Introduction to Artificial Intelligence

Optimization

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January 23, 2020

Outline

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At the beginning

We have have

- Fermat
  - "Methodus ad disquirendam maximam et minimam et de tangentibus linearum curvarum"
- Lagrange
  - He was one of the creators of the calculus of variations, deriving the Euler–Lagrange equations for extrema of functionals.

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- Dantzig
  - He published the Simplex algorithm in 1947
- John von Neumann in 1947
  - Developed the min-max
  - And the Theory of Duality

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Definition of the Problem

A mathematical optimization problem

$$minimize f_0(\boldsymbol{x})$$
$$s.t. f_i(\boldsymbol{x}) \leq b_i \; i = 1, ..., m$$

Here, the vector $x^T = (x_1, ..., x_n)$

It is the optimization variable of the problem problem

The function $f_0 : \mathbb{R}^n \longrightarrow \mathbb{R}$

It is the objective function.

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Furthermore

The function $f_i : \mathbb{R}^n \longrightarrow \mathbb{R}$

They are the (inequality) constraint functions, and the constants $b_1, ..., b_m$ are the limits.

We want to find a vector

A vector x^* is called optimal, or a solution of the problem.

If it has the smallest objective value among all vectors that satisfy the constraints

for any z with $f_1(z) \leq b_1, ..., f_m(z) \leq b_m$

$$f_0(z) \geq f_i(x^*)$$

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We have several

An Optimization Problem is called linear program

If the objective and constraint functions $f_0, ..., f_m$ are linear:

$$f_i(\alpha \boldsymbol{x} + \beta \boldsymbol{y}) = \alpha f_i(\boldsymbol{x}) + \beta f_i(\boldsymbol{y})$$

for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ and all $\alpha, \beta \in \mathbb{R}$.

If the optimization problem is not linear

It is called a nonlinear program.

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If the optimization problem is not linear

It is called a nonlinear program.

In our case, we go half way

We have the following type of functions

A convex optimization problem is one in which the objective and constraint functions $f_0, ..., f_m$ are convex:

$$f_i(\alpha \boldsymbol{x} + \beta \boldsymbol{y}) \leq \alpha f_i(\boldsymbol{x}) + \beta f_i(\boldsymbol{y})$$

for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$ and all $\alpha, \beta \in \mathbb{R}$.

Here, we have constraints

$$\alpha + \beta = 1$$
$$\alpha \geq 0$$
$$\beta \geq 0$$

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Example

In portfolio optimization

We seek the best way to invest some capital in a set of n assets.

Vector representation of Assets

The variable x_i represents the investment in the i^{th} asset:

$$x^T = (x_1, x_2, x_3, ..., x_n)$$

Where the constraints might represent a limit on the budget

A limit on the total amount to be invested

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We have the following

The efficient frontier is the curve that shows all efficient portfolios in a risk-return framework:

1. An efficient portfolio is defined as the portfolio that maximizes the expected return for a given amount of risk (standard deviation).
2. The portfolio that minimizes the risk subject to a given expected return.

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We need a little bit of notation

We have

- C_0 capital that can be invested
- C_{end} capital at the end of the period
- R_p total portfolio return
- μ_p expected portfolio return
- σ_p^2 variance of portfolio return
- r vector rate of return on assets
- μ vector expected rate of return on assets
- θ vector amount invested at each asset
- $\Sigma = [\sigma_{ij}]$ matrix of covariances of returns r

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Then, we have

The following equalities

- $C_{end} = C_0 + R_p$
- $R_p = \boldsymbol{r}^T \theta$
- $\mu_p = \mu^T \theta$
- $\sigma_p^2 = \theta^2 \Sigma \theta$

Cost Function

We have

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\begin{aligned}
var\left(C_{end}\right) &= var\left(C_0 + R_p\right)\\
&= var\left(R_p\right)\\
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Under the constraints

First, the expected return must be fixed, because we are minimizing the risk given this return

$$\mu^T \theta = \mu_p$$

The second constraint is that we can only invest the capital we have

$$1^T \theta = C_0$$

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Using a little bit of linear algebra

We have that

$$A = \begin{bmatrix} \mu & 1 \end{bmatrix} \text{ and } B = \begin{bmatrix} \mu_p \\ C_0 \end{bmatrix}$$

We have that we can rewrite our problem as

$$\min \left\{ \theta^T \Sigma \theta | A^T \theta = B \right\}$$

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Firstly

We have that

A solution method for a class of optimization problems is an algorithm that computes a solution of the problem.

