From Calculus to Machine Learning

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- Identify a space of "reasonable" models
- Construct a function which computes how well a given model fits the data
- Find the model(s) which maximize (or minimize) the function

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In this seminar we'll try to understand some of the theory behind all three steps.

The plan:

1. Optimization for functions of one variable
2. Linear algebra and PCA
3. Optimization for functions of several variables
4. Conditional probability and Bayesian statistics
5. Linear regression
6. Perceptrons
7. Back propagation and gradient descent

1.1 Optimizing quadratic functions of one variable

You wish to build a rectangular fence next to a river. You have 100m of fence to work with and you want to enclose as much area as possible. How do you do it?

What is the space of models?

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- Each possible fence is determined by its height x and its width y

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- Constraints: $x \geq 0$, $y \geq 0$, and $2x + y = 100$

What is the objective function?

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We want to maximize the area $A(x, y) = xy$

This is now just a math problem: maximize $A(x, y) = xy$ subject to the constraints $x \geq 0$, $y \geq 0$, and $2x + y = 100$

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The objective function is quadratic and the constraint is linear, so we can hope to solve it analytically.

Using the constraint, eliminate y to get:

$$A(x) = x(100 - 2x)$$

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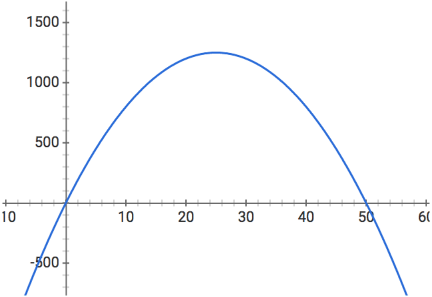

Algebraic magic:

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Since

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we get

$$A(x) \leq 1250$$

with equality if and only if $x = 25$

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Start with an expression of the form $x^2 + bx$.

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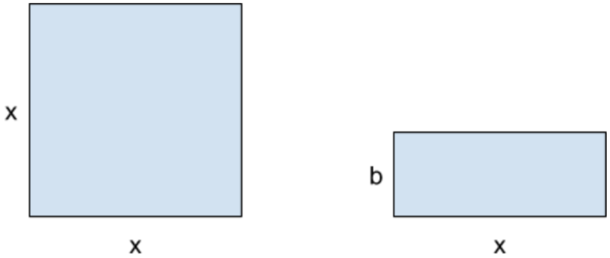

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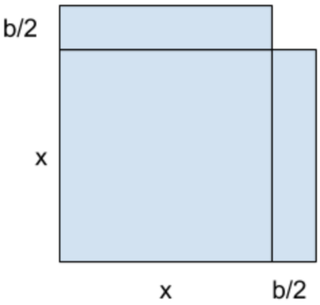

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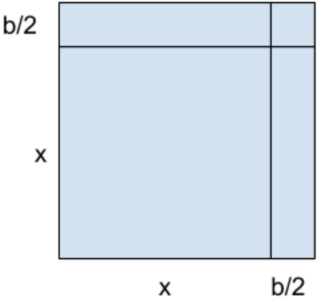

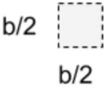

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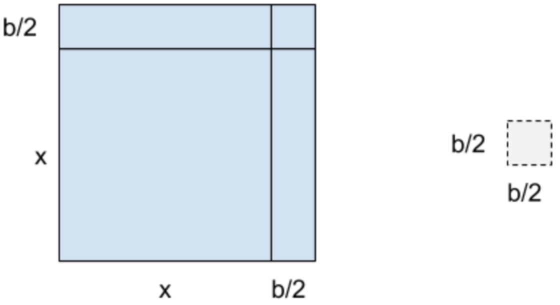

Conclusion:

$$x^2 + bx = \left(x + \frac{b}{2}\right)^2 - \left(\frac{b}{2}\right)^2$$

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Conclude with a little bit of simplifying:

$$A(x) = -2(x - 25)^2 + 2 \cdot 25^2 = -2(x - 25)^2 + 1250$$

Let's look at another optimization problem:

You want to build an open box with a square base which holds $25m^3$ of water. How much material do you need?

