

GOAL PROGRAMMING → find the  $x \in \mathbb{R}^n$  to get a particular value from  $[f_1(x), \dots, f_m(x)]$

MULTI-AGENT SYSTEMS → each agent can  
 1) harvest info from environment  
 2) act on environment  
 3) receive reward from environment

Then they need to cooperate or compete to reach a goal

OPTIMIZATION TYPES

- ① Local vs Global
    - local: gradient methods
    - global: space filling curves (effective in low dimensional spaces)
  - ② Deterministic vs Stochastic (eg. SLS or EA) or SIMULATED ANNEALING
  - ③ Single vs Multi Objective
  - ④ Single vs Multi Agent
  - ⑤ Heuristic vs Metaheuristic
    - Heuristic: problem specific methods like greedy
    - Metaheuristic: doesn't need domain knowledge, generates solutions typically with stochastic methods (nature inspired algorithms → GA, Ant colony, Swarm Intelligence)
- Swarm Intelligence (SI) → decentralized system of agents, interacting locally with one another and the environment  
 - emerges intelligence that is unknown from single agent

Multi Objective Optimization

$$\begin{cases} \min F(x) = (f_1(x), \dots, f_n(x)) \\ x \in D \end{cases}$$

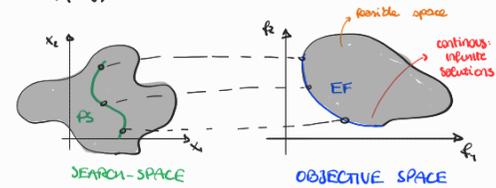
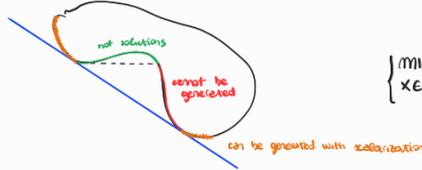
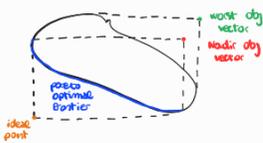
↖ search space

-  $x$  può essere continua, discreto o una mixing variables

$\vec{x}$  dominates  $\vec{y}$  ↔  
 1)  $f_i(x) \leq f_i(y) \forall i$   
 2)  $\exists j: f_j(x) < f_j(y)$

- strongly dominates if  $\forall i: f_i(x) < f_i(y)$

$\vec{x}$  is a pareto optimum if it is not dominated by any other solution  
 - objectives are conflicting, otherwise we have an ideal point  $\in D$



PS: pareto set  
 EF: efficient frontier

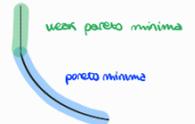
$$\begin{cases} \min \sum w_i \cdot F(x) \\ x \in D \end{cases} \text{ with } \sum w_i = 1 \wedge w_i \geq 0$$

can generate all the solutions ↔ P is convex

$$\begin{aligned} \bigcup_{w_i} S_{w_i} &= \{ \text{Weak minimum} \} \quad (\exists x \in S: f(x) \leq f(x^*) \forall i) \\ \bigcap_{w_i} S_{w_i} &\in \{ \text{Minimum} \} \\ &\downarrow \\ &\text{equal in the linear case} \end{aligned}$$

To obtain the final solution we need to weight the objectives

- 1) a priori → single obj optimization
- 2) a posteriori → get the pareto optimal set and then choose the preferred solution
- 3) interactive → providing feedback and zero to focus (from humans or AI)



Objectives of the optimizers

- 1) find solutions as close as possible to EF
  - 2) try to reach the extremes of EF
  - 3) solutions as uniform distributed as possible
- } META-TARGETS

Two algorithms 1) scalarization 2) population based → more solutions per iteration (eg. GA)

GA → avoid problems with non-convex P and generate with a single pass more points of EF  
 - handles well non-differentiable objectives

GENETIC ALGORITHMS → meta-heuristic optimization algorithms, taking inspiration by evolution

1) A solution may be encoded as string, if binary:  $\begin{matrix} 2^5 & 2^6 \\ 0100 & 010010 \\ \hline x_1 & x_2 \end{matrix}$  we can map them with  $x_i = x_i^{\min} + \frac{x_i^{\max} - x_i^{\min}}{2^{e_i} - 1} \text{BV}(s_i)$  (s: string int)

- cross over operator → select two strings and recombine them in two offspring by mix together the genetic materials
  - single point cross-over: randomly select a crossing site and exchange all bits on its right
  - uniform cross-over → select a bit from one of the two parents with p probability
 not all strings undergo the cross over, we use  $p_c$  to model the P to select a string
- mutation operator → randomly mutate some genes at random (probability of  $p_m$ )
- Elitist → when the best solution (or all the non dominated ones) can be selected without mutation and crossover to the next generation (will be selected if not outperformed by the offspring)

2) Vector of real numbers  $x \in \mathbb{R}^n$  → perturb with noise, combine  $x_i, x_n$  with averaging, ...

replace only a few individuals at each generation, more computationally efficient, but more generations needed to converge

1) Steady State + Mutation  
elitist

create randomly initial population of pop\_size  
evaluate their fitness (obj + penalization if not feasible)  
while (not termination condition)  
- choose at random (or  $\propto$  fitness) one individual from curr population  
- mutate and evaluate fitness  
- add to current population  
- remove worst individual

2) SS + Cross-Over + Mutation

→ inside the while:

- choose at random two individuals  
- cross-over to generate two offspring  
- mutate both, evaluate  
- remove the worst two

3) Generational GA + Cross-Over + Mutation

potential full population replacement in one generation → more aggressive

still elitist

$t=0$ , create  $P_t$  (randomly (pop\_size), evaluate  $P_t$   
while (not finish)  
- create  $Q_t$  of offspring from  $P_t$  of the same size (pop\_size)  
- evaluate  $Q_t$   
-  $R_t = Q_t \cup P_t$  (2 pop\_size)  
- create  $P_{t+1}$  by removing the worst pop\_size from  $R_t$

To create  $Q_t$ :

while (size  $Q_t <$  pop\_size)  
select first parent with BTS  
select second parent with BTS  
generate offsprings  
mutate and evaluate  
add to  $Q_t$

Binary Tournament Selection (if P constrained)

Pick two individuals at random from  $P_t$

- if both are feasible keep the best
- if only one is feasible keep that
- keep the one that updates less the contents

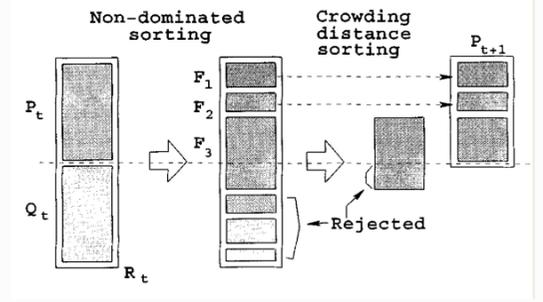
MOGA

- Family I → pareto dominance based algorithms (NSGA-II, PAES)
- Family II → indicator based algorithms (SMS-EMOA, HyPE, CHEA)
- Family III → decomposition based algorithms (MOEA/D)

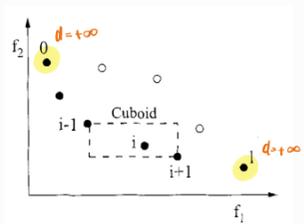
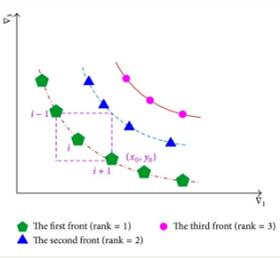
NSGA-II (non-dominated sorted GA)

params: pop\_size, n\_generation, p\_cross, p\_mut, elitist  
no niche size as I

$P_0$  ← random initial population of size pop\_size  
 $Q_0$  ← offsprings from  $P_0$  of size pop\_size  
for  $i=1$  to max\_gen  
 $R_t = P_t \cup Q_t$   
 $F$  ← fast-non dominated sort of  $R_t$  ( $F = (F_1, \dots)$ )  
 $i \leftarrow 1, P_{t+1} \leftarrow \{\emptyset\}$   
while  $|P_{t+1}| + |F_i| \leq$  pop\_size  
 $P_{t+1} = P_{t+1} \cup F_i$   
 $i \leftarrow i+1$   
compute crowding distance of  $F_i$  → last portion  
 $K \leftarrow$  pop\_size -  $|P_{t+1}|$  # elements to be added from  $F_i$   
 $P_{t+1} \leftarrow P_{t+1} \cup$  best  $K$  elements in  $F_i$   
 $Q_t \leftarrow$  generate offsprings from  $P_{t+1}$



**fast-non-dominated-sort( $P$ )**  
for each  $p \in P$   
 $S_p = \emptyset$   
 $n_p = 0$   
for each  $q \in P$   
if  $(p < q)$  then  
if  $p$  dominates  $q$   
 $S_p = S_p \cup \{q\}$   
Add  $q$  to the set of solutions dominated by  $p$   
else if  $(q < p)$  then  
Increment the domination counter of  $p$   
 $n_p = n_p + 1$   
 $p$  belongs to the first front  
if  $n_p = 0$  then  
 $p_{rank} = 1$   
 $F_1 = F_1 \cup \{p\}$  → non dominated solutions  
 $i = 1$   
while  $F_i \neq \emptyset$   
 $Q = \emptyset$   
Initialize the front counter  
Used to store the members of the next front  
for each  $p \in F_i$  → last frontier  
for each  $q \in S_p$   
 $n_q = n_q - 1$   
if  $n_q = 0$  then  
 $q$  belongs to the next front  
 $q_{rank} = i + 1$   
 $Q = Q \cup \{q\}$  → add to next frontier iff not dominated by any other, just  $F_1, \dots, F_i$   
 $i = i + 1$   
 $F_i = Q$



**crowding-distance-assignment( $I$ )**

$l = |I|$   
for each  $i$ , set  $I[i].distance = 0$   
for each objective  $m$   
 $I = \text{sort}(I, m)$   
 $I[1].distance = I[l].distance = \infty$   
for  $i = 2$  to  $(l-1)$   
 $I[i].distance = I[i].distance + (I[i+1].m - I[i-1].m) / (\frac{f_m^{\max}}{m} - \frac{f_m^{\min}}{m})$  → normalization  
number of solutions in  $I$   
initialize distance  
sort using each objective value  
so that boundary points are always selected  
for all other points  
equal weight among objectives

- selgo quelle con crowding distance maggiore perché zona meno affollata in quel fronte → soluzioni uniformi

- works also on non-convex ES

$(\mu-\lambda)$ -PAES  
 initially only mutation  
 Pareto ordered ES

→ mutation only (evolutionary strategies)

$\mu$ : number of current solutions

$\lambda$ : number of mutants generated from current solutions

when  $\lambda=1$ : steady state algorithm

(1-1) PAES

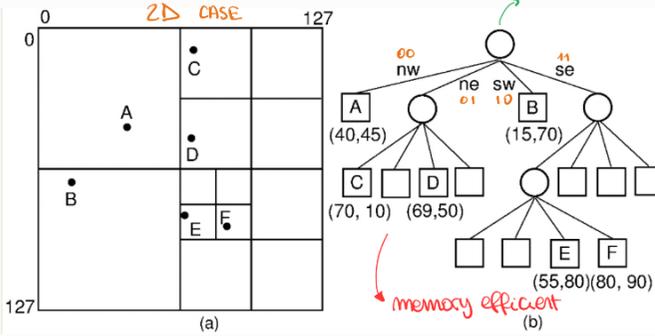
1 generate initial random solution  $c$  and add it to the archive  
 2 mutate  $c$  to produce  $m$  and evaluate  $m$   
 3 if ( $c$  dominates  $m$ ) discard  $m$   
 4 else if ( $m$  dominates  $c$ )  
 5 replace  $c$  with  $m$ , and add  $m$  to the archive  
 6 else if ( $m$  is dominated by any member of the archive) discard  $m$   
 7 else apply  $\text{test}(c, m, \text{archive})$  to determine which becomes the new current solution and whether to add  $m$  to the archive  
 8 until a termination criterion has been reached, return to line 2

test( $c, m, \text{archive}$ )

```

1 if the archive is not full
2 add  $m$  to the archive
3 if ( $m$  is in a less crowded region of the archive than  $c$ )
4 accept  $m$  as the new current solution
5 else maintain  $c$  as the current solution
6 else
7 if ( $m$  is in a less crowded region of the archive than  $x$  for
   some member  $x$  on the archive)
8 add  $m$  to the archive, and remove a member of the archive from
   the most crowded region
9 if ( $m$  is in a less crowded region of the archive than  $c$ )
10 accept  $m$  as the new current solution
11 else maintain  $c$  as the current solution
12 else
13 if ( $m$  is in a less crowded region of the archive than  $c$ )
14 accept  $m$  as the new current solution
15 else maintain  $c$  as the current solution
  
```

$m$  may be the current solution but  $\notin$  archive



- Assuming the range is defined for each objective I can repeatedly bisection each objective range

2<sup>nd</sup> hypercubes  $l$ : # of space bisection  $d$ : space dimension

Adaptive method: specify  $l$  but not the range  $\Rightarrow$  variable size hypercubes

- the range for  $m$  objective is the one of current solutions
- recompute the grid  $\Leftrightarrow$  the  $\Delta$  range  $>$   $\epsilon$