- Solving various classes of optimization problems.
- Analyzing their properties.
- Developing good software implementations.

- Particular forms of the objective function.
- Particular forms of the constraint functions.
- How many variables and constraints there are.

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A solution method for a class of optimization problems is an algorithm that computes a solution of the problem.

Since the late 1940s

A large effort has gone into developing algorithms for:

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In particular

Special structure

A problem is sparse if each constraint function depends on only a small number of the variables

Something Notable

Even when the objective and constraint functions are smooth

- The optimization is surprisingly hard to solve.

However, for a few problem

We have effective algorithms that can reliably solve even large problems (Thousand of variables and function)

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Introduction

Observation

we describe two very widely known and used special sub-classes of convex optimization:

- Least-Squares Problems
- Linear Programming

Least-Squares Error (LSE)

A least-squares problem is an optimization problem with no constraints

$$\min f_0(\boldsymbol{x}) = \sum_{i=1}^{k} \left(\boldsymbol{a}_i^T \boldsymbol{x} - b_i\right)^2 = \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2$$

Remember the Solution

$$\boldsymbol{x} = \left(A^T A\right)^{-1} A^T b$$

The least-squares problem can be solved in a time approximately proportional

$$O\left(n^2 k\right)$$

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In many cases we can solve even larger least-squares problems

Exploiting a special property of the problem

What if A is sparse?

It has far fewer than kn nonzero entries.

It is possible

To accelerate the solution of the LSE Problem

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Regularization

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Most of the inverse problems posed in science and engineering areas are ill posed.

- Basically if you have $Ax = b$ how do you find x?

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- Computational vision (Poggio, Torre, & Koch, 1985; Bertero, Poggio, & Torre, 1988),
- System identification (Akaike, 1974; Johansen, 1997),
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- etc

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The house example

Imagine the following data set

Now assume that we use LSE

For the fitting

$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{w}}\left(x_i\right)-y_i\right)^2$$

We can then run one of our machine to see what minimize better the previous equation

Question: Did you notice that I did not impose any structure to $h_w(x)$?

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Question: Did you notice that I did not impose any structure to $h_{\boldsymbol{w}}\left(x\right)$?

Then, First fitting

What about using $h_1(x) = w_0 + w_1 x + w_2 x^2$?

Second fitting

What about using $h_2(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$?

Therefore, we have a problem

We get weird over-fitting effects!!!

What do we do? What about minimizing the influence of w_3, w_4, w_5?

How do we do that?

$$\min_{w} \frac{1}{2} \sum_{i=1}^{N} \left(h_w \left(x_i \right) - y_i \right)^2$$

What about integrating those values to the cost function? Ideas

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Regularization intuition is as follow

Small values for parameters $w_0, w_1, w_2, ..., w_n$

It implies

1. "Simpler" function
2. Less prone to overfitting

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We can do the previous idea for the other parameters

We can do the same for the other parameters

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}}\left(x_i\right) - y_i\right)^2 + \sum_{i=1}^{d} \lambda_i w_i^2 \quad (1)$$

However handling such many parameters can be so difficult

Combinatorial problem in reality!!!

We can do the previous idea for the other parameters

We can do the same for the other parameters

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}}\left(x_i\right) - y_i\right)^2 + \sum_{i=1}^{d} \lambda_i w_i^2 \tag{1}$$

However handling such many parameters can be so difficult

Combinatorial problem in reality!!!

