Introduction to Artificial Intelligence

Search by Optimization

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Outline

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Optimization Searches

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3. Random Restart Hillclimbing
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The Hill Climbing Heuristic (Greedy Local Search)

What is Hill Climbing?

Hill climbing is a mathematical optimization technique which belongs to the family of local search.

Process

Iteratively it tries to improve the solution by changing one element of the solution so far.

- It is applicable to find a solution for the TSP.

Then

- If the change produces a better solution, an incremental change is made to the new solution.
  - Until no improvements can be made!!!

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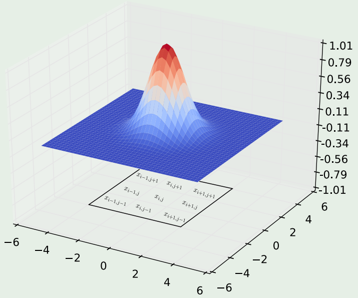
Example

Maybe you want to minimize something based in a Gaussian Function

$x_{i-1,j+1}$	$x_{i,j+1}$	$x_{i+1,j+1}$
$x_{i-1,j}$	$x_{i,j}$	$x_{i+1,j}$
$x_{i-1,j-1}$	$x_{i,j-1}$	$x_{i+1,j-1}$



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Algorithm

Discrete Space Hill Climbing Algorithm

1. currentNode = startNode
2. while true
3. $\quad L$ = NEIGHBORS(currentNode)
4. $\quad$ nextEval = $-\infty$
5. $\quad$ nextNode = NULL
6. $\quad$ for all $x \in L$
7. $\quad\quad$ if (EVAL(x) > nextEval)
8. $\quad\quad\quad$ nextNode = x
9. $\quad\quad\quad$ nextEval = EVAL(x)
10. $\quad\quad$ if nextEval <= EVAL(currentNode)
11. $\quad\quad\quad$ //Return current node since no better neighbors exist
12. $\quad\quad\quad$ return currentNode
13. $\quad\quad$ currentNode = nextNode

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Example: TSP

Goal

The main idea of TSP is the problem faced by a salesman to visit all towns or cities in an area, without visiting the same town twice.

The Simplest Version

- It assumes that each town is a point in the $\mathbb{R}^2$ plane.
- Thus a node in the problem is a sequence of cities to be visited in order

$$X_i = \langle x_1, x_2, ..., x_n \rangle$$

Where $x_1 == x_n$

The "Eval" function

$$Eval\left(\langle x_1, x_2, ..., x_n \rangle\right) = \sum_{i=1}^{n} \|x_{i+1} - x_i\|$$

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Something Notable

The definition of the neighborhoods is not obvious or unique in general.

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A new neighbor will be created by swapping two cities

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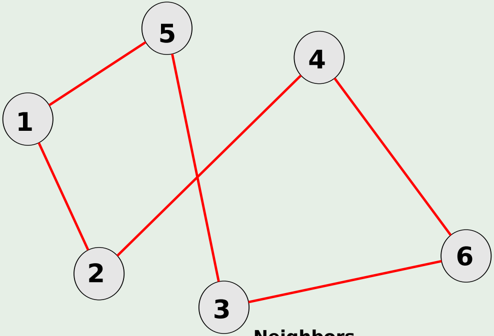
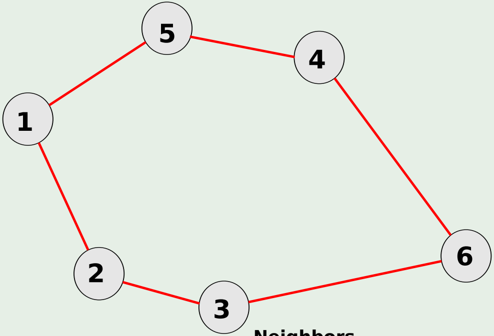


Neighbors

$$\langle 1, 5, \boxed{3}, 6, \boxed{4}, 2, 1 \rangle$$

Example

New Local State



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This idea of neighborhood

It is used for Genetic Algorithm (GA) for mutating elements in the population!!!

Thus

By looking at elements of the neighborhood

- New permutations by swapping cities

It is possible to obtain local improvements by improving

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- Heuristic search algorithms were developed that do not insist on the optimal solution.
- Some strategies even sacrifice completeness and may fail to find a solution of a solvable problem instance.
  - **But the have strategies to decrease the likelihood of such errors.**

- Enforced Hill Climbing
- Weighted A*
- Overconsistent A*
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We want something more stable

A more stable version is enforced hill-climbing.