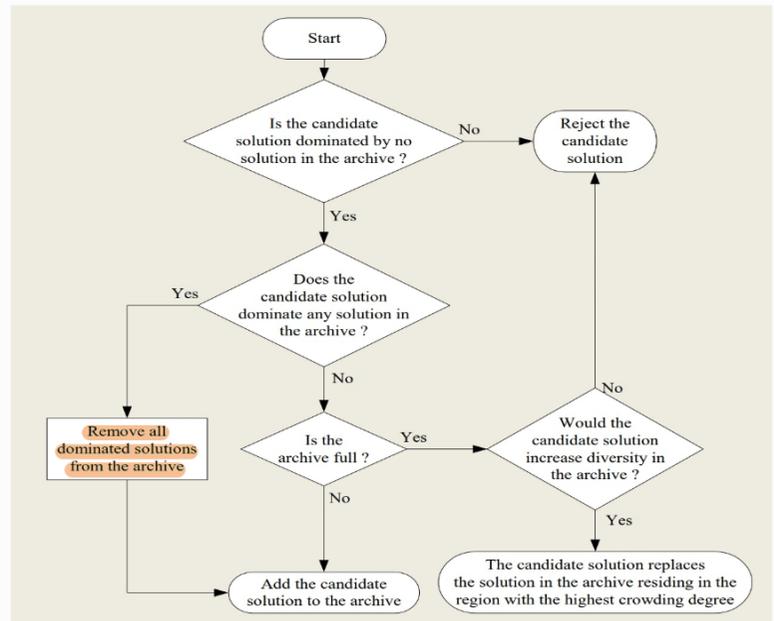
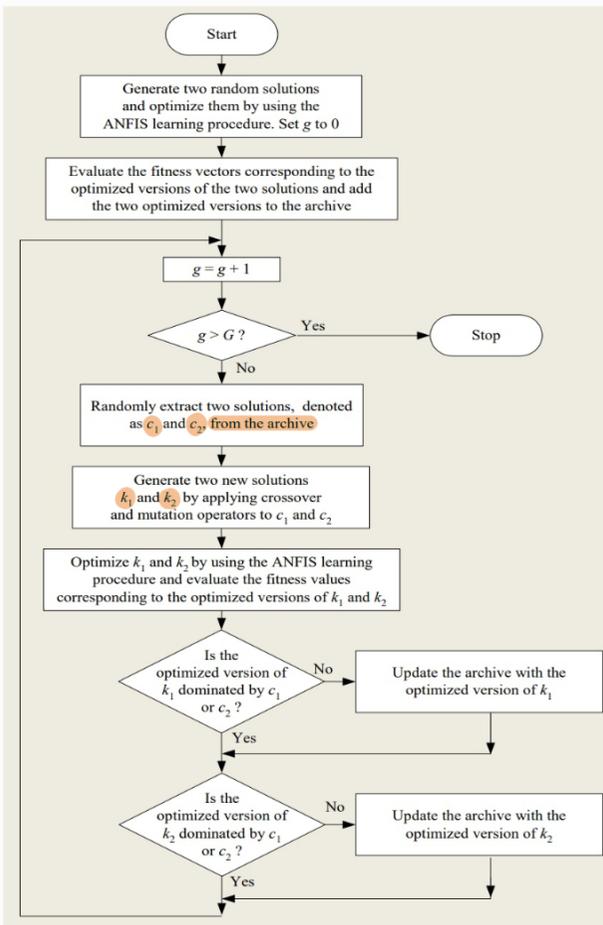
→ In  $n$ -D I would have need  $2^n$  split in the tree

• Then concat the binary strings obtained and use it as index for a map containing the crowding number

→ In case of known obj. space (eg. ROC space) we could use static grids to reduce complexity

• This CD is more efficient than standard one

(2-2) PAES



# SMS-EMOA → S-Metric Selection-based Evolutionary Multi-Objective Algorithm

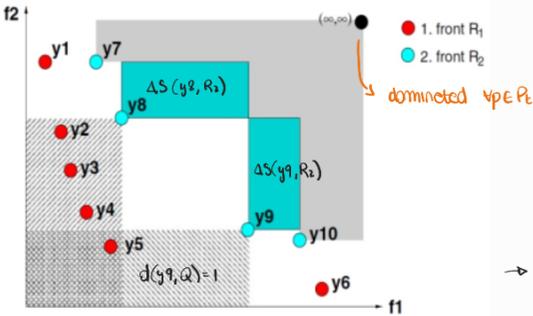
- Hypervolume is called **S measure** → several definitions (exact or approximate)
- it is an **elitist** algorithm  $S(P_t) \leq S(P_{t+1})$

$$S_z(P) = \int_{\{q \in \mathbb{R}^n : (\exists p \in P : p \leq q) \wedge (q \leq z)\}} \text{Lebesgue integral}$$

Maximize the Area between the pareto frontier and the Nadir Point

## Algorithm 1. SMS-EMOA

- 1:  $P_0 \leftarrow \text{init}()$  /\* Initialise random population of  $\mu$  individuals \*/
- 2:  $t \leftarrow 0$
- 3: repeat
- 4:  $q_{t+1} \leftarrow \text{generate}(P_t)$  → **steady state** /\* generate offspring by variation \*/
- 5:  $P_{t+1} \leftarrow \text{Reduce}(P_t \cup \{q_{t+1}\})$  /\* select  $\mu$  best individuals \*/
- 6:  $t \leftarrow t + 1$
- 7: until termination condition fulfilled



- 1) Algorithm 2. Reduce(Q)
  - 1:  $\{\mathcal{R}_1, \dots, \mathcal{R}_r\} \leftarrow \text{fast-nondominated-sort}(Q)$  /\* all  $r$  fronts of  $Q$  \*/
  - 2:  $r \leftarrow \text{argmin}_{s \in \mathcal{R}_r} [d(s, Q)]$   $\Delta S = S(\mathcal{R}_r) - S(\mathcal{R}_r \setminus \{s\})$  /\*  $s \in \mathcal{R}_r$  with lowest  $d(s, \mathcal{R}_r)$  \*/
  - 3: return  $(Q \setminus \{r\})$  /\* eliminate detected element \*/
- 2) Algorithm 3. Reduce(Q)
  - 1:  $\{\mathcal{R}_1, \dots, \mathcal{R}_r\} \leftarrow \text{nondominated-sort}(Q)$  /\* all  $r$  fronts of  $Q$  \*/
  - 2: if  $v > 1$  then
  - 3:  $r \leftarrow \text{argmax}_{s \in \mathcal{R}_r} [d(s, Q)]$  /\*  $s \in \mathcal{R}_r$  with highest  $d(s, Q)$  \*/
  - 4: else
  - 5:  $r \leftarrow \text{argmin}_{s \in \mathcal{R}_1} [d(s, \mathcal{R}_1)]$  /\*  $s \in \mathcal{R}_1$  with lowest  $d(s, \mathcal{R}_1)$  \*/
  - 6: end if
  - 7: return  $(Q \setminus \{r\})$  /\* eliminate detected element \*/

- 1) more computationally efficient
- 2) keep points that cover the gaps of prev fronts

$$d(s, Q) = |\{y \in Q : y \leq s\}|$$

number of point in Q that dominates s  
- more computationally efficient ( $d(s, Q)$  not usable when  $v=1$ )

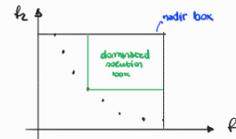
$$\Delta S \text{ function} \in O(\mu^2)$$

- maximize both the vicinity to the pareto point and also the sparseness of the solution

→ with first method I would prefer y8 with second y9

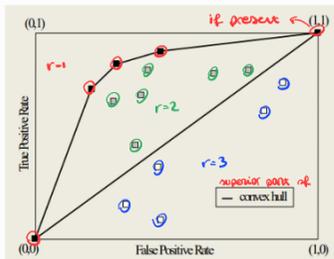
## MPE → Use a monte-carlo approach to compute S

- generation of random points inside nadir point box
- compute the ratio between points inside the dominated solution box and the total
- it gives an idea of the importance of the solution



## FV-MOEA → it is exact but faster than SMS-EMOA, since to compute $\Delta S(p, Q)$ we need just the neighbour of p, not the all set

## CHEA (convex-hull based algorithm)



**convex hull**: smallest convex set containing all the binary classifiers

- 1) Generate random initial population of size  $N_{pp}$ ,  $P_0$  and evaluate TPR, FPR. create offspring  $Q_0$  from  $P_0$  (random selection, crossover + mutation) of size  $N_{pp}$
  - 2) Evaluate FPR and TPR  $\forall q \in Q_k$ . build  $R_k \leftarrow P_k \cup Q_k$ . compute the convex hull of  $R_k \cup \{(0,0), (1,1)\}$
  - 3) assign a rank (1,2,3) to each solution and call  $N_1, N_2, N_3$  the # of points with i rank. rank 1 → points in the convex hull → they are also non-dominated. rank 2 → other candidate classifiers (above random line). rank 3 → non-candidate classifiers.
  - 4) Generate  $P_{k+1}$ . if  $N_1 > N_{pp}$  → randomly select, otherwise add all. if  $N_1 < N_{pp}$  if  $N_2 > N_{pp} - N_1$  → randomly select, otherwise move all. randomly extract  $N_{pp} - N_1 - N_2$  from rank 3 and move it, if still missing points.
  - 5) if  $k = k_{max}$  → stop, otherwise create  $Q_{k+1}$  offspring of size  $N_{pp}$  from  $P_{k+1}$  using **binary tournament** based on ranks and apply crossover + mutation.
- $k \leftarrow k+1$  and goto step 2

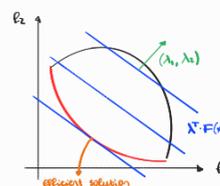
## MOEA/D → based on the decomposition into N single-objective sub-problems

- problems are solved **collaboratively** → best solution found so far by one can affect the best solution found by another one in its **neighborhood**
- it uses both a population of size N and an **unbounded archive** of non-dominated solutions found so far → **elitist algorithm**

↳ optional, get more than N solutions

It uses N lambda vectors (or weight vector) provided by the user

- in this way I will get N solutions  $\in$  ES
- WS (weighted sum scalarization) works well in convex problems



weighted sum scalarization

$$\min g^{WS}(x, \lambda) = \sum_{i=1}^n \lambda_i F_i(x)$$

where  $\sum \lambda_i = 1$  and  $\lambda_i \geq 0$

Chebyshev Scalarization (alternative to WS)

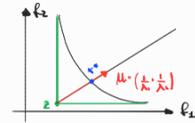
$$\min_{x \in Z} g^c(x | \lambda, z) = \min_{x \in Z} \max_{\lambda_i \in [0,1]} \{ \lambda_i | f_i(x) - z_i | \} = \min_{x \in Z} \| \lambda \circ (f(x) - z) \|_\infty$$

↑ this is not differentiable  
↑ each term is continuous w.r.t x (when divided ||)

$$z_i = \min_{x \in Z} f_i(x)$$

$$\sum \lambda_i = 1 \wedge \lambda_i \geq 0$$

- For any  $x^*$  Pareto optimal solution,  $\exists \lambda : x^*$  is optimal for the above problem
- $\rightarrow g^c(x | \lambda, z)$  is non-smooth w.r.t  $x$  and  $\lambda$ , so gradient method doesn't work
- $\rightarrow$  I can find any ideal point
- $\rightarrow$  works also for non-convex problems



The neighbour of  $i$ -th subproblem are the ones with similar weight vectors (that identifies the search direction)  
 - they have similar obj functions and with high probability a similar optimal solution

At each generation and sub-problem:

- Obtain the current solutions from some neighbours (T-1)
- Generate new solution by applying crossover + mutation from (its own solution and) the borrowed ones
- Replace its own solution with the newer one if improve its objective
  - Pass the new solution to some neighbours that will replace if it improves their objective

1) Initialization

- compute  $L_2$  distances between any pair of weight vectors and determine the  $T$  closest to each  $\lambda_i$
  - randomly generate the initial population and evaluate  $F(x_i) \forall i \in 1, \dots, N$  (for each individual(s))
  - initialize  $z$  as  $z_j = \min_{1 \leq i \leq N} f_j(x_i)$
- ↑ neighbourhood size  
↑ contains  $i$   
 $B(i) = \{i_1, \dots, i_T\}$   
↑  $N = \text{pop-size}$

2) UPDATE

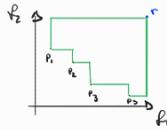
For  $i=1$  to  $N$  do: ↑ Neighbors

- randomly select  $e$  and  $k$  in  $B(i)$  and generate  $x_{\text{new}}$  from  $x_e$  and  $x_k$  with crossover + mutation
- repair with some heuristic if  $x_{\text{new}}$  violates the constraints
- evaluate  $F(x_{\text{new}})$
- $\forall j \in 1, \dots, m$  if  $z_j > f_j(x_{\text{new}})$  update it
- $\forall j \in B(i)$  if  $g^c(x_{\text{new}} | \lambda_j, z) < g^c(x_j | \lambda_j, z)$  update it (Neighbour/self update)
- here we could mention on archive of non-dominated solutions

3) STOPPING CRITERION  $\rightarrow$  if stop criterion satisfied return  $(\{x_1, \dots, x_N\}, \{F(x_1), \dots, F(x_N)\})$  else step 2

MOEA performance comparison  $\rightarrow$  can be done in different ways

1) Hyper-Volume  $\rightarrow$  exactly or by using monte-carlo methods (we need a reference point)



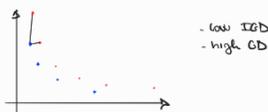
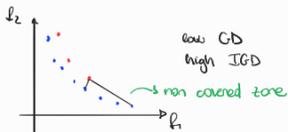
2) GD - generational distance  $GD(A) = \frac{1}{n} \left( \sum_{i=1}^n d_i^p \right)^{\frac{1}{p}}$  where  $A = \{a_1, \dots, a_n\}$  non-dominated objective vector set  
 $Z = \{z_1, \dots, z_m\}$  the reference set  
 $p \in \mathbb{N}$

↑ avg distance of A to Z  
↑  $L_2$  distance between  $a_i$  and nearest  $z_j \in Z$

3) IGD - inverted generational distance  $IGD(A) = \frac{1}{m} \left( \sum_{i=1}^m d_i^p \right)^{\frac{1}{p}}$   
↑  $L_2$  distance from  $z_i$  and NN in A

how well-spread are the solutions w.r.t reference points

4) Delta metric  $\Delta(A) = \max \{GD(A), IGD(A)\}$



# MANY OBJECTIVE OPTIMIZATION (from 4 to 30, if > 30 then massive-objective)

- Problems:
- 1) most of the solutions are non-dominated → no solutions to eliminate
  - 2) difficult to use crowding distance or hypervolume because becomes computationally heavy (and curse of dimensionality)
  - 3) difficult to visualize the ES and needs exponentially more points to be covered
  - 4) Ineffective recombination operations since two distant solutions tend to generate an offspring distant from both, not inheriting beneficial characteristics

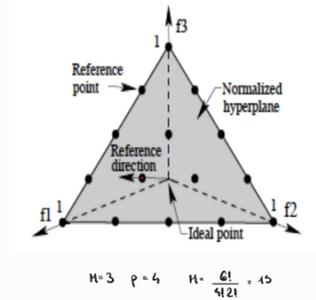
**NSGA-III** based on a set of reference points provided by the user

a generation of reference points (optional) <sup>just at start</sup> If not provided we can generate them on the **normalized hyperplane**

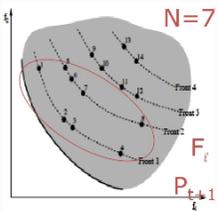
#reference points =  $\binom{M+p-1}{p}$  typically - pop size ↓  
 $M \rightarrow$  # of obj functions  
 $p \rightarrow$  # of divisions per edge of the simplex

**Des-Desimis Algorithm**

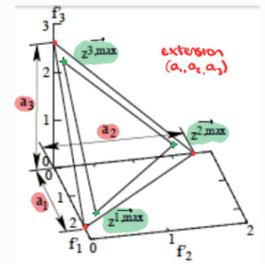
each point is associated with a reference (search) direction