Better, we can

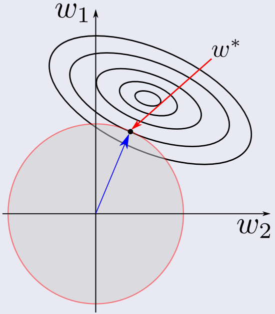
We better use the following

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}}\left(x_i\right) - y_i\right)^2 + \lambda \sum_{i=1}^{d} w_i^2 \tag{2}$$

Graphically

Geometrically Equivalent to

$\sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{w}\right)^2 + \lambda \sum_{i=1}^{d+1} w_i^2$



What about Thousands of Features?

There is a technique for that

Least Absolute Shrinkage and Selection Operator (LASSO) invented by Robert Tibshirani that uses $L_1 = \sum_{i=1}^{d} |w_i|$.

The Least Squared Error takes the form of

$$\sum_{i=1}^{N} \left(y_i - x^T w \right)^2 + \sum_{i=1}^{d} |w_i| \quad (3)$$

However

You have other regularizations as $L_2 = \sqrt{\sum_{i=1}^{d} |w_i|^2}$

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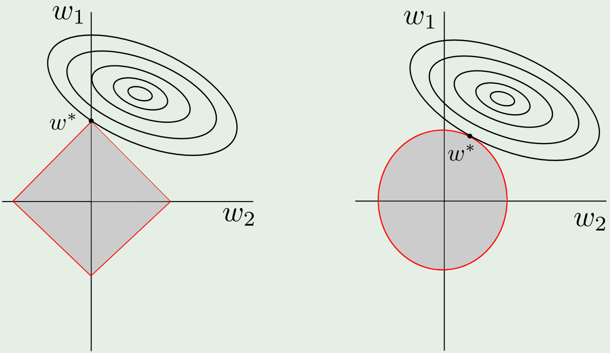
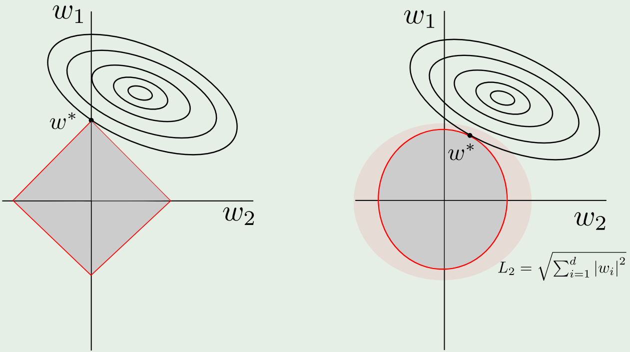
Graphically

The first area correspond to the L_1 regularization and the second one?



Graphically

Yes the circle defined as $L_2 = \sqrt{\sum_{i=1}^{d} |w_i|^2}$



Outline

Line Segments

Define a segment between two points

Suppose $\boldsymbol{x}_1 \neq \boldsymbol{x}_2$ are two points in $\mathbb{R}^n$. Points of the form

$$y = \lambda \boldsymbol{x}_1 + (1 - \lambda)\, \boldsymbol{x}_2$$

where $\lambda \in \mathbb{R}$ form a line passing through $\boldsymbol{x}_1, \boldsymbol{x}_2$.

In the case $\lambda \in (0, 1)$

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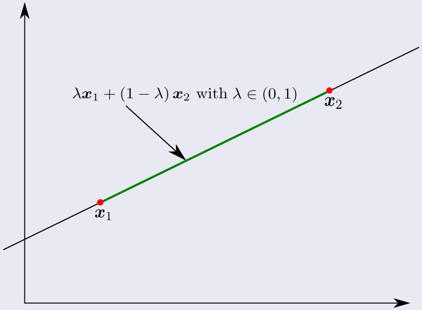
Example

We have in $\mathbb{R}^2$



Convex sets

Definition

A set C is convex if the line segment between any two points in C lies in C, i.e. if for any $\boldsymbol{x}_1, \boldsymbol{x}_2 \in C$ and any $\lambda \in [0,1]$

$$\lambda \boldsymbol{x}_1 + (1-\lambda)\,\boldsymbol{x}_2 \in C$$

Additionally

We call a point of the form

$$\lambda_1 \boldsymbol{x}_1 + \ldots + \lambda_n \boldsymbol{x}_n$$

a convex combination of points $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ with $\sum_{i=1}^{n} \lambda_i = 1$ and $\lambda_i \geq 0$

Denoted

$$conv\ C = \{\lambda_1 \boldsymbol{x}_1 + \ldots + \lambda_n \boldsymbol{x}_n | \boldsymbol{x}_i \in C$$
$$\lambda_i \in C \text{ and } \textstyle\sum_{i=1}^{n} \lambda_i = 1\}$$

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It is more

Something Notable

It can be shown that a set is convex if and only if it contains every convex combination of its points.

