

Lecture 7: Introduction to Optimization

COMP90049

Introduction to Machine Learning

Semester 1, 2024

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Last time... Probability

- estimate the (conditional, joint) probability of observations
- Bayes rule
- Marginalization
- Probabilistic models
- Maximum likelihood estimation (taster)
- Maximum a posteriori estimation (taster)

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Today... Optimization

- Curves, minima
- Gradients, derivatives
- Recipe for numerical optimization
- Maximum likelihood of the Binomial (from scratch!)



Optimization

We are all here to **learn** about Machine **Learning**.

- What is learning?
- It probably has something to do with **change** or **mastering** or **optimizing** performance on a specific task
- Machine learning typically involves to build models (like seen last time), and learning boils down to **finding model parameters that optimize some measure of performance**

But, how do we know what is optimal?



Finding Optimal Points I

Finding the **parameters** that optimize a **target**

Ex1: Estimate the **study time** which leads to the **best grade** in COMP90049.

Ex2: Find the **shoe price** which leads to **maximum profit** of our shoe shop.

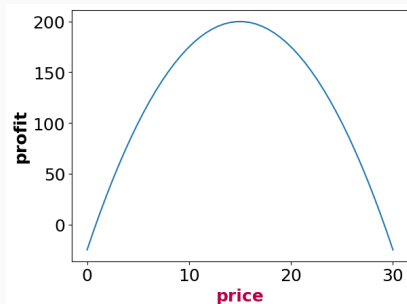


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Ex3: Predicting **housing prices** from a **weighted** combination of house age and house location

Ex4: Find the **parameters θ** of a spam classifier which lead to the **lowest error**

Ex5: Find the **parameters θ** of a spam classifier which lead to the **highest data log likelihood**



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Find parameter values θ that maximize (or minimize) the value of a function $f(\theta)$

- we want to find the **extreme** points of the **objective function**.
Depending on our **target**, this could be
- ...the **maximum**
E.g., the **maximum** profit of our shoe shop
E.g., the **largest** possible (log) likelihood of the data

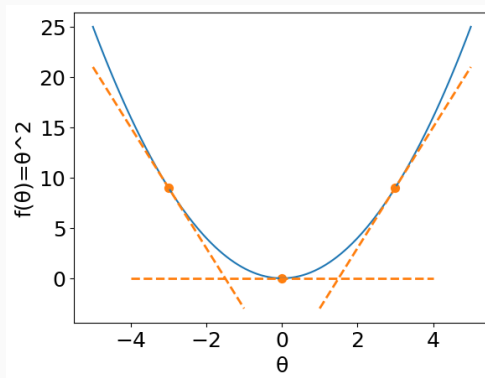
$$\hat{\theta} = \operatorname{argmax}_{\theta} f(\theta)$$

- ...or the **minimum** (in which case we often call f a **loss function**)
E.g., the **smallest** possible classification error

$$\hat{\theta} = \operatorname{argmin}_{\theta} f(\theta)$$

Finding extreme points of a function

- At its **extreme point**, $f(\theta)$ is 'flat': its **slope** is equal to **zero**.
- We can measure the **slope** of a function at any point through its first **derivative** at that point
- The derivative measures the change of the output $f(\theta)$ given a change in the input θ
- We write the derivative of f with respect to θ as $\frac{\partial f}{\partial \theta}$

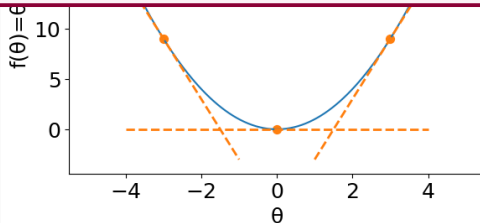


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In order to find the parameters that maximize / minimize an objective function, we find those inputs at which the derivative of the function evaluates to zero.

That's it!