1) Identifying the non-dominated frontiers → generation of  $P_{t+1}$



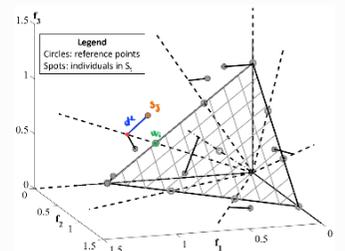
- Parent ( $P_t$ ) and offsprings ( $Q_t$ ) are combined into  $R_t$  <sup>crossover + mutation</sup>
- non-dominated sorting of  $R_t$
- collect old and new fronts from 1 to  $l$  to  $S_t$ , where  $l$  is the first integer that  $\sum_{i=1}^l |F_i| \geq N$  (elitism)
- if  $|S_t| > N \rightarrow P_{t+1} = S_t$  (return  $P_{t+1}$ )
- else  $P_{t+1} = \bigcup_{i=1}^l F_i$  then remaining points will be added to  $P_{t+1}$  from  $F_l$  but not using crowding distance (step 2 and 3)



2) Normalization of population members ( $|S_t| \neq N$ )

- identify ideal point of  $S_t$  ( $\bar{z}^{min}$ )  $z_i^{min} = \arg\min_{s \in S_t} f_i(s)$
  - translate everything, making the ideal point the origin  $f'_j(s) = f_j(s) - z_j^{min}$
  - identify extreme points for each objective (nadir points could be calculated)  $z^{i,max} = f(s^{i,max}), s^{i,max} = \arg\max_{s \in S_t} f_i(s)$
  - generate the  $M$ -dimensional hyperplane with this  $M$  extreme vectors, compute  $a_j \in \mathbb{R}$  as the intercepts of this plane with the axes
  - $f'_j(s) = \frac{f_j(s) - z_j^{min}}{a_j} = \frac{f_j(s)}{a_j} \quad \forall s \in S_t, j=1, \dots, M$
- ↳ can handle different scaled objectives

the reference points if generated in step 0 are already in this hyperplane, otherwise (provided by user) are projected in  $\Pi$



3) Association of population members ( $|S_t| \neq N$ )

Assign each  $s \in S_t$  to a reference point  $e \in Z$  using the minimum perpendicular distance

$$d^+(s, w) = \left\| \frac{e^T(s) - w^T(s)}{\|e - w\|} \right\|_2 \quad \text{assign } s \text{ to } \Pi(s) = \arg\min_{w \in Z^*} d^+(s, w)$$

↳ reference points set

- create the vector  $\bar{\pi}$  in this way:

$$\bar{\pi} = \begin{bmatrix} \pi_1 \\ \vdots \\ \pi_{|P_{t+1}|} \\ \vdots \\ \pi_{|F_l|} \end{bmatrix} \left\{ \begin{array}{l} s \in P_{t+1} \\ s \in F_l \end{array} \right\} S_t$$

4) Compute Niche Count

↳ reference point  $w \in Z^*$ :  $\rho_i = \sum_{s \in S_t, s \in P_{t+1}} \mathbb{I}(\Pi(s) = w)$

5) The niching procedure

- NSGA II/III no parameters needed, while MOEA/D requires  $T$  and  $\bar{\lambda}$
- NSGA-III uses niche meanwhile NSGA-II uses crowding distance to select points from  $F_l$ 
  - ↳ favors better spread since uses information of all  $P_{t+1}$  points selected
- with higher  $M$  exponentially more points are needed to cover correctly the space

- If there are constraints there is a **binary tournament selection** (using CV( $\rho_i$ ) if both infeasible or random if both feasible)

↳  $N - |P_{t+1}|$  (# of points to add)

```

Algorithm 4 Niching ( $K, \rho_j, \pi, d, Z, F_l$ ) procedure
Input:  $K, \rho_j, \pi(s \in S_t), d(s \in S_t), Z, F_l$ 
Output:  $P_{t+1}$  → niche count,  $Z^*$  → reference points
1:  $k = 1$ 
2: while  $k \leq K$  do
3:  $J_{min} = \{j : \arg\min_{j \in P} \rho_j\}$  → may be more than one
4:  $\bar{j} = \text{random}(J_{min})$ 
5:  $I_j = \{s : \pi(s) = \bar{j}, s \in F_l\}$ 
6: if  $I_j \neq \emptyset$  then
7: if  $\rho_{\bar{j}} = 0$  then → no  $p \in P_{t+1}$  associated with reference  $\bar{j}$ 
8:  $P_{t+1} = P_{t+1} \cup \{s : \arg\min_{s \in I_j} d^+(s)\}$  → because  $\bar{j}$  is under-represented
9: else
10:  $P_{t+1} = P_{t+1} \cup \text{random}(I_j)$ 
11: end if
12:  $\rho_{\bar{j}} = \rho_{\bar{j}} + 1, F_l = F_l \setminus s$ 
13:  $k = k + 1$ 
14: else
15:  $Z^* = Z^* \setminus \{\bar{j}\}$  → exclude reference point  $\bar{j}$  from further calculations
16: end if
17: end while
    
```

# PURE LEXICOGRAPHIC Multi-Objective OPTIMIZATION

$$\begin{cases} \text{lexmin} & f_1(x), \dots, f_m(x) \\ x \in \Omega \end{cases}$$

where the importance of minimizing  $f_1$  is infinitely more important than  $f_2$  and so on  
 → the **lexicographic order** allows to compare vectors  $[2, 4] \prec_{lex} [3, 7]$  → defines a **total order**

vectors  $[2, 4] \prec_{lex} [2, 8]$  ↔ exclusion scalars  $3 \cdot 7 \prec_{lex} 2 + 29$

**PRIORITY CHAINS (PC)** → there maybe some priority chains among objectives



$$\min \begin{bmatrix} \text{lexmin}(f_1^{(1)}(x), f_1^{(2)}(x), \dots, f_1^{(p_1)}(x)) \\ \text{lexmin}(f_2^{(1)}(x), f_2^{(2)}(x), \dots, f_2^{(p_2)}(x)) \\ \vdots \\ \text{lexmin}(f_m^{(1)}(x), f_m^{(2)}(x), \dots, f_m^{(p_m)}(x)) \end{bmatrix} \rightarrow \min \begin{bmatrix} f_1^{(1)}(x) + \mathbb{1}^{-1} f_1^{(2)}(x) + \dots + \mathbb{1}^{1-p_1} f_1^{(p_1)}(x) \\ f_2^{(1)}(x) + \mathbb{1}^{-1} f_2^{(2)}(x) + \dots + \mathbb{1}^{1-p_2} f_2^{(p_2)}(x) \\ \vdots \\ f_m^{(1)}(x) + \mathbb{1}^{-1} f_m^{(2)}(x) + \dots + \mathbb{1}^{1-p_m} f_m^{(p_m)}(x) \end{bmatrix} \triangleq \min \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_m(x) \end{bmatrix}$$

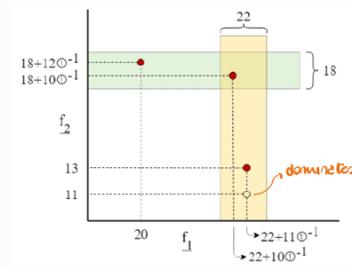
**Cross scalar**  $\mathbb{1} = S(x) \eta^q$  **PNM (polynomial arithmetic number)**  
 $f_i(x)$  is a chain in the directed graph

$f_1^1$  may be the profit  
 $f_1^2$  may be the profit from sustainable investments → secondary objective

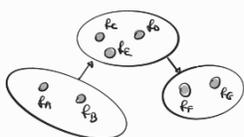
- $\mathbb{1}$  → gross number: cardinality of  $\mathbb{N}$
- $\mathbb{1}^{-1}$  → reciprocal of gross number: smallest number greater than zero

**Pareto lexicographic dominance (PL)**: A dominates B:  $A \prec B \Leftrightarrow \begin{cases} f_i(x_A) \prec f_i(x_B) \quad \forall i=1, \dots, m \\ \exists j: f_j(x_A) < f_j(x_B) \end{cases}$

• I could adapt both NSGA-II and MOEA/D Algorithms



## PRIORITY LEVELS (PL)



$$\text{lexmin} \left[ \min \begin{pmatrix} f_1^1(x) \\ \vdots \\ f_m^1(x) \end{pmatrix}, \dots, \min \begin{pmatrix} f_1^p(x) \\ \vdots \\ f_m^p(x) \end{pmatrix} \right] = \min \left( \begin{pmatrix} f_1^1(x) \\ \vdots \\ f_m^1(x) \end{pmatrix} + \dots + \mathbb{1}^{1-p} \begin{pmatrix} f_1^p(x) \\ \vdots \\ f_m^p(x) \end{pmatrix} \right)$$

• find pareto non-dominated solutions from  $L_i$  and those will be used to search on  $L_{i+1}$

**PL Dominance** Given A and B belonging to the subfronts  $F_i$  and  $F_j$ :  $A \prec^* B \Leftrightarrow i < j$

• **SUBFRONTS**: we take the points set of  $L_i$ , for each of them we further split based on the  $L_2$  and recursively until  $L_p$

$F_i$  front is defined by a gross scalar eg:  $i = 2 \cdot \mathbb{1}^0 + 7 \cdot \mathbb{1}^{-1} + 3 \cdot \mathbb{1}^{-2}$  all the solutions belonging to the second front of  $L_1$  objectives, 7<sup>th</sup> front to  $L_2$  objectives ---

problem: a posteriori nature of the definition. To compute  $F_i$  and  $F_j$  I need to find all other individuals

## PL-NSGA-II

determines fine rank, called with  $\text{cwl} = 0$

**Algorithm 1** Priority Levels fast non-dominated sort.

```

1: /* This function is recursive */
2: /* P is the population, lvl is the current level to consider */
3: procedure PL_FAST_NONDOMINATED_SORT(P, lvl)
4:   /* Base case of recursion */ eg = -2 if 2 levels are present
5:   if lvl < min_lvl then return P
6:   /* The first iteration also initializes all ranks to 0 */
7:   if lvl == 0 then
8:     for all p in P do
9:       prank = 0
10:   /* Ranking within the priority level to determine subfronts */
11:   F^(lvl) = fast_nondom_sort_in_level(P, lvl) = {F1, ...}
12:   /* Repeat for every subfront found */
13:   for all Fi in F^(lvl) do
14:     /* In the next priority level */
15:     Fi = PL_fast_nondominated_sort(Fi, lvl-1)
return F^(cwl)
    
```

```

1: procedure FAST_NONDOM_SORT_IN_LEVEL(P, lvl)
2:   for all p in P do
3:     Sp = ∅ → points that p dominates
4:     np = 0 → # of points that dominate p
5:     for all q in P do
6:       /* non-dominance at specified priority level */
7:       if p ≻^lvl q then
8:         Sp = Sp ∪ {q}
9:       else if q ≻^lvl p then
10:        np = np + 1
11:     if np == 0 then
12:       /* First subfront within P */
13:       Prank = prank + 1
14:       /* first subfront set */
15:       Fi = Fi ∪ {p}
16:       /* Start from the first subfront */
17:       i = 1
18:       while Fi ≠ ∅ do
19:         /* i-th subfront set accumulator */
20:         for all p in Fi do
21:           for all q in Sp do
22:             nq = nq + 1 → because we removed p
23:             if nq == 0 then
24:               /* q belongs to the i-th subfront */
25:               qranks = qranks + i + 1
26:               Q = Q ∪ {q}
27:             /* Index of the next subfront */
28:             i = i + 1
29:         Fi = Q
    
```

return  $\{F_1^{(cwl)}, \dots, F_i\}$

→ level 1 rank will have  $i \in \mathbb{N}$

$$cd = cd_x \cdot \mathbb{1}^0 + \dots + cd_p \cdot \mathbb{1}^{-p}$$

**Algorithm 2** Priority Levels crowding distance assignment.

```

1: /* F is a leaf-front in the hierarchy of population fronts partitioning */
2: procedure PL_CROWDING_DIST_ASSIGNMENT(F)
3:   n = |F|
4:   for all i in F do
5:     F[i].dist = 0
6:   /* For each level of priority q; p is the index of the last level */
7:   for q = 1 ... p do
8:     for j = 1 ... m_q do
9:       F = sort(F, fj^(q))
10:      /* +Inf means "full-scale" (IEEE 754 standard) */
11:      F[1].dist += +Inf * 1^(1-q)
12:      F[n].dist += +Inf * 1^(1-q)
13:      for i = 2 ... (n-1) do
14:        /* PL_crowd_dist_ass. has infinitesimal parts */
15:        F[i].dist += 1^(1-q) * (fj^(q)(F[i+1]) - fj^(q)(F[i-1])) / (fj^(q)max - fj^(q)min)
    
```

**Algorithm 3** PL-NSGA-II algorithm.

```

1: /* P0 is the starting population, T is the total number of iterations */
2: /* The function returns the approximated Pareto front P_T */
3: procedure PL_NSGA-II (P0, T)
4:   for t = 0 ... T - 1 do
5:     Qt = make_new_pop(Pt)
6:     Rt = Pt ∪ Qt
7:     /* F is the set of all the non-dominated subfronts */
8:     F = PL_fast_nondom_sort(Rt, 0) = [F1, ...]
9:     Pt+1 = ∅
10:    /* i is a gross-index, a.k.a. gross-scalar */
11:    i = 1 i ← first_index(F) (1 + ω^1 + ... + ω^i)
12:    while |Pt+1| + |Fi| ≤ N do
13:      /* Crowding distance is computed within subfront Fi */
14:      PL_crowding_dist_assignment(Fi)
15:      Pt+1 = Pt+1 ∪ Fi
16:      /* Move to the next subfront */
17:      i = next_index(F, i)
18:      Sort(Fi, by CD by CD)
19:      Pt+1 = Pt+1 ∪ Fi[1 : (N - |Pt+1|)]
20:   return P_T

```

Real world Application

- Vehicle crash Worthiness

$$\text{Exam} \min \left( \min \begin{pmatrix} \text{mass}(x) \\ \text{twe}(x) \end{pmatrix}, \min \begin{pmatrix} \text{twe}(x) \\ -\text{acc}(x) \end{pmatrix} \right)$$

↑ I cared at -acc(x) if a company wants  
↳ intrusion resistance

- Aircraft design: 10 objectives that could be divided by importance (eg. noise, mass, ...)