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If B is any convex set that contains C, then $conv\ C \subseteq B$.

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Intersection

Convexity is preserved under intersection:

- if S_1 and S_2 are convex, then $S_1 \cap S_2$ is convex.

Affine Transformation

If C is a convex set, $C \subseteq \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, then

$$AC + b = \{Ax + b | x \in C\} \subseteq \mathbb{R}^m$$

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Further

Translation and Scaling

$$C + b, \alpha C$$

Set sum

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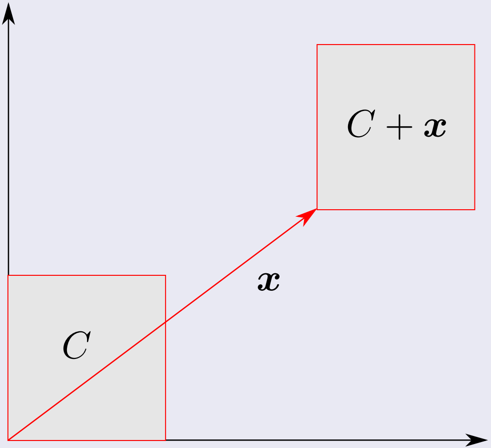
For Example

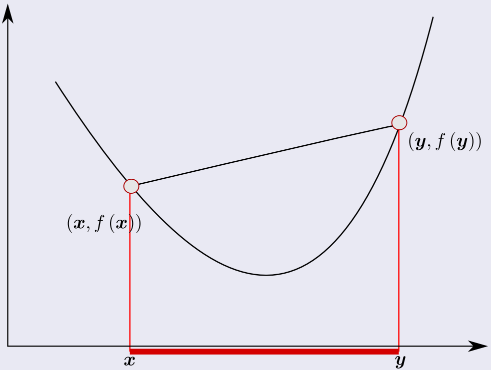
We have a convex set under translation



Outline

We have that

Intuition



Definition

Convex function

A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if $dom(f)$ is a convex set and if$\forall \boldsymbol{x}, \boldsymbol{y} \in dom(f), \forall \theta \in [0,1]$, we have:

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The epigraph of a function $f : \mathbb{R}^n \to \mathbb{R}$ is the set of points:

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Quite simple...

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Zeroth Order Property

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f is convex if and only if $\forall \boldsymbol{x} \in dom\left(f\right)$, $\forall \boldsymbol{u}$, the function

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Look at the board

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Remark

This property is useful

Checking the convexity of a multivariate function reduces to check the convexity of a univariate function.

1. Taking any point x on the $dom(f)$
2. Taking a vertical slice through the point x
3. The resulting plane intersects the domain of f on a line
4. Generating a new 2D function $g(t)$

Remark

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Example

1. A 3D convex cup-shaped function
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Outline

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Suppose f is differentiable

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Then f is convex if and only if $dom\left(f\right)$ is convex and

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We have the following situation

- Let $f : \mathbb{R}^n \to \mathbb{R}$ and consider the problem to minimize $f(\boldsymbol{x})$ subject to $\boldsymbol{x} \in S$.
- A point $x \in S$ is called a feasible solution to the problem.
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if $\nabla f(\boldsymbol{x}) = 0$

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Rearranging Terms

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Making $\alpha \longrightarrow 0$

$$g(t_1) \geq g(t_2) + g'(t_2)(t_1 - t_2)$$

Then $g(1) \geq g(0) + g'(0)$

$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$

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The other part of the proof

I leave you the part

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\boldsymbol{y} - \boldsymbol{x}) \implies f \text{ is convex}$$

Outline

Here, we assume

If f is twice differentiable

The Hessian exist!!!