- It picks a successor node, only if it has a strictly better evaluation than the current node.

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Algorithm

Enforced-Hill-Climbing$(s, h, Expand)$

Input: Implicitly given graph with start node s, successor generating function $Expand$ and a heuristic h

Output: Path to node $t \in T$

```
u = s
ht = h(s)
while (ht ≠ 0)
        (u', ht') = EHC-BFS(u, h, Expand)
        if (ht' = ∞) return ∅
        u = u'
        ht = ht'
return Path(u)
```

Algorithm

EHC-BFS$(u, h, Expand)$

Input: Node u with evaluation $h(u)$

Output: Node v with evaluation $h(v) < h(u)$ or failure

```
Enqueue (Q, u)
while (Q ≠ 0)
        v = Dequeue (Q)
        if (h(v) < h(u)) return (v, h (v))
        Succ (v) = Expand (v)
        for each w ∈ Succ (v)
                Enqueue (w)
return (·, ∞)
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The Problem with Dead-Ends

Definition

Given a planning task, a state S is called a dead end **if and only** if it is reachable and no sequence of actions achieves the goal from it.

We will look more about this in Classic Planning

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Theorem (Completeness Enforced Hill-Climbing)

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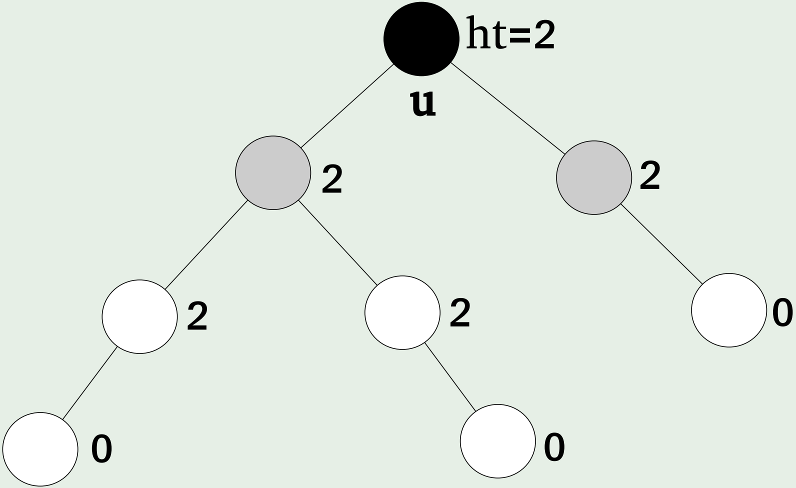
Example

Example of enforced hill-climbing (two iterations)



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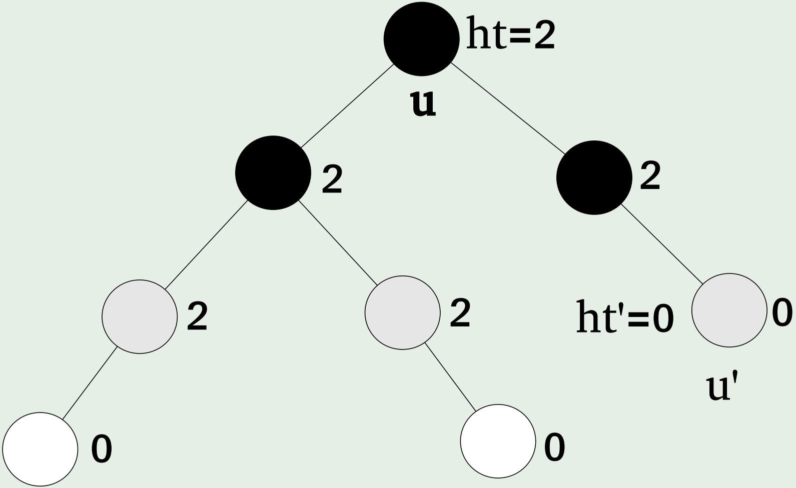
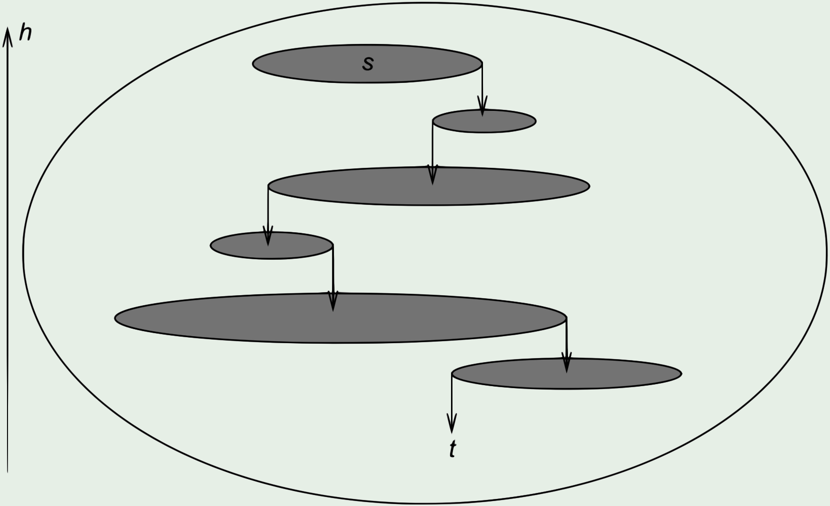


It is more

Search plateaus generated with enforced hill-climbing



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Pretty obvious what this is...

- Generate a random start state
- Run hill climbing and store answer
- Iterate, keeping the current best answer as you go
  - Stopping... when?

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We can do better by using Simulated Annealing

Definition of terms

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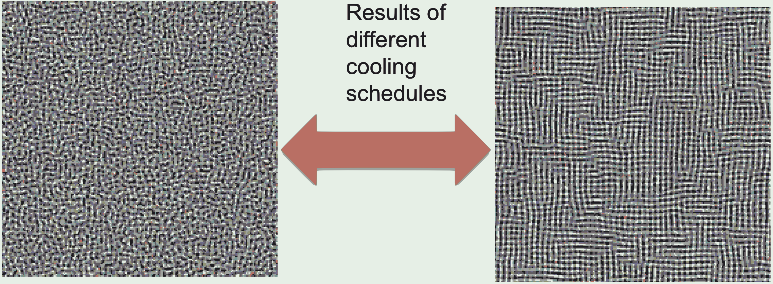
Analogy

Slowly cool down a heated solid, so that all particles arrange in the ground energy state

At each temperature wait until the solid reaches its thermal equilibrium