Example

- For our function, with a single 1-dimensional parameter θ

$$f(\theta) = \theta^2$$

Take the derivative

$$\frac{\partial f}{\partial \theta} = 2\theta$$

We want to find the point where this derivative is zero, so

$$2\theta = 0$$

and solve for θ

$$\theta = 0$$

Finding a Minimum / Maximum

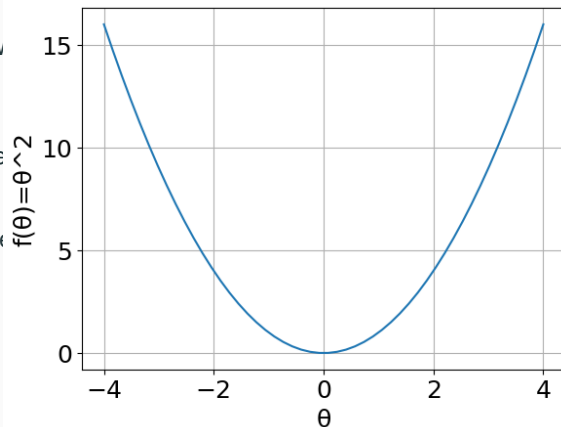
Example

- For our function, we

Take the derivative

We want to find the

and solve for θ



The global minimum of $f(\theta) = \theta^2$ occurs at the point where $\theta=0$.



Recipe for finding Minima / Maxima

1. Define your function of interest $f(\theta)$ (e.g., data log likelihood)
2. Compute its first derivative with respect to its input θ
3. Set the derivative equal to zero
4. Solve for θ

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Let's do this for a more interesting problem. Recall our binomial spam model from the last lecture?



1. Problem setup / identifying the function of interest

- Consider a data set of emails, where each email is an observation x which is labeled either as `spam` or `not spam`
- We have N observations, each with 2 possible outcomes. The data consequently follows a **binomial distribution** and the data likelihood is

$$\mathcal{L}(\theta) = p(X; N, \theta) = \frac{N!}{x!(N-x)!} \theta^x (1-\theta)^{N-x}$$

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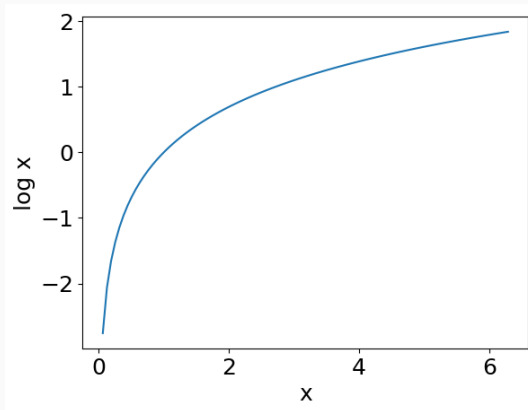
- So the parameter $\theta = P(\text{spam})$
- Imagine we have a data set of 100 emails: 20 are `spam` (and consequently 80 emails are `not spam`).
- In the last lecture, we agreed intuitively that $P(\text{spam}) = \theta = 20/100 = \frac{x}{N}$.
- We will now derive the same result mathematically, and show that $\theta = \frac{x}{N}$ is the $\hat{\theta}$ that maximizes the likelihood of the observed data



Maximum Likelihood Optimization of the Binomial Spam Model

(Log transformation aside)

- Log is a monotonic transformation: The same θ will maximize both $p(x, y)$ and $\log p(x, y)$
- Log values are less extreme (cf. x scale vs y scale)
- Products become sums (avoid under/overflow)



Maximum Likelihood Optimization of the Binomial Spam Model

$$\mathcal{L}(\theta) = p(X; N, \theta) = \frac{N!}{x!(N-x)!} \theta^x (1-\theta)^{N-x} \approx \theta^x (1-\theta)^{N-x}$$

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2. Computing its first derivative

$$\begin{aligned}\mathcal{L}(\theta) = p(X; N, \theta) &= \frac{N!}{x!(N-x)!} \theta^x (1-\theta)^{N-x} \\ &\approx \theta^x (1-\theta)^{N-x}\end{aligned}$$