Definition

Given a function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$, then the Jacobian of the derivatives

$$\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}$$

is called the Hessian Matrix H

I.e.

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A real matrix A is positive if

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For example

In the case for functions on $\mathbb{R}$

We have the simple condition $f''(x)$

- Which means that the first derivative $f'(x)$ is non-decreasing.

Outline

Then

Just as for convex sets

We consider standard operations which preserve function convexity.

Basically

We can say if a function is convex then it is constructed from simpler convex functions

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A way to test for convexity

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A way to test for convexity

We have

Non-negative weighted sum

$$\forall \alpha_i \geq 0, \; \sum_{i=1}^{k} \alpha_i f_i$$

Composition with affine mapping

$$f(Ax+b)$$

Composition with monotone convex

$g(f(x))$ is convex for f convex, g convex and non-decreasing.

We have

Non-negative weighted sum

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2. Hillclimbing
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We are interested in knowing those points $\boldsymbol{x} \in D \subseteq \mathbb{R}^n$ such that $f(\boldsymbol{x}_0) \leq f(\boldsymbol{x})$ of $f(\boldsymbol{x}_0) \geq f(\boldsymbol{x})$

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A minimum or a maximum point x_0.

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It is a search process using certain properties of the function.

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Local vs Global Minimum/Maximum

- Local minimum/maximum is the minimum/maximum in a neighborhood $L \subset D$.
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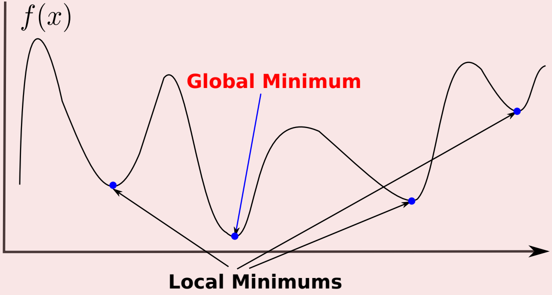

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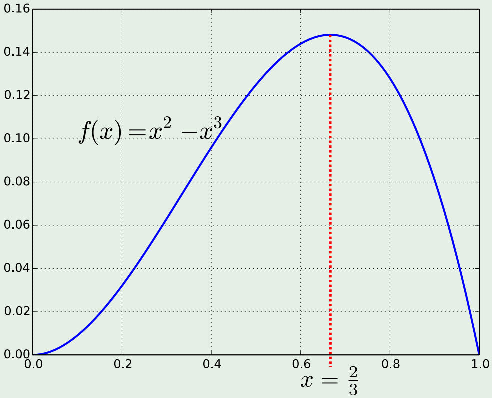

Do we have a Maximum or a Minimum

Second Derivative Test

The sign of the second derivative tells if each of those points is a maximum or a minimum:

1. If $\frac{d^2 f(x_i)}{dx^2} > 0$ for $x = x_i$ then x_i is a minimum.
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$$\frac{d^2 f(x)}{dx^2} = 2 - 6x$$

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$$\frac{d^2 f\left(\frac{2}{3}\right)}{dx^2} = 2 - 6 \times \frac{2}{3} = 2 - 4 = -2$$

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If the second derivative is 0 in a critical point x_i, then x_i may or may not be a minimum or a maximum of f. **WHY?**

We have for $x^3 - 3x^2 + x - 2$

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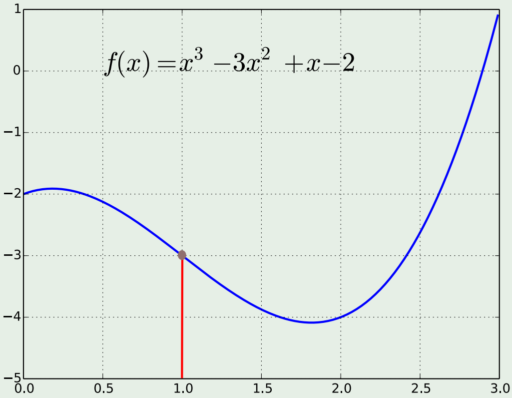

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Generalization

To move to higher dimensional functions, we will require to take partial derivatives!!!