PC-NSGA-II → it is completely identical to NSGA-II but substitute  $f_i$  with  $\underline{f}_i$  in CD  
 $F[j]_{\text{dist}} = \textcircled{1}$

PC-MOEA-D

```

1: procedure PC_MOEA/D
2:   EP = ∅
3:   for i = 1 ... N do
4:     λi1, ..., λiT = find_closest_weights(λi, T)
5:     Bi = {i1, ..., iT}
6:     x1, ..., xN = initialize_population(N)
7:     for i = 1 ... N do
8:       FVi = F(xi)
9:     z1, ..., zm = initialize_ref_point(m)
10:    while stop_criteria() = False do
11:      for i = 1 ... N do
12:        k, l = rand(Bi, 2)
13:        y = make_new_sol(xk, xl)
14:        y' = mutate(y)
15:        for j = 1 ... m do
16:          if zj < fj(y') then
17:            zj = fj(y')
18:        for all j ∈ Bi do
19:          if gte(y' | λj, z) ≤ gte(xj | λj, z) then
20:            xj = y'
21:            FVj = F(y')
22:            DD = PC_find_dominated_sol(EP, F(y'))
23:            DG = PC_find_dominating_sol(EP, F(y'))
24:            EP = EP \ DD
25:            if DG = ∅ then
26:              EP = EP ∪ F(y')

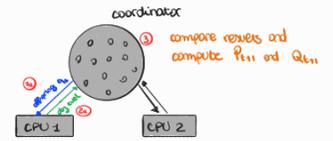
```

archive

→ dominated by  $\underline{f}_j$   
 if no one dominates  $\underline{f}_j$   
 add to archive

## PARALLELIZATION of MOEA

→ typically is really simple to // MOEA



### COORDINATOR WORKERS APPROACH

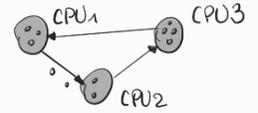
- a coordinator generates the offspring population and distributes the computation to the workers
- the workers compute the solution of the current generation that are collected by the coordinator that will generate the next generation

} needs coordination

### THE ISLAND MODEL

-decentralized (if a CPU fails we can continue) -population is spreaded

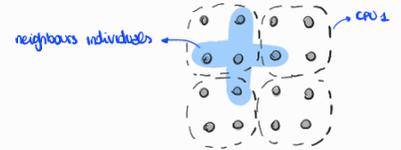
- on each CPU (island) evaluate a sub-population independently
- After  $K$  generations shares the best solutions with other islands → random or determined migration



### THE CELLULAR MODEL

-decentralized -population is spreaded

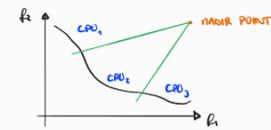
- The individuals are spatially arranged → solutions of one migrates only to the neighbours (defined by a pre-det. scheme)



### CONE SEPARATION MEA (cspMEA)

→ is not general purpose as the others, but specific (redefined the NSGA-II algorithm)

- Divide the objective space in  $n$  cones  $n = \#CPU$
- usable for 2D/3D problems
- At each population  $P_t$  the nadir point change (dynamic)



Typically a master-slave approach (or just a decentralized communication)

● → requires inter-process communication

## Algorithm 1 Cone-separated NSGA-II

Initialize the different sub-populations

- *Normalize fitness values* → All  $F_i$  within unit square (or unit hypercube) → NADIR POINT
- *Determine region constraints* → divide  $90^\circ$  in equal parts

Non-dominated sorting → needed for TS in the offspring generation

CROWDED TS:

- 1) compare the two front ranks
- 2) if equal use crowding distance

REPEAT

Generate Offspring

IF (migration)

- *Normalize fitness values*
- *Determine region constraints*
- *Migrate individuals violating constraints*

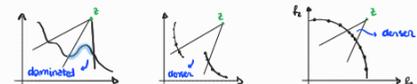
Non-dominated sorting

Prune population to original size → via CD

UNTIL stop-condition

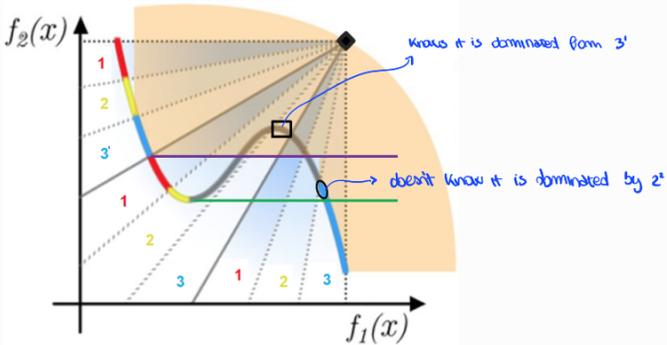
- It is better than random individuals assignments since it exploits the search space

- Local pareto front may be dominated by other front (≠ global front)
- The solutions of the global pareto front may be unevenly distributed
- The migration rate can be really high



**MICRO-CONE SEPARATION PARALLEL MOEA (mspMEA)** → Do not only divide the unit square into  $n$  cones, but each cone is divided in  $N_{micro}$  **microcones** → each of them a CPU  
 - when  $N_{micro} = 1$  → cspMEA  $\approx$  mspMEA

- drawback → the offspring generated is more likely to fall outside the microcones of the CPU (parents may come from different microcones)
- thus the constraint is considered as **soft** instead of hard
- at each generation a fixed number of random individuals violating the soft constraints are migrated to the right CPU
- allow to control the migration rate
- added the **binary tournament** to favour recombination of the individuals falling inside the microcones assigned to the CPU

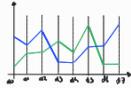


→ Each CPU has an idea on the global front (**global front**)

- 1) get  $P_i$  and compute global extremes
  - 2) Perform non dominated sort between all microcones of a CPU
  - 3) For best front select iteratively one point for microcone until reached pop-size or no more point
- To select the point for each microcone:
- a) If  $\exists$  points inside → use crowding distance
  - b) If  $\nexists$  points inside → use **microcone distance** (angular)
- 4) Once pop-size reached perform the random migration

**VISUALIZE DATA IN HIGH DIMENSION**

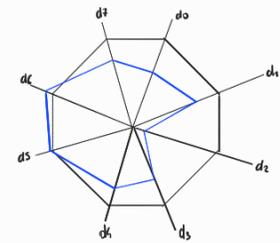
1) **Parallel coordinate**



→ Two non-dominated solutions

2) **Radar Chart**

- if they **intersect** they are non-dominated



3) **Scatter plot matrix**

→ triangular matrix of plots ( $dim_1$  vs  $dim_2$ )

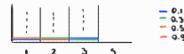
4) **Nested Axes Plot**

for 4 and 5b → works particularly well if some are discrete

5) **Heatmap**

→ similar to // coordinates but instead of lines the points are represented with different colored segment

- no dominance can be seen



6) **Bubble chart**

→ 4D = 2D + bubble size + colour

7) **Self Organizing Maps (SOM)**

→ NN that lower the dimension from  $M$  to 2

- can't show many points fell inside each cell → visualize them in a 2D grid

- their problems is that close cells could map very distant zone of a manifold if it overlap

→ **iSOM** was been introduced for efficient sets → near cells maps for mean points in the original manifold

8) **RadViz**

→ normalize the obj between  $[0,1]$ , map each obj to the vertex of a polygon

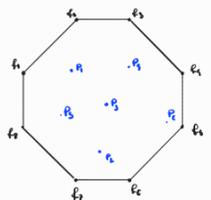
- the single point position can be understood imagine it connected by all the obj vertices by a spring

**3D RadVis**

→ adds a dimension as the distance of the solution to the hyperplane

$(1,0,\dots), (0,1,\dots), \dots$

- in this way we understand the dominated/non-dominated solutions



# QUANTUM COMPUTING

A **qubit** is a physical entity (electron, atom, ...) that can be at the same time in two distinct states

→ It is in a **superposition** of two states

· Decays when measured → it destroys superposition

Wave function measures the probability the electron is in a specific point in space at a given time

→ follows a PDE called Schrödinger Equation → **wave equation**

state pure state  
 $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$

·  $\alpha, \beta \in \mathbb{C}$ ,  $\alpha^2 + \beta^2 = 1$

·  $\alpha^2$  is the probability of being in state  $|0\rangle$

· Super position can be represented using a sphere

· Quantum Physics can be axiomatized

When we have 2 qubits (4 pure states) they can also **entangle**

→ the two are not independent → some superstate is preferred

two can prepared H-T, if I see one I immediately know the second, the outcome was decided at start

Different from classical correlation (when two states have common causes and knowing one, reveals the other)

- 1) violates local realism (Bell Inequalities) → object influenced only by it's surroundings
- 2) instantaneous but info max at speed of light
- 3) Measurement has an effect

Since Schrödinger is a wave equation then exists **interference** between paths

→ eg. Mac-Zender Interferometer or double-slit

→ used in quantum computing to increase the probability of finding the qubits in the correct final state for the problem

**Tunneling** → when a particle goes on energy barrier even with not sufficient energy (thanks to its wave nature)

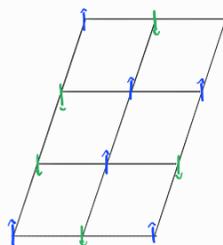
- 1) In optimization can be used to escape local minima (by a thermal jump)
- 2) In sensing can be used to denoise the signal and reach the true one

## ADIABATIC QUANTUM COMPUTERS

→ some NP-hard problems could be solved in polynomial time

Problems are written in terms of the **Ising Model** (spin  $\uparrow$  or  $\downarrow$ )

- each possible arrangement is a candidate solution
- total energy of the arrangement → quality of the solution



Condition: the energy needs to change slowly and smoothly → **ADIABATIC**

- if rush the system could jump in the wrong state

· Quite tolerant to noise wirt other implementations

Problem is solved via **Quantum Annealing**

- 1) start via a simple landscape with obvious global minimum
- 2) slowly reshape the landscape until the one that encode the problem → quantum tunneling helps to not get stuck

Applications

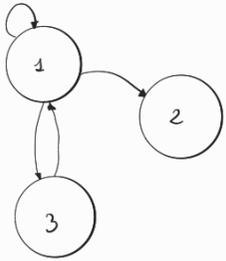
1) Quantum NN

2) Quantum Kernel Methods

3) QRL

4) Q Generative Models

**MARKOV PROCESS** → Stochastic Process that satisfies the Markov property



**Markovian property**  $P(S_t = s | S_{t-1}, \dots, S_1) = P(S_t = s | S_{t-1})$

can be defined a **transition matrix**  $P \in \mathbb{R}^{|\mathcal{S}| \times |\mathcal{S}|}$  where  $P_{ij} = P(S_t = i | S_{t-1} = j) \geq 0$ ,  $\sum_{i=1}^{|\mathcal{S}|} P_{ij} = 1 \forall j$

Starting distribution  $S^{(0)} \in \mathbb{R}^{|\mathcal{S}|}$  (eg  $S^{(0)} = [1, 0, 0]^T$ )

$S^{(t+1)} = P S^{(t)} \rightarrow S^{(t+1)} = P^t S^{(0)}$

The **stationary distribution**  $S^*$  satisfy:  $S^* = P S^* \Rightarrow S^*$  is an eigenvector of  $P$  associated with  $\lambda = 1$   
 $S^*$  represents the probability of being in each state in the long run

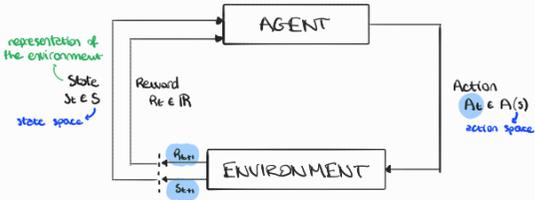
**Ergodic Theorem**: If a chain is irreducible (can reach any state from any other) and a-periodic (not locked in cycles)

State space  $\mathcal{S} = \{1, 2, 3\}$

- 1)  $\exists! S^*$ :  $S^* = P^t S^*$
- 2)  $S^{(t)} \rightarrow S^*$  regardless  $S^{(0)}$

- Implications
- 1) Sampling long run episodes estimates  $\mathbb{E}_{S^*}$
  - 2) Policy gradient exists uniquely  $[\forall \theta \exists \alpha \sum_{s \in \mathcal{S}} d_{\theta_0}(s) \sum_{a \in \mathcal{A}(s)} \alpha(a, s)]$  and independently from  $S^{(0)}$

**RL** → branch of ML where an agent learns to take actions within an environment, by maximizing the rewards obtained



$P(S_t = s', R_t = r | S_{t-1} = s, A_{t-1} = a)$  depends only on last state and action

**dynamics function**  $p: \mathcal{S} \times \mathcal{R} \times \mathcal{S} \times \mathcal{A} \rightarrow [0, 1]$   
 $\sum_{s' \in \mathcal{S}} \sum_{r \in \mathcal{R}} p(s', r | s, a) = 1 \quad \forall s, a \in \mathcal{S} \times \mathcal{A}$

To satisfy the **Markov property**  $S$  must carry all the important historical info

$p(s' | s, a) = P(S_t = s' | S_{t-1} = s, A_{t-1} = a) = \sum_{r \in \mathcal{R}} p(s', r | s, a)$   
**state transition function**  $p: \mathcal{S} \times \mathcal{S} \times \mathcal{A} \rightarrow [0, 1]$

$r(s, a) = \mathbb{E}[R_t | S_{t-1} = s, A_{t-1} = a] = \sum_{r \in \mathcal{R}} r \sum_{s' \in \mathcal{S}} p(s', r | s, a)$   
**reward function**  $r: \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$

The objective is to maximize the cumulative reward it received in the long run

**simplest one**  $G_t = R_{t+1} + R_{t+2} + \dots + R_T$  (episode time step (could be finite eg TicTacToe or  $T = +\infty$ ))  
 reward (must be a function of the reward sequence)

$G_t = R_{t+1} + \delta R_{t+2} + \dots = \sum_{k=0}^{\infty} \delta^k R_{t+k+1}$   
 consider expanding final state  $t+T$  with  $R_t = 0$   
**discount rate**  $\delta \in [0, 1]$

- 1)  $R_{t+k}$  is worth only  $\delta^k R_{t+k}$  when it would be received immediately
- 2) If  $\delta < 1 \wedge \{R_t\}$  bounded  $\Rightarrow G_t$  has a **finite value**  
 If  $\delta = 0$  the agent is "myopic", trying to maximize only immediate rewards
- 3)  $G_t = R_{t+1} + \delta(R_{t+2} + \delta R_{t+3} + \dots) = R_{t+1} + \delta G_{t+1}$

**Policy**:  $\pi(a|s) = P(A_t = a | S_t = s)$  IR agent is following policy  $\pi \Rightarrow p(a|s) = \pi(a|s)$

$r(s, \pi) \cdot V_{\pi}^s = \sum_{a \in \mathcal{A}} \pi(a|s) r(s, a) \quad V_{\pi}^s = \mathbb{E}_{\pi} [V_{\pi}^s]$   
 $P_{ss'}^{\pi} = \sum_{a \in \mathcal{A}} \pi(a|s) P_{ss'}^a = \mathbb{E}_{\pi} [P_{ss'}^a]$   
 $P_{ss'}^a = p(s'|s, a)$