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The Metropolis Acceptance Criterion

Something Notable

The criterion models how a thermodynamic system moves from the current solution $\omega \in \Omega$ to a candidate solution $\omega' \in N(\omega)$.

Acceptance Probability

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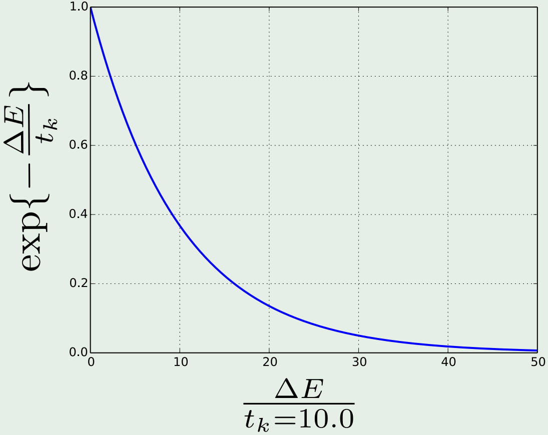

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If $\frac{\Delta E}{t_k} \to \infty$

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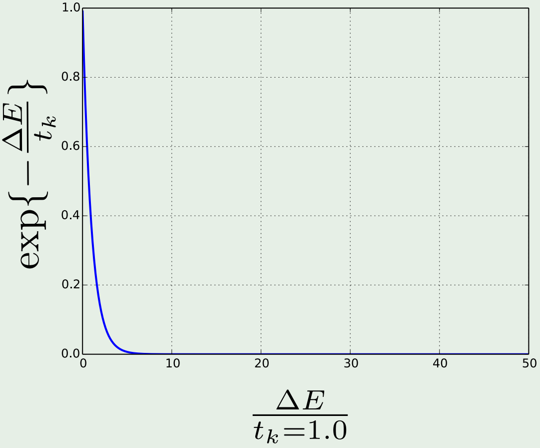

Meaning

The larger is the t_k

The more probable we accept larger jumps from $f(\omega)$.

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The system will reach an equilibrium at certain iteration k

This equilibrium follows the Boltzmann distribution

It is the probability of the system being in state $\omega \in \Omega$ with energy $f(\omega)$ at temperature T such that

$$P\left\{\text{System in state } \omega \text{ at temp } T\right\} = \frac{\exp\left\{-\frac{f(\omega)}{t_k}\right\}}{\sum_{\omega'' \in \Omega} \exp\left\{-\frac{f(\omega'')}{t_k}\right\}}$$

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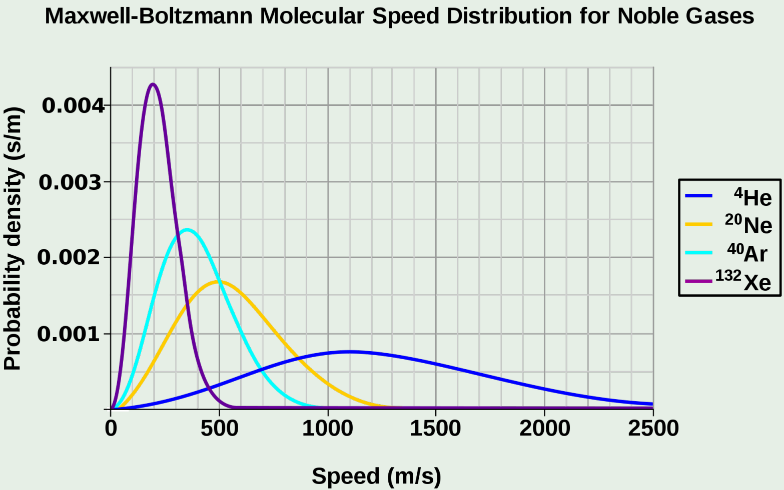
Example of Boltzmann distribution

For Gases



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We have

1. M_k number of steps at each temperature t_k
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Algorithm

Simulated_Annealing$(\omega, M_k, \epsilon_t, \epsilon, t_k, f)$

$\Delta E = \infty$

while $|\Delta E| > \epsilon$

  for $i = 0, 1, 2, ..., M_k$

    Randomly select ω' **in** $N(\omega)$

    $\Delta E = f(\omega') - f(\omega)$

    if $\Delta E \leq 0$

      $\omega = \omega'$

    if $\Delta E > 0$

      $\omega = \omega'$ **with probability** $Pr\{Accepted\} = \exp\left\{\frac{-\Delta E}{t_k}\right\}$

  $t_k = t_k - \epsilon_t$ **# We can also use** $t_k = \epsilon_t \cdot t_k$

Meaning of probability $Pr\left\{Accepted\right\} = \exp\left\{\frac{-\Delta E}{t_k}\right\}$

Basically

You draw a random value α from the distribution $U\left(0,1\right)$

Then if