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A system of equations!!!

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For a bounded D the only possible points of maximum/minimum are critical or boundary ones, so, in principle, we can find the global extremum.

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A lot of them

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Taylor's Expansion

Using the first order Taylor's expansion around point $x \in \mathbb{R}^n$ for $f : \mathbb{R}^n \to \mathbb{R}$

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \nabla f(\boldsymbol{x}_0)^T \cdot (\boldsymbol{x} - \boldsymbol{x}_0) + O\left(\|\boldsymbol{x} - \boldsymbol{x}_0\|^2\right)$$

Note:

- Actually the Taylor's expansions are polynomial approximation to the function!!!
- $\nabla f(x) = \left[\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, ..., \frac{\partial f(x)}{\partial x_n}\right]^T$ with $x = (x_1, x_2, ..., x_n)^T$

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With $h' = \frac{h}{\|\nabla f(\boldsymbol{x}_0)\|}$

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Outline

Gradient Descent

In the method of Gradient descent, we have a cost function $J(\boldsymbol{w})$ where

$$\boldsymbol{w}(n+1) = \boldsymbol{w}(n) - \eta \nabla J(\boldsymbol{w}(\boldsymbol{n}))$$

How, we prove that $J(\boldsymbol{w}(n+1)) < J(\boldsymbol{w}(n))$?

We use the first-order Taylor series expansion around $\boldsymbol{w}(n)$

$$J(\boldsymbol{w}(n+1)) \approx J(\boldsymbol{w}(n)) + \nabla J^T(\boldsymbol{w}(\boldsymbol{n}))\Delta\boldsymbol{w}(n) \quad (5)$$

Remark: This is quite true when the step size is quite small!!! In addition, $\Delta\boldsymbol{w}(n) = \boldsymbol{w}(n+1) - \boldsymbol{w}(n)$

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The equation of the tangent line to the curve $y = J(w(n))$

$$L(w(n)) = J'(w(n))[w(n+1) - w(n)] + J(w(n)) \tag{6}$$

Example

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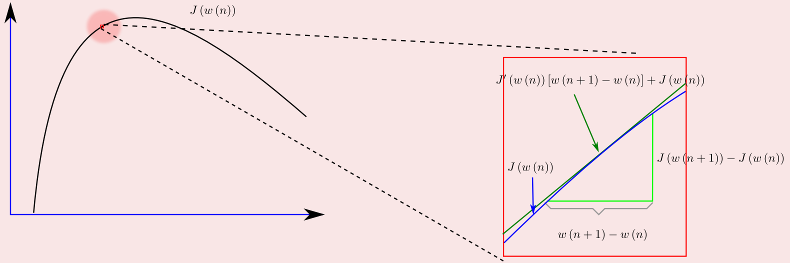

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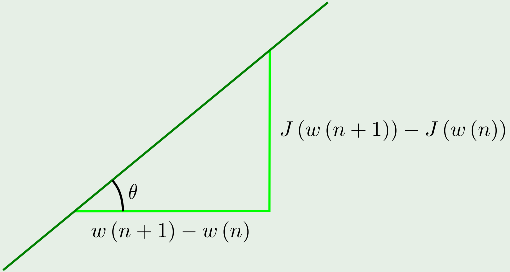
Remember Something quite Classic



$$\tan\theta = \frac{J(w(n+1)) - J(w(n))}{w(n+1) - w(n)}$$

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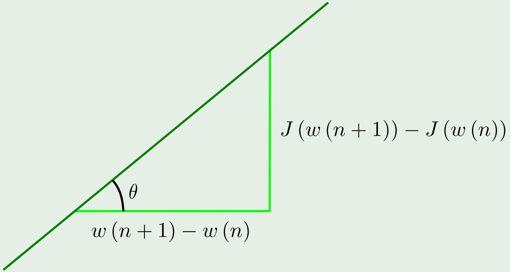