Move to log space (makes our life easier)

$$\log \mathcal{L}(\theta) = x \log \theta + (N-x) \log(1-\theta)$$

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Move to log space (makes or life easier)

$$\log \mathcal{L}(\theta) = x \log \theta + (N-x) \log(1-\theta)$$

Take the derivative of \mathcal{L} wrt the parameters θ

$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{x}{\theta} - \frac{N-x}{1-\theta}$$

3. Set the derivative to zero

$$0 = \frac{x}{\theta} - \frac{N-x}{1-\theta}$$

4. Solve for θ

$$\frac{x}{\theta} = \frac{N-x}{1-\theta} \quad [\times (1-\theta)]$$

$$\frac{x \times (1-\theta)}{\theta} = N-x \quad [\times \frac{1}{x}]$$

$$\frac{1-\theta}{\theta} = \frac{N-x}{x} \quad [\text{rearrange}]$$

$$\frac{1}{\theta} - 1 = \frac{N}{x} - 1 \quad [+1]$$

$$\frac{1}{\theta} = \frac{N}{x} \quad [\text{flip}]$$

$$\hat{\theta} = \frac{x}{N}$$

Which corresponds to our estimate of $\frac{x}{N} = \frac{20}{100} = 0.2$ for our spam classification problem.

Please go to

<https://pollev.com/krisehinger432>

for a quick quiz on optimization / MLE!

Can you think of scenarios where this approach breaks down?

Can you think of scenarios where this approach breaks down?

- Our loss function is not differentiable
- It is mathematically impossible to set the derivative to 0 and solve for the parameters θ . “No closed-form solution”.
- Our function has multiple ‘extreme points’ where the slope equals zero. Which one is the correct one?

to be continued...

Summary

- What is optimization?
- Objective function / loss function
- Gradients, derivatives, and slopes

Next: Naive Bayes



Solution subject to Constraints

Constrained Optimization

Finding the **parameters** that optimize a **target** subject to one or more constraints.

- Buy **3 pieces of fruit** which lead to the best **nutritional value**. But we only have a budget of 3\$.
- I want to estimate the **parameters of a Categorical distribution** to maximize the **data log likelihood** and I know that **the parameters must sum to 1**.



It often happens that the parameters we want to learn have to obey constraints

$$\begin{aligned} & \underset{\theta}{\operatorname{argmin}} f(\theta) \\ & \text{subject to } g(\theta) = 0, \end{aligned}$$

- ideally, we would like to incorporate such constraints and still be able to follow the general recipe for optimization discussed before
- **Lagrangians** allow us to do exactly that in the case of **equality constraints** (there are also boundary constraints, which we won't cover)
- we combine our target functions with (sets of) constraints multiplied through **Lagrange multipliers** λ

$$\mathcal{L}(\theta, \lambda) = f(\theta) - \lambda g(\theta)$$

- proceed as before: derivative, set to zero, solve for θ



Example

- Find an optimal parameter vector θ such that each all θ_i sum up to a certain constant b .
- Formalize the constraint:

$$\sum_i \theta_i = b$$

- Set the constraint to zero

$$0 = \sum_i \theta_i - b = -b + \sum_i \theta_i$$

- set the constraint and write the Lagrangian

$$g_c(\theta) = -b + \sum_i \theta_i$$

$$\begin{aligned}\mathcal{L}(\theta, \lambda) &= f(\theta) - \lambda g_c(\theta) \\ &= f(\theta) - \lambda(-b + \sum_i \theta_i)\end{aligned}$$

- proceed as before: derivative, set to zero, solve for θ



Jacob Eisenstein. Introduction to Natural Language Processing, Appendix B (up to B.1)

Dan Klein. Lagrange Multipliers without Permanent Scarring. <https://people.eecs.berkeley.edu/~klein/papers/lagrange-multipliers.pdf> .
Sections 1, 2 (up to 2.4), 3.1, 3.5

