_{ik}}$$

$$= p_1^{m_1} \, p_2^{m_2} \cdots p_k^{m_k}$$

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

How do we maximize this likelihood?

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

Now we have $p_j, j = 1, 2, \ldots, k$ 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 $p_k = 1 - \sum_{j=1}^{k-1}$ and then optimize over $(p_1, p_2, \ldots, p_{k-1})$.

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:

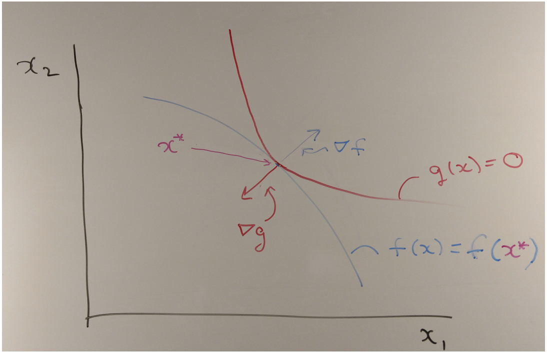
$$g(x) = 0$$

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:

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

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

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

$$\Rightarrow \quad p_k \propto m_k$$

$$\Rightarrow \quad \hat{p}_k = \frac{m_k}{\sum m_k} = \frac{m_k}{n}.$$

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

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

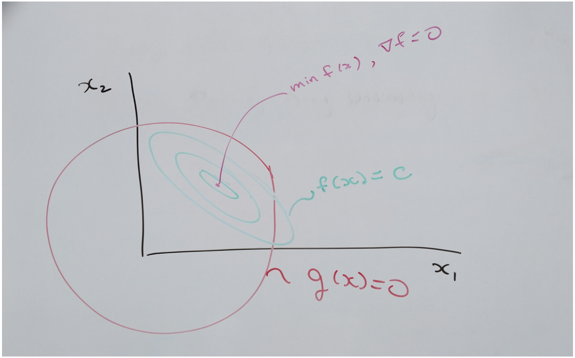
is called the "lagrangian" and α is the lagrange multiplier.

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

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

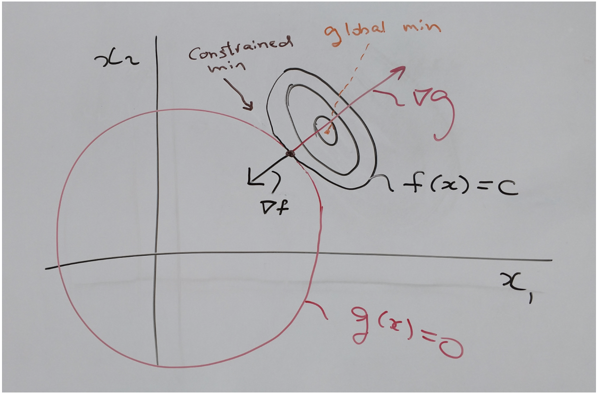
Here is the case where the constraint is not binding.

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.

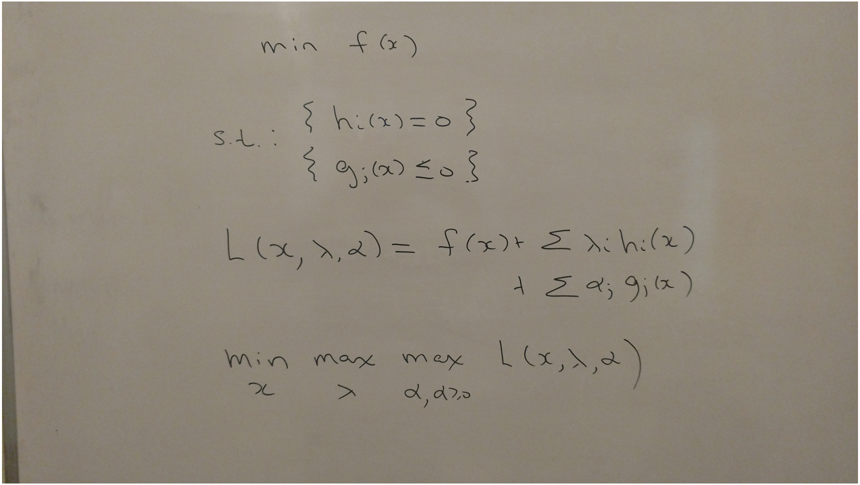
Remember, ∇f is the direction in which f goes up the fastest!!
∇f points perpendicularly to the contour of f.



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.



Example:

What happens when we do

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

What happens when we do

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

$$g(x) = x_1^2 + x_2^2 - 1$$

$$f(x) = a^T x = [a_1, a_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = a_1 x_1 + a_2 x_2$$

$$\nabla g(x) = [2x_1, 2x_2]$$

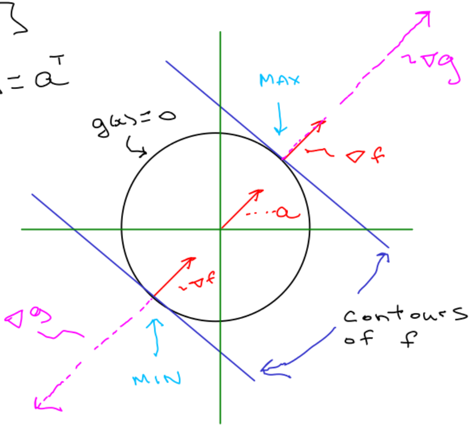
$$\nabla f(x) = [a_1, a_2] = a^T$$

At min:

$$\nabla f + \alpha \nabla g = 0$$
$$\alpha > 0$$

At max

$$\nabla f + \alpha \nabla g = 0$$
$$\alpha < 0$$



Solve for MIN

$\nabla f + \alpha \nabla g \quad \alpha > 0$

$$[a_1, a_2] + 2\alpha [x_1, x_2] = 0$$

$$a_i + 2\alpha x_i = 0$$

$$x_i = \frac{-a_i}{2\alpha}$$

$x_1^2 + x_2^2 = 1 \Rightarrow$

$$x_i = \frac{-a_i}{\sqrt{a_1^2 + a_2^2}}$$

$$x^* = -\frac{a}{\|a\|}$$

Solve for MAX

$$[a_1, a_2] - 2\alpha [x_1, x_2] = 0 \quad \alpha > 0$$

$$x_i = \frac{a_i}{2\alpha} \Rightarrow x_i = \frac{a_i}{\sqrt{a_1^2 + a_2^2}}$$

$$x^* = \frac{a}{\|a\|}$$

Note

From the MAX we have

$$a^T \frac{x}{\|x\|} \leq a^T \frac{a}{\|a\|} = \|a\|$$

So $$\frac{a^T x}{\|a\| \, \|x\|} \leq 1$$

From the MIN we have $-1 \leq \frac{a^T x}{\|a\| \, \|x\|}$

So $$-1 \leq \frac{\langle a, x \rangle}{\|a\| \, \|x\|} \leq 1$$

the Cauchy-Schwartz inequality !!

Note Let (x_i, y_i) $i = 1, 2, \ldots n$

be data on x and y.

We often demean data:

$$x_i \to \tilde{x}_i = x_i - \bar{x}$$
$$y_i \to \tilde{y}_i = y_i - \bar{y}$$

$$\frac{\langle \tilde{x}, \tilde{y} \rangle}{\|\tilde{x}\| \, \|\tilde{y}\|} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2} \sqrt{\sum (y_i - \bar{y})^2}}$$ = the sample correlation $\equiv r_{xy}$

$$\boxed{-1 \le r_{x,y} \le 1}$$