Space of models:

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Constraints: $x \geq 0$, $y \geq 0$, Volume $= x^2 y = 25$

Objective function:

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The amount of material needed is determined by the surface $S(x, y) = x^2 + 4xy$ of the box.

Constrained optimization problem: minimize $S(x, y) = x^2 + 4xy$ subject to the constraints $x \geq 0$, $y \geq 0$, and $x^2 y = 25$.

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The objective function is quadratic, but the constraint $x^2y = 25$ is cubic, so we expect this to be harder.

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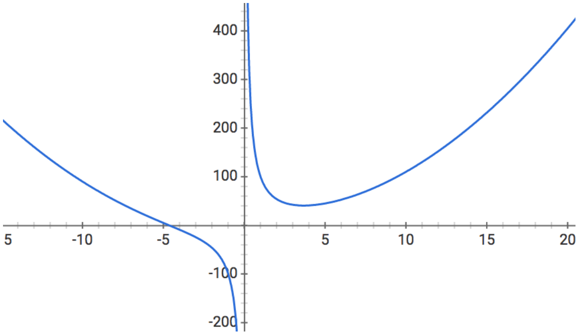

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Main idea: approximate a general function with linear and quadratic functions.

1.2 Optimization via linear approximation

Our objective now is to solve optimization problems of the following form:

Find the maximum and/or minimum value of a function $f : A \to \mathbb{R}$ where $\mathbb{R}$ is the set of all real numbers and A is a subset of $\mathbb{R}$.

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This problem is completely hopeless in general, but there are lots of techniques which work in special cases which come up in applications.

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Assume that f is defined on an interval (or finite collection of intervals) in $\mathbb{R}$; we will look at:

- The *local behavior* of f near points of interest in the interior of its domain

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Assume that f is defined on an interval (or finite collection of intervals) in $\mathbb{R}$; we will look at:

- The *local behavior* of f near points of interest in the interior of its domain
- The *boundary behavior* of f near the endpoints of its domain

Definition

A point $x_{\max \in A}$ is said to be a *local maximum* for f if

$$f(x_{\max}) \geq f(x)$$

for all x sufficiently close to $x_{\max}$.
Similarly, $x_{\min}$ is said to be a local minimum if $f(x_{\min}) \leq f(x)$ for all x near $x_{\min}$.

To find local extrema, we will use *local linear approximations*.

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Main idea: if x_0 is a local extremum of f and f can be well approximated by a line near x_0 then that line is flat (has slope zero).

1.3 Lines

Before approximating functions by lines, let us review some basic facts about them.

Definition

A function L is said to be *linear* if it satisfies the following conditions:

$$L(x+y) = L(x) + L(y), \quad L(ax) = aL(x)$$

for every x, y, and a.

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Fact: every linear function $L\colon \mathbb{R} \to \mathbb{R}$ has the form $L(x) = mx$ for some constant m called the *slope* of L.

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It is standard to simply refer to an affine function as a line and write its equation as $y = mx + b$.

Given a point (x_0, y_0) in the plane and a slope m, one can construct a line which passes through (x_0, y_0) with slope m by solving the following equation for y:

$$y - y_0 = m(x - x_0)$$

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Example

Find a line with slope -2 which passes through the point $(3, 5)$.

Given two points (x_0, y_0) and (x_1, y_1) in the plane (not on the same vertical line), one can construct a line which passes through both points by using the slope:

$$m = \frac{y_1 - y_0}{x_1 - x_0}$$

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Example

Find a line which passes through the points $(1, 4)$ and $(7, 5)$.

1.4 Linear approximation and limits

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Such a linear approximation does not necessarily exist:

Assuming it does exist, how would we find it?