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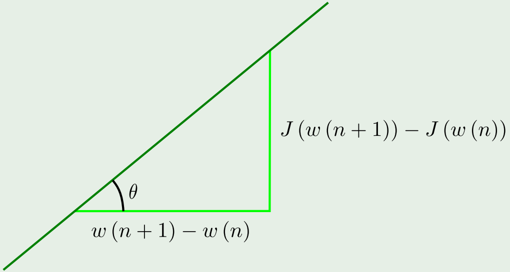

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Now, for Many Variables

An hyperplane in $\mathbb{R}^n$ is a set of the form

$$H = \left\{ \boldsymbol{x} | \boldsymbol{a}^T \boldsymbol{x} = b \right\} \tag{8}$$

Given $\boldsymbol{x} \in H$ and $\boldsymbol{x}_0 \in H$

$$b = \boldsymbol{a}^T \boldsymbol{x} = \boldsymbol{a}^T \boldsymbol{x}_0$$

Thus, we have that

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Definition (Differentiability)

Assume that J is defined in a disk D containing $\boldsymbol{w}(n)$. We say that J is differentiable at $\boldsymbol{w}(n)$ if:

1. $\frac{\partial J(\boldsymbol{w}(n))}{\partial w_i}$ exist for all $i = 1, ..., n$.
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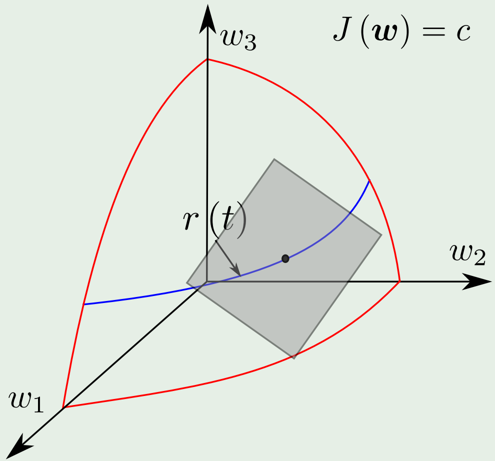
Thus, we have

$$\begin{aligned}\nabla J(\boldsymbol{w}(n)) &= \left(\frac{\partial J(\boldsymbol{w}(n))}{\partial w_1}, \frac{\partial J(\boldsymbol{w}(n))}{\partial w_2}, ..., \frac{\partial J(\boldsymbol{w}(n))}{\partial w_m}\right) \\ &= \sum_{i=1}^{m} \hat{w}_i \frac{\partial J(\boldsymbol{w}(n))}{\partial w_i}\end{aligned}$$

Where: $\hat{w}_i^T = (1, 0, ..., 0) \in \mathbb{R}$

Now

Given a curve function $r(t)$ that lies on the level set $J(\boldsymbol{w}(n)) = c$ (When is in $\mathbb{R}^3$)



Level Set

Definition

$$\{(w_1, w_2, ..., w_m) \in \mathbb{R}^m | J\,(w_1, w_2, ..., w_m) = c\} \quad (10)$$

Remark: In a normal Calculus course we will use x and f instead of $\boldsymbol{w}$ and J.

Where

Any curve has the following parametrization

$$r : [a, b] \to \mathbb{R}^m$$
$$r(t) = (w_1(t), ..., w_m(t))$$

With $r(n+1) = (w_1(n+1), ..., w_m(n+1))$

We can write the parametrized version of it

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Differentiating with respect to t and using the chain rule for multiple variables

$$\frac{dz(t)}{dt} = \sum_{i=1}^{m} \frac{\partial J(\boldsymbol{w}(t))}{\partial w_i} \cdot \frac{dw_i(t)}{dt} = 0 \quad (12)$$

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Given $y = f(\boldsymbol{u}) = (f_1(\boldsymbol{u}), ..., f_l(\boldsymbol{u}))$ and $\boldsymbol{u} = g(\boldsymbol{x}) = (g_1(\boldsymbol{x}), ..., g_m(\boldsymbol{x}))$.