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What happen if you have the following

What if you have a cost function with the following characteristics

- It is parametrically defined.
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What we want

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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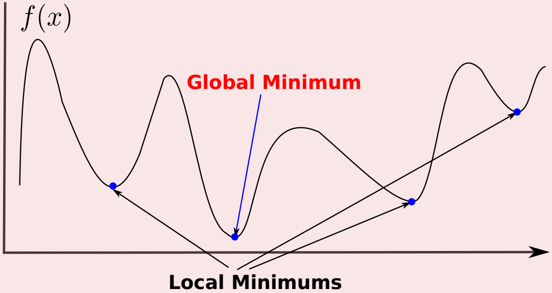

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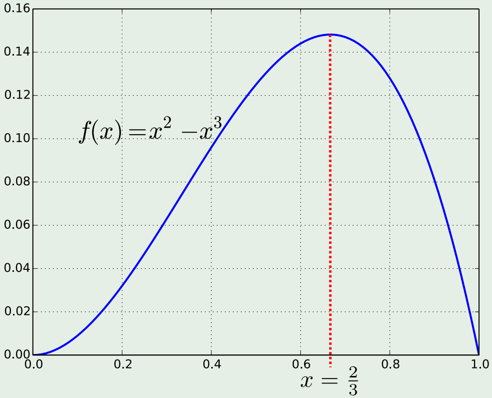

Do we have a Maximum or a Minimum

Second Derivative Test

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

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

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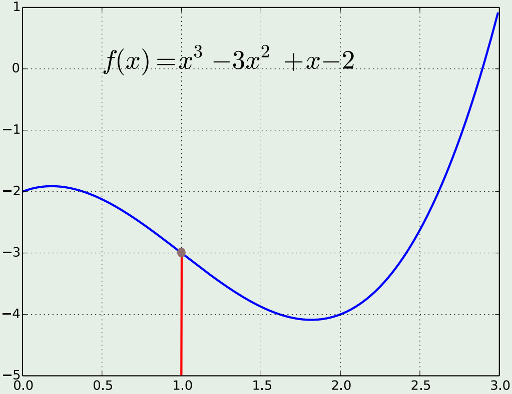

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Generalization

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A system of equations!!!

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A lot of them

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Taylor's Expansion

Using the first order Taylor's expansion around point $\boldsymbol{x} \in \mathbb{R}^n$ 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!!!
- $\nabla f(\boldsymbol{x}) = \left[\frac{\partial f(\boldsymbol{x})}{\partial x_1}, \frac{\partial f(\boldsymbol{x})}{\partial x_2}, \ldots, \frac{\partial f(\boldsymbol{x})}{\partial x_n}\right]^T$ with $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$

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$$f\left(\boldsymbol{x}_0 + h\boldsymbol{u}\right) - f\left(\boldsymbol{x}_0\right) \approx h\nabla f\left(\boldsymbol{x}_0\right)^T \cdot \boldsymbol{u}$$

Then

We minimize

$$\nabla f\left(\boldsymbol{x}_0\right)^T \cdot \boldsymbol{u}$$

Thus, the unit vector that minimize

In order to obtain the largest difference

$$\boldsymbol{u} = -\frac{\nabla f\left(\boldsymbol{x}_0\right)}{\left\|\nabla f\left(\boldsymbol{x}_0\right)\right\|}$$

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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 $\boldsymbol{w}(n)$

$$J(\boldsymbol{w}(n+1)) \approx J(\boldsymbol{w}(n)) + \nabla J^T(\boldsymbol{w}(n)) \Delta \boldsymbol{w}(n) \quad (2)$$