**Value function**:  $V_{\pi}(s) = \mathbb{E}_{\pi} [G_t | S_t = s] = \mathbb{E}_{\pi} \left[ \sum_{k=0}^{\infty} \delta^k R_{t+k+1} | S_t = s \right]$   
 $p(a_{t+1}, r_{t+1}, s_{t+1}, \dots, s_T, r_T | s_t) = \prod_{k=0}^{T-t-1} \pi(a_{t+k+1} | s_{t+k}) p(s_{t+k+1}, r_{t+k+1} | s_{t+k}, a_{t+k+1})$   
 distribution over trajectories from  $s_t$

Expected return when in  $s$  and follow the  $\pi$  policy  
 - how good is to be in that state, it doesn't inform on what action is better

$V_{\pi}$  and  $q_{\pi}$  can be estimated from experience → **Monte Carlo Approximation**  
 $q_{\pi}$  says also what is the best action to take

**Action-Value function**  $q_{\pi}(a, s) = \mathbb{E}_{\pi} [G_t | S_t = s, A_t = a]$   
 after  $a$ , follow  $\pi$  policy

$V_{\pi}(s) = \mathbb{E}_{\pi} [q_{\pi}(s, a)] = \sum_{a \in \mathcal{A}} \pi(a|s) q_{\pi}(s, a)$

**Markov Decision Process** MDP =  $\langle \mathcal{S}, \mathcal{A}, p, r, \gamma \rangle$  (state space)

model that formalizes decision making in scenarios where outcomes are partially random and partly under control of a decision maker → MDP is the environment  
 - follows the Markov property  
 - solving a MDP means to find an optimal policy  $\pi^*$

can be seen as an extension of Markov Chains with  $a_t$  and  $r_t$

**Agent**  $\langle \pi, V_{\pi} \rangle$  or  $\langle \pi, q_{\pi} \rangle$  - evaluate and improve  $\pi$  under  $\epsilon$  MDP

**POLICY Evaluation** → how worth a policy  $\pi$  is - since  $V_{\pi}$  is unknown we can keep track of rewards achieved through time following  $\pi$ , in this way we can estimate  $V_{\pi}$  by taking the mean of  $G_t$  following a visit to  $s$

$V_{\pi}(s) = \mathbb{E}_{\pi} [G_t | S_t = s] = \mathbb{E}_{\pi} [R_{t+1} + \delta V_{\pi}(S_{t+1}) | S_t = s] = \mathbb{E}_{\pi} [R_{t+1} + \delta \mathbb{E}_{\pi} [G_{t+1} | S_{t+1}]] | S_t = s = \mathbb{E}_{\pi} [R_{t+1} + \delta V_{\pi}(S_{t+1}) | S_t = s]$   
 total expectation  $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X|A]]$

**BELLMAN EQUATIONS**

$= \sum_{a \in \mathcal{A}} \pi(a|s) \sum_{s'} p(s'|s, a) [r(s, a) + \delta V_{\pi}(s')] = \sum_{a \in \mathcal{A}} \pi(a|s) [r(s, a) + \delta \sum_{s'} p(s'|s, a) V_{\pi}(s')]$

$= \sum_{a \in \mathcal{A}} \pi(a|s) [R_s^a + \delta \sum_{s'} P_{ss'}^a V_{\pi}(s')] = R_s^{\pi} + \sum_{s'} P_{ss'}^{\pi} V_{\pi}(s')$

$Q_{\pi}(s_t, a_t) = \mathbb{E}_{\pi} [R_{t+1} + \delta Q_{\pi}(s_{t+1}, a_{t+1}) | S_t = s_t, A_t = a_t] = R_s^a + \delta \sum_{s'} P_{ss'}^a \sum_{a' \in \mathcal{A}} \pi(a'|s') Q_{\pi}(s', a')$

## Closed form solution of Bellman Equation

Can be rewritten in matrix form  $V_{\pi} = R^{\pi} + \gamma P^{\pi} V_{\pi} \rightarrow V_{\pi} = (I - \gamma P^{\pi})^{-1} R^{\pi}$

$R^{\pi}$  vector with entries  $r_s^{\pi}$   
 $P^{\pi}$  matrix with entries  $p_{ss'}^{\pi}$

Intractable to solve in real world scenarios

**Optimal Policy** A policy  $\pi$  is **better than**  $\pi'$  ( $\pi \succ \pi'$ )  $\Leftrightarrow V_{\pi}(s) \geq V_{\pi'}(s) \forall s \in S$   
 • VMDP exists at least one optimal policy  $\pi^* = \operatorname{argmax}_{\pi} \mathbb{E}_{\pi} [G_1 | s_1 \sim \mathcal{P}(s)] = \operatorname{argmax}_{\pi} \mathbb{E}_{\pi} [V_{\pi}(s_1)]$

**Optimal Value Functions**  $V_*(s) = \max_{\pi} V_{\pi}(s) \rightarrow$  largest expected return achievable from each  $s$   
 $q_*(s, a) = \max_{\pi} q_{\pi}(s, a)$

Th: VMDP  $\exists \pi^*(s)$  a deterministic optimal policy:  $\pi^*(a|s) = \begin{cases} 1 & \text{if } a = \operatorname{argmax}_{a \in A} Q^*(s, a) \\ 0 & \text{otherwise} \end{cases}$

**Bellman Optimality Equation** •  $V^*(s) = \max_{a \in A} q^*(s, a) = \max_{a \in A} [R_s^a + \gamma \sum_{s'} P_{ss'}^a V^*(s')]$   
 •  $q^*(s, a) = R_s^a + \gamma \sum_{s'} P_{ss'}^a V^*(s') = R_s^a + \gamma \sum_{s'} P_{ss'}^a \max_{a' \in A} q^*(s', a')$   
 → implies deterministic optimal policy with max  
 → Independent from  $\pi$

→ These equations are non-linear, so in general  $\nexists$  a closed solution  $V_*$   
 • we need ways to approximate → iterative approaches

## DYNAMIC PROGRAMMING

→ can be used to solve problems that:

- 1) can be decomposed in sub-problems → bellman equations
- 2) can store and reuse sub-problems solutions → done by value function (computation of  $\mathbb{E}$  return over a trajectory)

• Assume full MDP knowledge and finite MDP (finite  $A, S$ )

① **Policy Iteration** → alternates policy evaluation and improvement until convergence → Each iteration is called **GPI** (generalized policy iteration)

$$\pi_0 \xrightarrow{E} V_{\pi_0} \xrightarrow{I} \pi_1 \xrightarrow{E} V_{\pi_1} \rightarrow \dots \xrightarrow{E} V_{\pi_k} \xrightarrow{I} \pi_{k+1}$$

1) **Policy Evaluation**: Input  $S, A, R, P, \pi, \gamma$

→ I could compute  $V_{\pi}$  exactly but it is computationally heavy → iterative method  
 $O(|S|^3)$  vs.  $O(|S| \cdot |A|)$  per iteration

$V_k(s) = 0 \quad \forall s \in S$   
 $k = 0$   
 while  $k = 0 \vee \|V_k - V_{k-1}\| > \epsilon$ :  
 $V_k = V_{k-1}(s) = \sum_{a \in A} \pi(a|s) [R_s^a + \gamma \sum_{s'} P_{ss'}^a V_{k-1}(s')]$   
 $k++$   
 return  $V_k$

2) **Policy Improvement**  $\pi'(s) \leftarrow \operatorname{argmax}_{a \in A} [R_s^a + \gamma \sum_{s'} P_{ss'}^a V_k(s')]$   
 deterministic  $q^*(a, s)$  computed using old  $\pi$   $\forall s \in S$

• improve just by looking a step-ahead  
 → typically  $V_k$  takes more to converge w.r.t  $\pi$   
 → do not need  $q_{\pi}$  actually

Th: **Policy Improvement** lets  $\pi' \leftarrow \operatorname{greedy}(V_{\pi}) \wedge \pi \neq \pi' \Rightarrow V_{\pi'} > V_{\pi}$   
 in case of equality  $V_k(s) = \max_{a \in A} Q_{\pi}(s, a) \rightarrow V_k - V_{k-1} = V_k \rightarrow \pi - \pi' = \pi^*$   
 1)  $q_{\pi}(s, \pi'(s)) = \max_{a \in A} q_{\pi}(s, a) \geq q_{\pi}(s, \pi(s)) = V_{\pi}(s)$   
 2)  $V_{\pi'}(s) \leq Q_{\pi}(s, \pi'(s)) = \mathbb{E}_{\pi} [r_{t+1} + \gamma V_{\pi}(s_{t+1}) | s_t, a_t = \pi'(s_t)] = \mathbb{E}_{\pi} [r_{t+1} + \gamma q_{\pi}(s_{t+1}, a_{t+1}) | s_t] = \mathbb{E}_{\pi} [r_{t+1} + \gamma q_{\pi}(s_{t+1}, a_{t+1}) | s_t] \leq \dots \leq V_{\pi}(s_t)$

Th: **Policy Iteration Convergence** -  $|S|$  and  $|A|$  must be finite  
 -  $R$  must be bounded  
 -  $0 < \gamma < 1$   
 $\Rightarrow \{V_k\}$  converges to  $V_*$   $\wedge \{\pi_k\} \rightarrow \pi^*$

② **Value Iteration** → do not model  $\pi(s)$ , computes it only at the end  
 • uses Bellman Optimality Equation and not Bellman Equation

$$V_1 \rightarrow V_2 \rightarrow \dots \rightarrow V_k$$

$$V_{k+1}(s) = \max_{a \in A} [R_s^a + \gamma \sum_{s'} P_{ss'}^a V_k(s')] \text{ and then compute } \pi_k \leftarrow \operatorname{greedy}(V_{k+1})$$

### ASYNCHRONOUS DP

- some state may not need to have their values updated as often as others
- in place updates of  $V$  and  $\pi$
- Early stopping → do not wait for full convergence

} improve performances

### PROBLEMS of DP

- high computational effort, seeing all  $S$  and  $A$  each iteration  $O(|S| \cdot |A|)$  → do not scale with  $|S|$
- new approaches must be considered **sample-based**
  - model-free
  - model-based

→ DP method performs bootstrapping and not sampling

# MODEL FREE EVALUATION → algorithms that do not need to know transition probabilities $p(s'|s, a)$

- episode → list of experiences made between initial and final state (or max # of experiences T)
- experience<sub>i</sub> = < State, Action, Reward, Next State > → sample

1) MONTE-CARLO RL  $V_{\pi}(s) = \mathbb{E}_{\pi} [G^T | s_t = s]$   $G^T = \sum_{k=t}^{\infty} \gamma^{k-t} r_{k+1}$

In order to estimate  $V_{\pi}$  we have two possibilities:

- First-Encounter:**  $V_{\pi}(s)$  is the avg of returns following first visit to  $s$  across episodes.  $\hat{V}(s) = \frac{1}{N} \sum_{i=1}^N G_i \rightarrow V_{\pi}(s)$  as  $N \rightarrow +\infty$  for large number law.   
 (across N episodes, first encounter return in episode i)
- Every-Encounter:** consider all the visit to  $s$  across a single episode

**Input:**  $\pi$ , num-episodes

$N(s) \leftarrow 0 \quad \forall s \in S$   
 $Returns(s) \leftarrow 0 \quad \forall s \in S$

for  $e \leftarrow 1$  to num-episodes do  
 generate using  $\pi$  on episode  $S_0, A_0, R_1, \dots, S_{T-1}, A_{T-1}, R_T, S_T$   
 $G \leftarrow 0$   
 for  $t \leftarrow T-1$  to 0 do:  
 $G \leftarrow \gamma G + R_{t+1}$   
 [if  $S_t \notin \langle S_0, \dots, S_{t-1} \rangle$  then] \* → only present in first-encounter  
 $Returns(S_t) \leftarrow Returns(S_t) + G$  → sum across episodes  
 $N(S_t) \leftarrow N(S_t) + 1$

$V(s) \leftarrow \frac{Returns(s)}{N(s)} \quad \forall s \in S$        $[G(s_t, a_t) \leftarrow \frac{Returns(s_t, a_t)}{N(s_t, a_t)}]$  → needs two different counters the if is updated with  $\langle S_t, a_t \rangle \notin \langle S_0, a_0, \dots, S_{t-1}, a_{t-1} \rangle$

return  $V$

I could use the **incremental mean** to avoid storing  $Returns(S_t)$

$$V(S_t) \leftarrow V(S_t) + \frac{1}{N(S_t)} [G - V(S_t)]$$

In **non-stationary MBP** (transitions and rewards changes),  $V$  cannot converge and we will use **exponential decay** to forget about the past  $V(S_t) \leftarrow V(S_t) + \alpha (G_t - V(S_t))$   $\alpha \in (0, 1)$   
 (fixed regardless  $N(S_t)$  → prioritize recent observations)

- Offline learning** because wait the end of episode to update  $V$ , since I need to compute  $G_t$
- Unbiased** since we are computing correctly the expected value
- High Variance** wrt TD learning

## 2) TEMPORAL-DIFFERENCE (TD) LEARN → MC methods needs to wait the end of an episode to make an update, meanwhile TD methods only wait the next timestep

**TD(0):**  $V(S_t) \leftarrow V(S_t) + \alpha [R_{t+1} + \gamma V(S_{t+1}) - V(S_t)]$   
 (new estimation for  $G_t$ )

- Converges to optimality with high probability  $\Leftrightarrow 0 < \alpha \leq 1$
- sample order affects the result
- TD **converges faster** than MC in practice → **online learning**

- given  $\pi$ , TD(0) **converges** to  $V_{\pi} \Leftrightarrow$ 
  - $\pi$  induces on irreducible Markov chain (reach any state from any other)
  - finite MDP
  - $\sum_{k=1}^{\infty} \alpha \gamma^{k-1} < +\infty \wedge \sum_{k=1}^{\infty} \alpha \gamma^{k-1} > 0$  [ $\alpha \gamma < 1$ ]

**Input:**  $\pi, \alpha \in (0, 1], \text{num-ep}, \gamma$

Initialize  $V(s) \in \mathbb{R}$  randomly except  $V(\text{terminal}) = 0$

for  $e \leftarrow 1$  to num-ep  
 $S_0 \leftarrow$  initial state  $t \leftarrow 0$   
 while  $S_t \neq$  terminal  
 $a_t \leftarrow \pi(S_t)$   
 Take action  $a_t$  and observe  $(S_{t+1}, r_{t+1})$   
 $V(S_t) \leftarrow V(S_t) + \alpha [r_{t+1} + \gamma V(S_{t+1}) - V(S_t)]$   
 $t \leftarrow t + 1$

**Biased** since we use **bootstrapping** (use of estimated values in update) meanwhile MC samples **biased towards the current estimation**

$$V_{\pi}(s) = \mathbb{E}_{\pi} [G_t | S_t = s] \leftarrow \text{MC biased}$$

$$= \mathbb{E}_{\pi} [R_{t+1} + \gamma V_{\pi}(S_{t+1}) | S_t = s] \leftarrow \text{TD biased}$$