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Certainly it should pass through the point $(a, f(a))$, so if we can find the slope m then the line has the form

$$y = f(a) + m(x - a)$$

Look at the slope of the line passing through $(a, f(a))$ and $(x, f(x))$ for x close to a:

$$m = \frac{f(x) - f(a)}{x - a}$$

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$$\begin{aligned}\frac{f(x) - f(a)}{x - a} &= \frac{x^2 - a^2}{x - a} \\ &= \frac{(x - a)(x + a)}{x - a} \\ &= x + a\end{aligned}$$

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So as x approaches a the slope approaches $a + a = 2a$.

Thus part of the fundamentals of linear approximation lies in the notion of a *limit*.

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Informally, we say that a function g approaches a number m as x approaches a point a, written

$$\lim_{x \to a} g(x) = m$$

provided that the values of g can be made arbitrarily close to m by restricting the inputs x to some neighborhood of a.

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However, scientists and mathematicians happily used calculus to solve hard problems for over two centuries before the rigorous definition was discovered, so we will follow their lead in this seminar and reason from intuition when it is necessary to work with limits.

Definition

- The *derivative* of a function f at a point a is the number

$$f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a}$$

if the limit exists. In this case f is said to be *differentiable* at a.

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- If f is differentiable at a then the *local linear approximation* of f at a is the function

$$\ell(x) = f(a) + f'(a)(x - a)$$

Intuition: $f'(a)$ represents the factor by which f stretches tiny intervals centered at a:

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Example

Use the previous definition to compute the local linear approximation of the given function at the given point.

- $f(x) = x^2$, $a = 2$

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- $f(x) = x^2$, $a = 2$
- $f(x) = \sqrt{x}$, $a = 4$
- $f(x) = \frac{1}{x}$, $a = 1$

1.5 Computing derivatives

Did you struggle a little with $\sqrt{x}$ and $\frac{1}{x}$?
Imagine trying $\frac{x^5}{\sqrt{4x^2-7}}$!

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There are a number of handy rules for recovering the derivative of a complicated function from the derivatives of simpler pieces, and this is normally how one handles functions like the above.

Power functions

For $p \neq 1$, the derivative of $f(x) = x^p$ is given by

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Example

- Differentiate $f(x) = x^3$
- Differentiate $f(x) = \frac{1}{x^3}$
- Differentiate $f(x) = \sqrt[3]{x}$

Linearity

Given $f(x) = ag(x) + bh(x)$ we have

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Example

Differentiate $f(x) = x^3 + \frac{2}{x^3} - 4\sqrt[3]{x}$

Chain rule

Let $f = h \circ g$, meaning $f(x) = h(g(x))$. Then:

$$f'(x) = g'(x)h'(g(x))$$

if g is differentiable at x and h is differentiable at $g(x)$.

Chain rule

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if g is differentiable at x and h is differentiable at $g(x)$.

Intuition: if g stretches by a factor of m near x and h stretches by a factor of n near $h(x)$ then $g \circ h$ stretches by a factor of mn.

Example

- Differentiate $f(x) = (x - 5)^2$

Example

- Differentiate $f(x) = (x-5)^2$
- Differentiate $f(x) = \frac{1}{x^3+2x}$

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- Differentiate $f(x) = \sqrt[3]{x^2+1}$

Product rule

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- Differentiate $f(x) = (x-5)^2(x-2)^5$

Example

- Differentiate $f(x) = (x-5)^2(x-2)^5$
- Differentiate $f(x) = \frac{\sqrt{x}}{x+2}$

Quotient rule

Given $f(x) = \frac{g(x)}{h(x)}$, we have:

$$f'(x) = \frac{g'(x)h(x) - g(x)h'(x)}{h(x)^2}$$

if g and h are differentiable at x and $h(x) \neq 0$.

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Example

- Differentiate $f(x) = \frac{x^2}{\sqrt{x-1}}$.
- Differentiate $f(x) = \frac{x^5}{\sqrt{4x^2-7}}$.