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We have that

$$\nabla J\left(\boldsymbol{w}\left(n\right)\right) \cdot r'\left(n\right) = 0 \tag{14}$$

This proves that for every level set the gradient is perpendicular to the tangent to any curve that lies on the level set

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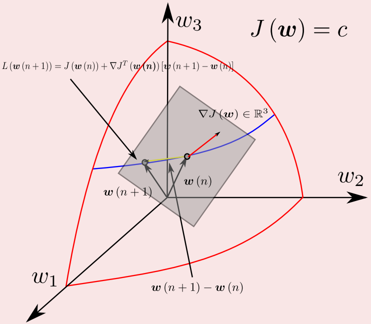

Proving the fact about the Gradient Descent

We want the following

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Outline

Algorithm of Gradient Descent

Initialization

1. Guess an init point x_0
2. Use a N_{max} iteration count
3. A gradient norm tolerance ϵ_g to know if we have arrived to a critical point.
4. A step tolerance ϵ_x to know if we have done significant progress
5. α_t is known as the step size.
   1. It is chosen to maintain a balance between convergence speed and avoiding divergence.

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Finally

Gradient_Descent($\boldsymbol{x}_0, N_{max}, \epsilon_g, \epsilon_t, \alpha_t$)

1. **for** $t = 0, 1, 2, \ldots, N_{max}$
2. $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \alpha_t \nabla f(\boldsymbol{x}_t)$

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2. $\quad \boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \alpha_t \nabla f(\boldsymbol{x}_t)$
3. $\quad$ **if** $\|\nabla f(\boldsymbol{x}_{t+1})\| < \epsilon_g$
4. $\quad\quad$ **return “Converged on critical point”**
5. $\quad$ **if** $\|\boldsymbol{x}_t - \boldsymbol{x}_{t+1}\| < \epsilon_t$
6. $\quad\quad$ **return “Converged on an x value”**
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  if $\|\boldsymbol{x}_t - \boldsymbol{x}_{t+1}\| < \epsilon_t$

    return “Converged on an x value”

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    return “Diverging”

return “Maximum number of iterations reached”

Finally

Gradient_Descent$(\boldsymbol{x}_0, N_{max}, \epsilon_g, \epsilon_t, \alpha_t)$

```
for t = 0, 1, 2, ..., N_max
        x_{t+1} = x_t − α_t ∇f(x_t)
        if ‖∇f(x_{t+1})‖ < ε_g
                return "Converged on critical point"
        if ‖x_t − x_{t+1}‖ < ε_t
                return "Converged on an x value"
        if f(x_{t+1}) > f(x_t)
                return "Diverging"
return "Maximum number of iterations reached"
```

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Given that the Canonical Solution has problems

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Gradient Descent

The basic procedure is as follow

1. Start with a random weight vector $\boldsymbol{w}(1)$.
2. Compute the gradient vector $\nabla J(\boldsymbol{w}(1))$.
3. Obtain value $\boldsymbol{w}(2)$ by moving from $\boldsymbol{w}(1)$ in the direction of the steepest descent:

$$\boldsymbol{w}(k+1) = \boldsymbol{w}(k) - \eta(k)\nabla J(\boldsymbol{w}(k)) \quad (16)$$

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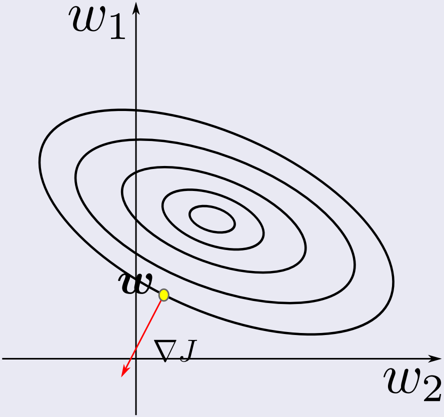
Geometrically

We have the following



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For our full regularized equation

We have

$$J(\boldsymbol{w}) = \frac{1}{2}\sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{d+1} x_j^i w_j\right)^2 + \frac{\lambda}{2}\sum_{j=1}^{d+1} w_j^2 \tag{17}$$

Then, for each w_j

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