(approximation)

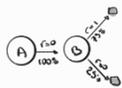
**Low variance** since a lot of updates (shorter stochastic chains)  
 eg. MC:  $\text{Var} [G_t | S_t] = \text{Var} [R_{t+1} + \gamma R_{t+2} + \dots]$

**DIFFERENCES TD vs. MC**

- MC converges to **MSE** solution  $V_{\pi} = \text{argmin} \sum_{s \in S} \sum_{a \in A} (G_s - V(s))^2$ , meanwhile TD(0) to maximum likelihood MDP
- MC doesn't respect **Markovian Property** → update  $V_{\pi}$  on all the episode meanwhile TD(0) does → update  $V_{\pi}$  only on  $s_t$  and  $s_{t+1}$

because TD(0) assumes and uses the MDP structure in one-step update

$$\begin{cases} \hat{P}_{SS'}^a = \frac{1}{N(s,a)} \sum_{t=1}^{T-1} \mathbb{I}(s_t = s, a_t = a, s_{t+1} = s') \\ \hat{R}_s^a = \frac{1}{N(s,a)} \sum_{t=1}^{T-1} \mathbb{I}(s_t = s, a_t = a) r_t \end{cases}$$



A, 0, B, 0	B, 1
B, 1	B, 1
B, 1	B, 1
B, 1	B, 0

MC:  $V_{\pi}(A) = 0$   
 TD:  $V_{\pi}(A) = \frac{3}{4}$

→ as if I first estimate  $\hat{P}_{SS'}^a$  and  $\hat{R}_s^a$  and then compute  $\mathbb{E}[G_t | S_t = A]$

**MODEL FREE OPTIMIZATION**

- ON-POLICY OPTIMIZATION** → There are two types of policies:
- 1) **Target policy**: used to optimize decision making (typically greedy)
  - 2) **Behavioural policy**: used to navigate the env (could be random or  $\epsilon$ -greedy)
- In on-policy algorithms the two are equal, meanwhile different in off-policy ones

→ Problems of Greedy approaches for updating the policy in on-policy algorithms:  $T_{\pi_{k+1}}(a|s) \leftarrow \text{argmax}_{a \in A} R_s^a + \gamma \sum_{s' \in S} P_{SS'}^a V_{\pi_k}(s')$

- 1)  $R_s^a$  and  $P_{SS'}^a$  are unknown → use  $Q$  instead of  $V$ :  $T_{\pi_{k+1}}(a|s) = \text{argmax}_{a \in A} Q_{\pi_k}(s,a)$
- 2) There is no exploration of the possible actions since only greedy choices are made
  - $\epsilon$ -greedy select with  $p=1-\epsilon$  the greedy choice and with  $p=\epsilon$  a choice at random
  - **Exploration** (get info about the world) - **Exploitation** (getting rewards) **tradeoff**

not deterministic

$$T_{\pi_{k+1}}(a|s) = \begin{cases} \frac{\epsilon}{|A(s)|} + (1-\epsilon) & \text{if } a = \text{argmax}_{a \in A} Q_{\pi_k}(s,a) \text{ (greedy action)} \\ \frac{\epsilon}{|A(s)|} & \text{otherwise} \end{cases}$$

$m = |A(s)|$

**Th:  $\epsilon$ -greedy policy improvement**:  $\epsilon$ -greedy generates a policy  $\pi_{k+1}$  that  $V_{\pi_{k+1}} \geq V_{\pi_k}$

$\max_{a \in A} Q_{\pi_k}(s,a) \geq \sum_{a \in A} w_a Q_{\pi_k}(s,a)$  with  $\sum w_a = 1$  and  $w_a \geq 0$

**Proof**:  $\mathbb{E}_{\pi_{k+1}}[Q_{\pi_k}(s,a)] \geq \sum_{a \in A} T_{\pi_{k+1}}(a|s) Q_{\pi_k}(s,a) = \frac{\epsilon}{m} \sum_{a \in A} Q_{\pi_k}(s,a) + (1-\epsilon) \max_{a \in A} Q_{\pi_k}(s,a) \geq \frac{\epsilon}{m} \sum_{a \in A} Q_{\pi_k}(s,a) + (1-\epsilon) \sum_{a \in A} \frac{T_{\pi_{k+1}}(a|s) - \frac{\epsilon}{m}}{1-\epsilon} Q_{\pi_k}(s,a) = \sum_{a \in A} T_{\pi_{k+1}}(a|s) Q_{\pi_k}(s,a) = V_{\pi_k}(s)$

- recursively apply this inequality for policy improvement theorem  $V_{\pi_{k+1}} \geq V_{\pi_k}$

**GUE PROPERTY (Greedy in the Limit with Infinite Exploration)**:

$\pi$  has GUE property  $\Rightarrow$  Q-style update rule converges ( $\pi^*, Q^*$ )

**DEF** a stochastic policy has GUE property if:

- 1)  $\lim_{k \rightarrow \infty} N_k(s,a) = +\infty$
- 2)  $\lim_{k \rightarrow \infty} T_k(a|s) = \mathbb{I}(a = \text{argmax}_{a \in A} Q_k(s,a))$

each state-action pair is visited infinitely many times

policy converges to the greedy one → guarantee the GUE converges to optimum  $\pi^*$

→ If  $\epsilon$ -greedy has  $\epsilon_k \in \Theta(\frac{1}{k}) \Rightarrow$  it has GUE property since:

- 1)  $\sum_{k=1}^{\infty} \epsilon_k = \sum_{k=1}^{\infty} \frac{1}{k} = +\infty \rightarrow$  infinite exploration
- 2) since  $\epsilon_k \rightarrow 0$ , tends to greedy selection

**1) ON-POLICY MC**

Initialize  $Q(s,a) \in \mathbb{R}$  arbitrarily  $\forall s,a \in S \times A$ ,  $\pi_t(s) \in A(s)$  arbitrarily ( $Q \approx Q^*$ )  
 for  $e \leftarrow 1$  to max-ep  
 generate an episode following  $\pi_e$ :  $s_0, a_0, r_1, \dots \rightarrow \pi$  both behavioural and target policy  
 $G \leftarrow 0$   
 for  $t \leftarrow T-1$  to 0:  
 $G \leftarrow \gamma G + R_{t+1}$   
 $N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$   
 $Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \frac{1}{N(s_t, a_t)} [G - Q(s_t, a_t)]$   
 $E \leftarrow \frac{1}{E}$   
 $\pi_e(a|s) \leftarrow \epsilon$ -greedy with  $Q \forall s, a$

**2) SARSA** → similar to TD evaluation on  $Q$  instead of  $V$

sample:  $i = \langle S, A, R, S', A' \rangle \rightarrow$  transitions of  $\langle S, A \rangle$  pairs

Update Rule:  $Q(s,a) \leftarrow Q(s,a) + \gamma [r + \delta Q(s',a') - Q(s,a)]$

→ **converges** (as all the weighted averages methods) to  $q^*(s,a)$  just sufficient exploration is needed

$\Leftrightarrow \sum_{t=1}^{\infty} \gamma^t = +\infty \wedge \sum_{t=1}^{\infty} \gamma^{2t} < +\infty \wedge$  GUE policy  $\pi_{\epsilon}(a|s)$

**EXPECTED SARSA**  $Q(s,a) \leftarrow Q(s,a) + \gamma [r + \delta \sum_{a' \in A} \pi(a'|s') Q(s',a') - Q(s,a)]$

→ fails when  $|A|$  is too large to compute

→ prevents the randomness of  $\alpha \pi$  to increase the variance by talking on  $\mathbb{E}_{\alpha \pi}$   
 • has the same bias but lower variance wrt SARSA  
 ↳ more robust updates  $\Rightarrow$  faster convergence

Input ( $\alpha \in (0,1]$ , num-ep,  $\gamma$ ) (estimate  $q^*$ )

Initialize  $Q(s,a) \in \mathbb{R}$  randomly except  $Q(\text{terminal}) = 0$   
 for  $e \leftarrow 1$  to num-ep  
 $S_0 \leftarrow$  initial state  $t \leftarrow 0$   $Q_0 \leftarrow \pi(S_0, A)$   
 while  $S_t \neq$  terminal  
 Take action  $a_t$  and observe  $(S_{t+1}, R_{t+1})$   
 $Q_{t+1} \leftarrow \pi(S_{t+1}, Q)$  → target policy in this iteration or  $\epsilon$ -greedy on the next one [L-9]  
 $Q(S_t, a_t) \leftarrow Q(S_t, a_t) + \alpha [R_{t+1} + \gamma Q(S_{t+1}, a_{t+1}) - Q(S_t, a_t)]$   
 $t \leftarrow t + 1$

# OFF-POLICY OPTIMIZATION

## 1) MC OPTIMIZATION

### Importance Sampling

$$\mathbb{E}_\pi [f(x)] \approx \frac{1}{N} \sum_{i=1}^N f(x_i) \quad \text{with } x_i \sim \mu(x)$$

Law of big numbers

$$\frac{1}{N} \sum_{i=1}^N f(x_i) - \mu \xrightarrow{\text{emp. N}} N(\mu, \sigma^2) = \begin{cases} \mu = \mathbb{E}_\pi [f(x)] \rightarrow \text{unbiased} \\ \sigma^2 = \frac{1}{N} \text{Var} [f(x)] \end{cases}$$

random variable since changing sample change  $\sigma$

$$\mathbb{E}_\pi [f(x)] = \sum_x \pi(x) f(x) = \sum_x \pi(x) \frac{p(x)}{q(x)} f(x) = \mathbb{E}_q \left[ \frac{p(x)}{q(x)} f(x) \right]$$

target policy  $\pi(x)$ , behavioral policy  $q(x)$

requirements:  $p(x) > 0, q(x) > 0$  otherwise cannot sample from some areas

I can estimate  $\mathbb{E}_\pi$  with samples from  $x \sim q$

$$\mathbb{E}_q \left[ \frac{p(x)}{q(x)} f(x) \right] \approx \frac{1}{N} \sum_{i=1}^N \frac{p(x_i)}{q(x_i)} f(x_i) = r \rightarrow \text{unbiased but different variance} \quad \text{Var}[r] = \frac{1}{N} \text{Var} \left[ \frac{p(x)}{q(x)} f(x) \right]$$

There are two samples:

1)  $G_t^\mu$  = return from  $\mu$  (behavioral)

2)  $G_t^\pi$  = return of target policy computed by  $\mu$  experiences

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha [G_t^\pi - Q(s_t, a_t)]$$

$$P(A_t, S_{t+1}, A_{t+1}, \dots, S_T | S_t, A_{t-1}, \dots) = \prod_{k=t}^{T-1} \pi(A_{k+1} | S_{k+1}, \text{past}) p(S_{k+1} | S_k, A_k, \text{past})$$

chain rule

$$= \prod_{k=t}^{T-1} \pi(A_k | S_k) p(S_{k+1} | S_k, A_k) \rightarrow \text{Markovian property}$$

$$\Rightarrow W_{t:T-1} = \frac{\prod_{k=t}^{T-1} \pi(A_{k+1} | S_{k+1}) p(S_{k+1} | S_k, A_k)}{\prod_{k=t}^{T-1} \mu(A_{k+1} | S_{k+1}) p(S_{k+1} | S_k, A_k)} = \frac{\prod_{k=t}^{T-1} \pi(A_{k+1} | S_{k+1})}{\prod_{k=t}^{T-1} \mu(A_{k+1} | S_{k+1})}$$

importance ratio

$$\mathbb{E}_\mu [W_{t:T-1} G_t^\pi | S_t = s] = \mathbb{E}_\pi [G_t^\pi | S_t = s] = V_\pi(s)$$

→ unfortunately  $W_t$  and the episodes increases the variance

- $W_t \neq 1 \rightarrow$  when  $\pi$  and  $\mu$  behave differently
- $\mu$  and  $\pi$  should be as close as possible (use  $\epsilon$ -greedy and greedy)

using  $\mu$  sample on episode  $s_0, a_0, r_1, \dots$

$$W_T \leftarrow 1, G^T \leftarrow 0$$

for  $t \leftarrow T-1$  to 0

$$W_t \leftarrow W_{t+1} \cdot \frac{\pi(A_t | S_t)}{\mu(A_t | S_t)}$$

typically deterministic

$$G^t \leftarrow R_{t+1} + \gamma G^t$$

typically stochastic

$$G^T \leftarrow W_t G^t$$

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha [G^t - Q(s_t, a_t)]$$

$$\pi(s_t) \leftarrow \text{argmax}_{a \in A} Q(s_t, a)$$

## 2) TD Optimization

depends on  $\mu$  for  $\alpha$  (influence only  $r_{t+1}$ )

reward  $r_{t+1}$  just depends on current  $\langle a, s \rangle$  pairs not on all trajectory

$$V(s_t) \leftarrow V(s_t) + \alpha \left[ \frac{\pi(a_t | s_t)}{\mu(a_t | s_t)} (r_{t+1} + \gamma V(s_{t+1})) - V(s_t) \right]$$

$$V_\pi(s) = \mathbb{E}_\mu [W_t (r_{t+1} + \gamma G_t^\mu) | S_t = s]$$

→ scaling by just one factor lower significantly the variance

## 3) Q-LEARNING

→ do not use importance sampling

$$\pi(s) = \text{argmax}_{a \in A} Q(a, s)$$

$$\mu(a | s) = \begin{cases} \frac{\epsilon}{|A(s)|} + (1-\epsilon) & \text{if } a = \text{argmax}_{a \in A} Q(a, s) \\ \frac{\epsilon}{|A(s)|} & \text{otherwise} \end{cases}$$

doesn't depend on  $\mu$

importance sample is not needed because  $a_t$  is given

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha \left[ \frac{\pi(a_t | s_t)}{\mu(a_t | s_t)} (r_{t+1} + \gamma \max_{a \in A} Q(s_{t+1}, a)) - Q(s_t, a_t) \right]$$

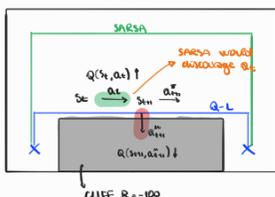
$$= r_{t+1} + \gamma \max_{a \in A} Q(s_{t+1}, a)$$

optimal convergence with GLIE and  $\sum \alpha_t = +\infty \wedge \sum \alpha_t^2 < +\infty$

Q-learning is a tabular method since I can express  $Q$  by a  $|S| \times |A|$  matrix

## SARSA vs Q-Learning

(on-policy vs off-policy)