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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Why? Look at the case in $\mathbb{R}$

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

$$L\left(w\left(n\right)\right) = J'\left(w\left(n\right)\right)\left[w\left(n+1\right) - w\left(n\right)\right] + J\left(w\left(n\right)\right) \tag{3}$$

Example

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

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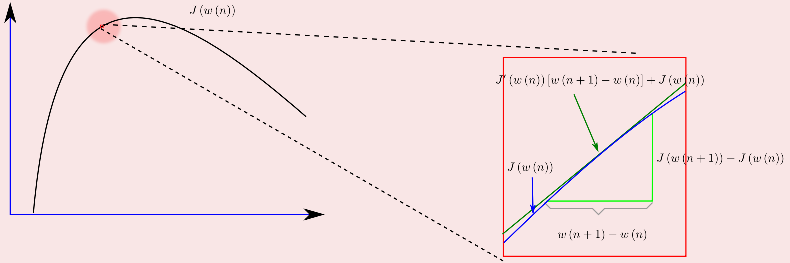

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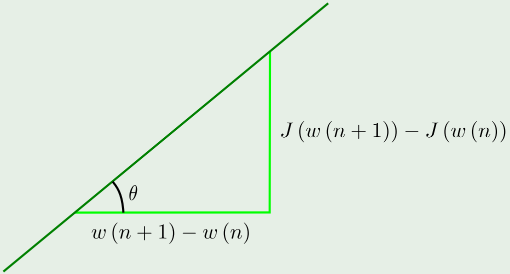

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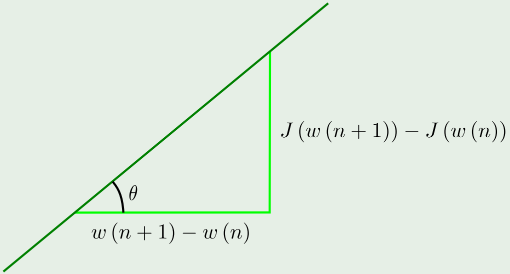

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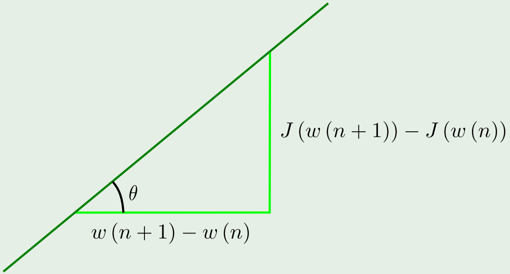

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Now, for Many Variables

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

$$H = \left\{ \boldsymbol{x} | \boldsymbol{a}^T \boldsymbol{x} = b \right\} \tag{5}$$

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

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

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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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We know that we have the following operator

$$\nabla = \left(\frac{\partial}{\partial w_1}, \frac{\partial}{\partial w_2}, ..., \frac{\partial}{\partial w_m}\right) \tag{6}$$

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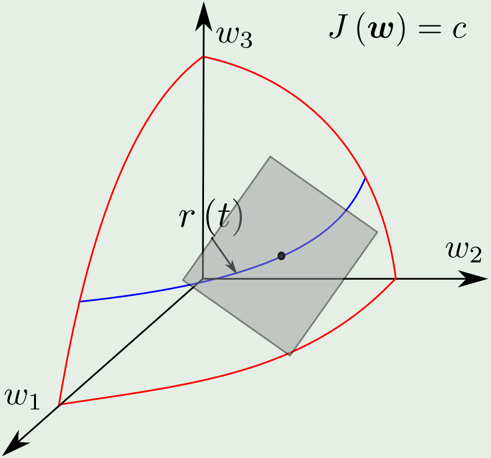
Thus, we have

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

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

$$\{(w_1, w_2, ..., w_m) \in \mathbb{R}^m | J\,(w_1, w_2, ..., w_m) = c\} \quad (7)$$

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

$$z(t) = J(w_1(t), w_2(t), ..., w_m(t)) = c \tag{8}$$

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

$$\frac{dz(t)}{dt} = \sum_{i=1}^{m} \frac{\partial J(\boldsymbol{w}(t))}{\partial w_i} \cdot \frac{dw_i(t)}{dt} = 0 \tag{9}$$