Q-learning is learning the actual optimal path (greedy) → optimistic

SARSA is learning the safest path from  $\epsilon$ -greedy → more conservative in dangerous situations

it learns a sub-optimal policy

**N-STEPS BOOTSTRAPPING** → n between MC methods with  $n \rightarrow \infty$  and TD(0)

$$G_t = \overbrace{R_{t+1} + \gamma R_{t+2} + \dots + \gamma^n R_{t+n}}^{n+1 \text{ rewards}} + \underbrace{\gamma^{n+1} R_{t+n+1} + \dots + \gamma^{T-t} R_T}_{\gamma^{n+1} V(S_{t+n}) \text{ bootstrapping}}$$

**1) TD(n)**

$$G_t^{(n)} = \sum_{k=0}^n \delta^k R_{t+k+1} + \delta^n V(S_{t+n})$$

$G_t^{(n)} = R_{t+1} + \gamma V(S_{t+1})$  will be the one of  $t+n$  steps ahead

→ typically the best result is in between  $n=1$  and  $n=\infty$

The first time  $R_{t+n+1}$  is available is  $n$  timesteps forward (online but delay)

$$V(S_t) \leftarrow V(S_t) + \alpha [G_t^{(n)} - V(S_t)]$$

**2) TD( $\lambda$ )**

→ weighted mean of  $G_t^{(n)}$  for different n  
 → **offline**

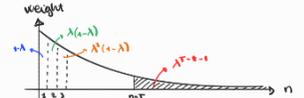
$$G_t^{(\lambda)} = (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} G_t^{(n)}$$

or long N (slide)

→  $\lambda$  controls bias-variance trade-off

$$\lambda \in (0,1) \rightarrow \sum_{n=1}^{\infty} (1-\lambda) \lambda^{n-1} = 1$$

short term rewards long term rewards



$\lambda=0 \Rightarrow G_t^{(\lambda)} = G_t^{(0)} \quad \text{TD}(0)$

$\lambda=1 \Rightarrow G_t^{(\lambda)} = (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} G_t^{(n)} + (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} G_t^{(n)}$

episodic (end of T)  $\lambda=1$  post-termination contributions =  $G_t$  because it sees all the timesteps  $t:T$

$= G_t (1-\lambda) \sum_{m=0}^{\infty} \lambda^{m+T-t-1} = G_t (1-\lambda) \lambda^{T-t-1} \sum_{m=0}^{\infty} \lambda^m$  → geometric serie

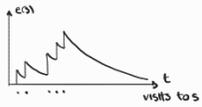
$= G_t (1-\lambda) \lambda^{T-t-1} \cdot \frac{1}{1-\lambda} = G_t \cdot \lambda^{T-t-1} = G_t \quad \text{MC}$

**3) Backward TD ( $\lambda$ )**

→ implement TD( $\lambda$ ) in an **online** way

Associated with each state there is what is called an **eligibility trace**  $e_t(s) \in \mathbb{R}^+$

→  $e_t(s)$  records which states have been recently visited



At each step update  $e_t(s)$  w.r.t  $s$  in this way:  $e_t(s) = \begin{cases} \gamma \lambda e_{t-1}(s) & \text{if } s \neq s_t, t > 0 \\ \gamma \lambda e_{t-1}(s) + 1 & \text{if } s = s_t, t > 0 \\ 0 & \text{if } t = 0 \end{cases}$

→ decay factor

We define  $\delta_t = R_{t+1} + \gamma V_t(S_{t+1}) - V_t(S_t)$

The update policy is  $V(s) \leftarrow V(s) + \alpha \delta_t e_t(s)$   $\forall s \in S$

→ constant  $\forall s \in S$

•  $\text{BTD}(0)$  has  $e_t(s) = \mathbb{I}(s=s_t)$ , thus equivalent to TD

• meanwhile with  $\text{BTD}(\lambda)$  you get MC, but better → online + extendable to continuing tasks

→ can be shown that TD( $\lambda$ ) and  $\text{BTD}(\lambda)$  are **equivalent** (with  $\gamma \lambda < 1$ )

$$V \left[ \sum_{k=0}^{\infty} (\gamma \lambda)^k \delta_{t+k} \right] = V \left[ G_t^{(\lambda)} - V(S_t) \right]$$

total update of  $V(S_t)$  from  $\text{BTD}(\lambda)$       TD( $\lambda$ ) update of  $V(S_t)$

→ At the end of the episode they produced the same updates

**4) SARSA ( $n$ )**

Defining  $Q_t^{(n)} \leftarrow \sum_{k=0}^{n-1} \gamma^k r_{t+k+1} + \gamma^n Q(S_{t+n+1}, a_{t+n+1})$

We got the update  $Q(S_t, a_t) \leftarrow Q(S_t, a_t) + \alpha [Q_t^{(n)} - Q(S_t, a_t)]$

**5) SARSA ( $\lambda$ )**

Defining  $Q_t^{(\lambda)} \leftarrow (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} G_t^{(n)}$

we got the update  $Q(S_t, a_t) \leftarrow Q(S_t, a_t) + \alpha [Q_t^{(\lambda)} - Q(S_t, a_t)]$

**6) Backward SARSA ( $\lambda$ )**

$Q(S_t, A_t) \leftarrow Q(S_t, A_t) + \alpha \delta_t E_t(S_t, A_t) \quad \forall s, a \in S \times A(s)$

$\delta_t = R_{t+1} + \gamma Q(S_{t+1}, a_{t+1}) - Q(S_t, a_t)$

$e_t(s, a) = \gamma \lambda e_{t-1}(s, a) + \mathbb{I}(s_t=s, a_t=a)$

**Episode**

$e(s) \leftarrow 0 \quad \forall s \in S$

So ← initialize  $t \leftarrow 0$

while  $S_t \neq \text{terminal}$

$a \leftarrow \pi(S_t)$

take action  $a$  and observe  $(r_t, S_{t+1})$

$S \leftarrow r + \gamma V(S_{t+1}) - V(S_t)$

$e(S_t) \leftarrow e(S_t) + 1$

$\forall s \in S:$

$V(s) \leftarrow V(s) + \alpha \delta e(s)$

$e(s) \leftarrow \gamma \lambda e(s)$

$t \leftarrow t+1$  → exponential decay

# Approximate Solutions Methods

Tabular methods have difficulties for large spaces (images) or continuous ones  
 - they lack the ability to recognize similar states and **generalize**

No more tabular version of V and Q but we define two **parametric functions**

$$\hat{V}: S \times \Theta \rightarrow \mathbb{R} \quad \hat{Q}: S \times \Theta \rightarrow \mathbb{R}^{|A|}$$

→ solution to generalize from unseen states  
 → needs to be **differentiable** for GD

Two problems

1) **Non-stationary data**

→ environment may change (thus the policy should change too)

2) **Non-IID data**

→ correlated events that could cause some problem with the convergence of GD

MSE: 
$$\mathcal{L}(\theta) = \mathbb{E}_{\mu} [(\underbrace{V_{\pi}(s)}_{\text{unknown}} - \hat{V}(s, \theta))^2]$$

$\mu$ : state probability distribution (how much we care about the error in state s)

## LINEAR APPROXIMATORS

$$\hat{V}(s, \theta) = \phi(s)^T \theta$$

↑ state space encoding function

-  $\mathcal{L}(\theta)$  is quadratic

$$\nabla_{\theta} \mathcal{L} = -2(V_{\pi}(s) - \hat{V}(s, \theta)) \cdot \frac{\partial \hat{V}(s, \theta)}{\partial \theta} = -2(V_{\pi}(s) - \hat{V}(s, \theta)) \phi(s) \Rightarrow$$

$$\theta_{t+1} \leftarrow \theta_t + \alpha [V_{\pi}(s) - \hat{V}(s, \theta)] \phi(s)$$

↑ gradient descent

- linear approximator is enough thanks to **Representer Theorem** (different part is to find the kernel  $\phi$ )

Since  $V_{\pi}(s)$  is unknown we need to replace it with the empirical target  $G_t$

**MC**:

$G_t$  is unbiased but noisy  
 $\mathbb{E}[G_t | S_t] = V_{\pi}(S_t)$   
 - strong convergence property

```

loop:
    generate with  $\pi$  on episode  $S_0, A_0, R_1, \dots$ 
    for each step  $t$ :
         $\theta \leftarrow \theta + \alpha [G_t - \hat{V}(S_t, \theta)] \phi(S_t)$ 
    
```

**TD(0)**:

$G_t$  is reliable but biased  
 - weak convergence property (for biased GD but faster)  
 • TD(0) under linear approximations converges

```

loop (episodes):
     $S_0 \leftarrow$  initialize
    loop (steps):
         $A \sim \pi(a|S)$ 
        take action  $A$  and observe  $R, S'$ 
         $\theta \leftarrow \theta + \alpha [R + \gamma \hat{V}(S', \theta) - \hat{V}(S, \theta)] \phi(S)$ 
         $S \leftarrow S'$ 
    
```

→ Since the target depends on current  $\theta$  the GD will be biased  
 → **semi-gradient methods** because the gradient is not the true gradient but an approximation  
 • All the bootstrapping are affected

The eligibility for TD( $\lambda$ ) can be defined as:  $E_t = \gamma \lambda E_{t-1} + \phi(S_t)$

- We can use **batched episodes** to generate more **stable** gradients → solves iid problems with dataset sampling from **experience replay buffer** ( $s, a, r, s' \sim D$ )  
 • I could add a **temporal weight** to overcome the non-stationary data

instead of iterative methods

## DNN APPROXIMATORS

Deep Q-Network (**DQN**) is a DNN to approximate Q

- it uses an **experience replay buffer** → breaks correlation between consecutive experience  
 - uses  **$\epsilon$  greedy policy**

cannot be done with Deep-SARSA since it depends on  $a' \sim \pi_{old}$

- It uses a separate NN to estimate Q-values target ( $\theta^-$  parameters) → prevents rapid oscillations caused by moving targets (diverges otherwise)  
 • it is updated **periodically** (not on every epoch  $\theta \leftarrow \theta^-$ ) → it reduces the bias  

$$\theta = T \theta + (1-T) \theta^- \quad \text{if } T=1 \Rightarrow \text{hard update, otherwise soft}$$

over replay buffer → semi-gradient update  
 simple DQN: 
$$\mathcal{L}(\theta) = \mathbb{E}_D [(r + \gamma \max_{a \in A} \hat{Q}(s', a, \theta^-) - \hat{Q}(s, a, \theta))^2]$$

• Problem: **upward positive bias** from taking the maximum of a noisy estimate  $\hat{Q}(s, a, \theta^-)$   
 → splits action selection ( $\hat{Q}_\theta$ ) and action evaluation ( $\hat{Q}_{\theta^-}$ ) and then vice-versa

→ problem is solved if the noise on  $\hat{Q}_\theta$  and  $\hat{Q}_{\theta^-}$  are decorrelated

double DQN:

$$\mathcal{L}(\theta) = \mathbb{E}_D [(r + \gamma \hat{Q}(s', \arg \max_{a \in A} \hat{Q}(s, a, \theta^-)) - \hat{Q}(s, a, \theta))^2]$$

• randomly select if updating  $\theta$  or  $\theta^-$  at each iteration

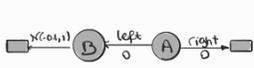
$$\mathcal{L}(\theta) = \mathbb{E}_D [(r + \gamma \hat{Q}(s', \arg \max_{a \in A} \hat{Q}(s, a, \theta^-)) - \hat{Q}(s, a, \theta^-))^2]$$

Dueling Networks  $\hat{Q}(s,a,\theta) = \hat{V}(s,\theta) + [\hat{A}(s,a,\theta) - \max_{a' \in A} \hat{A}(s,a',\theta)]$

- Uses two function:
- 1) Value function  $\hat{V}(s,\theta) \rightarrow$  expected reward for being in a state  $s$
  - 2) Advantage function  $\hat{A}(s,a,\theta) \rightarrow$  quantifies the advantage to choose a particular action in state  $s$   
 $\hat{A}(s,a) = Q(s,a) - V(s)$

In this way the model can learn **independently** what states are the best and what actions are advantageous and then combine them in the Q value  $\hat{Q}(s,a,\theta) = \hat{V}(s,\theta) + \hat{A}(s,a,\theta)$

- $\rightarrow$  more stable and robust
- 1) can estimate Q-values from unseen action better, because it has a stronger starting point than  $\hat{q}(s,a)$
  - 2) faster convergence when a lot of similar actions since  $V(s)$  will be shared and fixed and only  $\hat{A}$  will change



$\rightarrow$  once experienced a positive reward going left  $\rightarrow$  bias towards B

- no guarantees of convergence, higher variance,  $\pi$  diff

**POLICY GRADIENT METHODS**  $\rightarrow$  learn a parametrized policy  $\pi(a|s,\theta)$  not a value function to get the policy  $\rightarrow$  more direct

- typically  $\pi^*$  approximation converges faster than  $V^*$
- can be used in continuous A space
- wrt  $\epsilon$ -greedy the value of  $\pi_0$  change continuously with  $d\theta$  changes  $\rightarrow$  stronger convergence

I would like to  $\theta_{t+1} \leftarrow \theta_t + \alpha \nabla_{\theta} \pi_0(a^*|s)$  Unfortunately  $a^*$  is unknown  $\rightarrow$  weight the updates  $\theta_{t+1} \leftarrow \theta_t + \alpha \hat{Q}(s,a) \frac{\nabla_{\theta} \pi_0(a|s)}{\pi_0(a|s)}$  correction in order to not update too much more probable a

$\cdot \theta_t + \alpha \hat{Q}(s,a) \forall a \in \pi_0(a|s)$

**POLICY GRADIENT THEOREM**  $\hat{\pi} \in C^1(\mathbb{R}^n)$  In any policy gradient method where  $L(\theta) \propto \mathbb{E}_{\hat{\pi}}[V(s)] = \sum_{s \sim d_{\hat{\pi}}(s)} d_{\hat{\pi}}(s) V(s) = \sum_{s \sim d_{\hat{\pi}}(s)} \sum_a \pi(a|s,\theta) q_{\hat{\pi}}(s,a) \Rightarrow$

$\nabla_{\theta} J(\theta) \propto \sum_s d_{\hat{\pi}}(s) \sum_a q_{\hat{\pi}}(s,a) \nabla_{\theta} \pi(a|s,\theta) = \mathbb{E}_{\hat{\pi}} \left[ \sum_a \nabla_{\theta} \pi(a|s,\theta) q_{\hat{\pi}}(s,a) \right] = \mathbb{E}_{\hat{\pi}} \left[ \sum_a \nabla_{\theta} \pi(a|s,\theta) V_0 \pi(a|s,\theta) q_{\hat{\pi}}(s,a) \right]$

$\nabla_{\theta} J(\theta)$  depends both on:

- 1) action selection ( $\pi_0$ )
- 2) state distribution ( $d_{\hat{\pi}}$ )  $\rightarrow$  its change is a function of the environment, and thus unknown

$\cdot$  we do not need  $\nabla d_{\hat{\pi}}$  for previous theorem and neither  $\nabla q_{\hat{\pi}}(s,a)$