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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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Evaluating at $t = n$

$$\sum_{i=1}^{m} \frac{\partial J\left(\boldsymbol{w}\left(n\right)\right)}{\partial w_i} \cdot \frac{dw_i(n)}{dt} = 0$$

We have that

$$\nabla J\left(\boldsymbol{w}\left(n\right)\right) \cdot \boldsymbol{r}'\left(n\right) = 0 \qquad (11)$$

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

In particular to the point $\boldsymbol{w}\left(n\right)$.

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Now the tangent plane to the surface can be described generally

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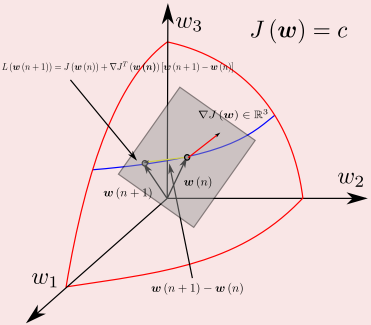

Proving the fact about the Gradient Descent

We want the following

$$J\left(\boldsymbol{w}\left(n+1\right)\right) < J\left(\boldsymbol{w}\left(n\right)\right)$$

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Outline

Algorithm of Gradient Descent

Initialization

1. Guess an init point $\boldsymbol{x}_0$
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.
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Gradient_Descent($x_0, N_{max}, \epsilon_g, \epsilon_t, \alpha_t$)

1. **for** $t = 0, 1, 2, ..., N_{max}$
2. $\quad x_{t+1} = x_t - \alpha_t \nabla f(x_t)$

Finally

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

1. **for** $t = 0, 1, 2, ..., N_{max}$
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"**
7. $\quad$ **if** $f(\boldsymbol{x}_{t+1}) > f(\boldsymbol{x}_t)$
8. $\quad\quad$ **return "Diverging"**
9. **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"
```

Finally

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

for $t = 0, 1, 2, ..., N_{max}$

  $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \alpha_t \nabla f(\boldsymbol{x}_t)$

  if $\|\nabla f(\boldsymbol{x}_{t+1})\| < \epsilon_g$

    return "Converged on critical point"

  if $\|\boldsymbol{x}_t - \boldsymbol{x}_{t+1}\| < \epsilon_t$

    return "Converged on an x **value"**

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$\nabla f(x)$ give us the direction of the fastest change at x.

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