**MC policy gradient**  $G_t$  is an unbiased sample of  $Q_{\hat{\pi}}(s,a) \rightarrow G_t = \mathbb{E}_{\hat{\pi}}[Q_{\hat{\pi}}(s,a) | s_t, a_t]$

By sampling the gradient policy theorem  $\nabla_{\theta} L(\theta) \propto \frac{1}{N} \sum_{i=1}^N \sum_{a=1}^{|A|} \nabla_{\theta} \pi(a|s_i, \theta) G_t^i \Rightarrow \theta_{t+1} \leftarrow \theta_t + \alpha \nabla_{\theta} L(\theta)$

**Weighted Maximum Likelihood**

$\cdot$  on-policy approach (otherwise importance sampling, but higher variance)

**ACTOR CRITIC METHODS** We want to **reduce** MC policy gradient variance

- Two entities:
- 1) Actor  $\pi$  that generates actions
  - 2) Critic  $\hat{Q}$  that evaluates the quality of the action taken
- $\rightarrow$  estimated by TD, MC, ... methods or using DNN if  $w \neq \theta$  two distinct NN, no gradient conflicts
- $\rightarrow$  Using a function to estimate  $G$  instead of the environment (stochastic) has lower variance but higher bias

**COMPATIBLE FUNCTION APPROXIMATION THEOREM**

If

- 1)  $\nabla_w \hat{Q}(s,a,w) = \nabla_{\theta} \pi(a|s,\theta)$  [compatibility hyp.] holds when:  $Q(s,a,w) = \nabla_{\theta} \pi(a|s,\theta)^T w$
- 2)  $\mathbb{E}_{\hat{\pi}}[(\hat{Q}_{\hat{\pi}} - \hat{Q})^2] \xrightarrow{w \rightarrow 0} 0$  [unbiased property]

$\Rightarrow$  The policy gradient theorem still holds true  $\nabla_{\theta} L(\theta) \propto \mathbb{E}_{\hat{\pi}}[\nabla_{\theta} \pi(a|s,\theta) \hat{Q}(s,a,w)]$

The variance can be further reduced using a **baseline**  $B(\cdot)$   $\rightarrow$  represents empirical knowledge about the model

$\nabla_{\theta} L(\theta) \propto \mathbb{E}_{\hat{\pi}} \left[ \sum_a \nabla_{\theta} \pi(a|s,\theta) (\hat{Q}_{\hat{\pi}} - B(\cdot)) \right]$   $\rightarrow$  keep only the variance about the action, not future states

- $\cdot$  If  $B(\cdot)$  depends only on  $s \Rightarrow$  doesn't change the gradient since  $\mathbb{E}_{\hat{\pi}}[\sum_a \nabla_{\theta} \pi(a|s,\theta) B(s)] = \mathbb{E}_{\hat{\pi}}[B(s) \sum_a \nabla_{\theta} \pi(a|s,\theta)] = \mathbb{E}_{\hat{\pi}}[B(s) \nabla_{\theta} 1] = 0$
- $\cdot$  Common choice  $B(s) = V_{\hat{\pi}}(s) \rightarrow$  reducing the variance of gradient updates (no bias introduced)  $\rightarrow$  faster convergence
- $\cdot$  becomes the Advantage function
- $\rightarrow$  Without baseline if  $Q_{\hat{\pi}}(s,a) > 0 \forall (s,a) \Rightarrow$  the network couldn't learn to do less of an action but just more the others

**Advantage function**  $A_{\pi}(s,a) = Q_{\pi}(s,a) - V_{\pi}(s)$  measures the value added by action a to state s

• advantage policy gradient reformulation  $\nabla_{\theta} L(\theta) \propto \mathbb{E}_{\pi} [\nabla_{\theta} \ln \pi(a|s, \theta) A_{\pi}(s,a)]$

→ In actor-critic scenario:  $\hat{A}(s,a, \omega, \rho) = \hat{Q}(s,a, \omega) - \hat{V}(s, \rho)$

• thus we should learn  $(\theta, \omega, \rho)$  but in reality:  $A_{\pi}(s,a) = \mathbb{E}_{\pi} [r + \delta V_{\pi}(s') - V_{\pi}(s) | s, a]$   
 $Q_{\pi}(s,a) = \mathbb{E}_{\pi} [r + \delta V_{\pi}(s') | s, a]$   
 $\downarrow$   
 $A_{\pi}$  could be biased if  $V_{\pi}$  estimate is not perfect

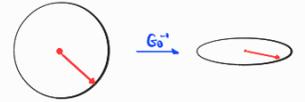
**NATURAL POLICY GRADIENT**

Policy gradients could perform poorly because of plateaus or discontinuities in policy space → small  $\theta$  change causes big  $\hat{\pi}$  changes  
 → critic  $\hat{Q}$  not valid anymore

Solution: make changes to  $\theta$  proportional to policy variation

$$\begin{cases} d^* = \underset{d}{\text{argmin}} L(\theta_0 + d) \\ \text{s.t. } D_{\theta}(\hat{\pi}(\theta_0) \parallel \hat{\pi}(\theta_0 + d)) \leq \epsilon \end{cases}$$

$D_{\theta}(\hat{\pi}(\theta_0) \parallel \hat{\pi}(\theta_0 + d)) = \int_{s \times A} \hat{\pi}(a|s, \theta_0) \ln \frac{\hat{\pi}(a|s, \theta_0)}{\hat{\pi}(a|s, \theta_0 + d)} ds da$   
→ limits the loss of information (penalize d that alters a lot  $\hat{\pi}$ )



Using the Taylor approximation of second order of  $D_{\theta}$  we can find that  $\Delta \theta_{t+1} - \Delta \theta_t \propto G_{\theta}^{-1} \nabla_{\theta} L(\theta)$  policy loss  
 $G_{\theta}^{-1} \nabla_{\theta} \ln \pi(a|s, \theta) Q_{\pi}(s,a)$

With  $G_{\theta}$  the **Fisher information matrix**  $G_{\theta} = \mathbb{E}_{\pi} [\nabla_{\theta} \ln \pi(a|s, \theta) \nabla_{\theta} \ln \pi(a|s, \theta)^T]$

→ It's like a covariance matrix, where big entry in  $G_{\theta}$  means small change in  $\theta$  → big change in  $\hat{\pi}$   
 → Its inverse helps to normalize the **parameters search space** by making all equally important

If **compatibility** holds we know that  $Q(s,a, \omega) = \nabla_{\omega} \ln \hat{\pi}(a|s, \theta)^T \omega$

$$\Rightarrow \Delta \theta_t \propto G_{\theta}^{-1} \nabla_{\theta} \ln \hat{\pi}(a|s, \theta) \nabla_{\omega} \ln \hat{\pi}(a|s, \theta)^T \omega = G_{\theta}^{-1} G_{\omega} \omega = \omega$$

→ learn faster with fewer data

**MODEL-BASED RL** → learns the model and from it get the value function from simulated experience (**peering**)

• needs to learn  $P_{ss'}^a$  and  $R_s^a$   
 • The simplest one is table lookup:  $P_{ss'}^a = \frac{1}{N(s,a)} \sum_{t=1}^T \mathbb{I}(s_t, a_t, s_{t+1})$      $R_s^a = \frac{1}{N(s,a)} \sum_{t=1}^T \mathbb{I}(s_t, a_t) r_t$

$M_{\pi} = \langle P_{\pi}, R_{\pi} \rangle$  model variables

• **Inaccurate models lead to inaccurate policies** → **two source of errors** ( $M_{\pi}$  and  $\hat{\pi}$ )

→ If the uncertainty is too high, go back to model-free or use an integrated approach

**Integrated Approach:**  
 1)  $M_{\pi}$  learning from real experience  
 2)  $\hat{V}, \hat{Q}, \hat{\pi}$  learning from both  $M_{\pi}$  and real experience

**BACKWARD SEARCH**

**Dyna-Q** → **integrated approach + deterministic environment**

It has an extension **Dyna-Q+** to add on exploration bonus

→ Dyna-Q fails if the env is not static (r changes)

$$(r + K \sqrt{P_{sa}}, s') \leftarrow \text{Model}(s,a)$$

$\downarrow$   
# times we've tried (s,a)

• Increasing the reward induces the policy to follow those a tried a long time ago

• In the sides is said that  $(s,a) \sim$  weighed distribution  $w_{(s,a)} = R_s^a + K \sqrt{P_{sa}}$

**Dyna-2** → Uses two Q functions:

- 1)  $Q^T$  (transient) → adjusted from simulation
- 2)  $Q^P$  (persistent) → learned only from real data

• Takes action combining both  $Q^T$  and  $Q^P$

**Input:**  $S, A, \delta$

Initialize  $Q(s,a)$  and  $M(s,a)$      $V(s,a) \in S \times A$

**loop:**

$S \leftarrow$  current state

$A \leftarrow \epsilon$ -greedy( $s, a$ )

execute A and observe  $(R, s')$

$Q(s,a) \leftarrow Q(s,a) + \alpha [R + \delta \max_{a'} Q(s', a') - Q(s,a)]$     # TD(0)

model  $M(s,a) \leftarrow (r, s)$     # Assuming deterministic env.

**for n times:**

choose  $s \in S$  from  $H$  → arbitrary

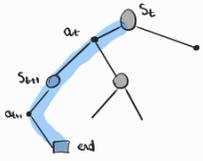
choose  $a \in A$  from  $M(s,a)$

$(r, s') \leftarrow M(s,a)$

$Q(s,a) \leftarrow Q(s,a) + \alpha [R + \delta \max_{a'} Q(s', a') - Q(s,a)]$

$$a_{t+1} \leftarrow \epsilon\text{-greedy}(Q^T(s_t, \cdot) + Q^P(s_t, \cdot))$$

## FORWARD SEARCH



builds a search tree with current state  $s_t$  as root  $\rightarrow$  uses  $M_{\eta}$  as look ahead  
 $\rightarrow$  simulates episodes from now with the model  
 $\rightarrow$  apply model-free methods to simulated episodes

## NAIVE MC Search

you are not learning  $\hat{\pi}$  from the simulations  
 $\rightarrow$  inefficient

**Input:**  $M, \pi, s_t$

for all  $a \in A$  do:  
 simulate  $k$  episodes  $\{s_t, a, R_{t+1}^k, s_{t+1}^k, a_{t+1}^k, \dots, s_T^k\} \sim M_{\eta}, \pi$   
 $Q(s_t, a) = \frac{1}{k} \sum_{i=1}^k G_i^k \rightarrow$  mean return on simulation  
 $a_t \leftarrow \arg \max_a Q(s_t, a)$   
completely from simulations

## MC TREE-SEARCH $\rightarrow$ Builds a search tree with visited states and actions

1) **Selection:** start from root  $s_0$  and traverse the tree using a **tree policy**  $\rightarrow$  use UCS to balance exploration and exploitation  
starting point where I want to take an action initially empty strategy to select which node to visit after:  $\epsilon$ -greedy

- stops when:
- reach a node with an action that is not expanded
  - using tree policy the next node to visit is not on the tree
  - terminal state is reached  $\rightarrow$  in this case skip to backpropagation

2) **Expansion:**  
 case a)  $\rightarrow$  add action node and a sampled state from  $M_{\eta}$   
 case b)  $\rightarrow$  action was already present, add only  $s \rightarrow$  stochastic result state after  $a$

3) **Simulation:** from the state  $s_t$  simulate using a **default policy**  $\rightarrow$  greedy until terminal state reached  
 $\{s_t, A_t^k, R_{t+1}^k, \dots, s_T^k\} \sim M_{\eta}, \pi$

4) **Backpropagation:** update every  $(s, a)$  along the path from selected node to root

- Increment visit count  $N(s, a)$  by one
- $G_t^k \leftarrow r_t^k + \gamma G_{t+1}^k$  (initial  $G$  is the return of selected node along the generated path)
- Update  $Q$  estimate

$$Q(s, a) = \frac{1}{N(s, a)} \sum_{k=1}^k \sum_{u=1}^{I_k} \mathbb{I}(s_u = s, A_u^k = a) G_u^k \rightarrow \text{could be done more efficiently with incremental mean}$$

# of simulations done

Repeat the four phases until there is computation time, then take  $a_t$  and discard the tree (some implementation could reuse it)

- $\rightarrow$  Exhaustive search is impracticable in complex spaces
- $\rightarrow$  Highly parallelizable
- $\rightarrow$  The two policies improves

**TD-SEARCH**  $\rightarrow$  uses bootstrapping instead of sampling simulation: apply SARSA from  $(s_t, a_t)$   
 $\Delta Q(s_t, a_t) = \alpha [R_{t+1} + \gamma Q(s_{t+1}, a_{t+1}) - Q(s_t, a_t)]$  . could be use to simulate  $n$  steps ahead like TD( $n$ )

From  $s_t$  update  $Q$  at each iteration  $\rightarrow$  lower variance  
 Dyna2 learns  $Q^{\pi}$  in this way

# EXPLORATION-EXPLOITATION TRADE-OFF

In  $\epsilon$ -greedy the exploration is random (noise + greedy).

Two strategies available:

- 1) **Optimism** → estimates action-state uncertainty and explore the more uncertain
- 2) **Information State** → uses history knowledge to explore

## MULTI-ARMED BANDIT SCENARIO

- deterministic starting state  $S_0$
- multiple actions that brings to a different terminal state (no state space) with rewards that depends on each probability distribution
- we want to find  $R_{S_0}^a$  (expected reward) in order to maximize  $\sum_{t=1}^T r_t$  (cumulative return over actions)

- using greedy we are exploiting our current knowledge to maximize one-step-ahead return, but we are not exploring
- using  $\epsilon$ -greedy may produce greater total reward in the long run

→ true action value (unknown)

$$V^* = Q(a^*) = \max_a Q(a)$$

→ regret: expected em doing suboptimal a

$$I_t = \mathbb{E}[V^* - Q(a_t)]$$

→ total regret

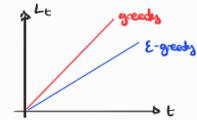
$$L_T = \sum_{t=1}^T I_t$$

minimize  $\sum_{t=1}^T I_t \iff$  maximize  $\sum_{t=1}^T r_t$

number of selection of a action  $T$  timesteps (depends on  $\pi$ )

$$L_T = \sum_{t=1}^T \mathbb{E}[V^* - Q(a_t)] = \sum_a \mathbb{E}[N_T(a)] (V^* - Q(a))$$

greedy (no exploration) or  $\epsilon$ -greedy (random exploration) has **linear regret**



- in greedy  $\mathbb{E}[N_T(a^*)]$  can be  $T$  for a single  $a^* \rightarrow L_T = T(V^* - Q(a^*))$
- in  $\epsilon$ -greedy  $\mathbb{E}[N_T(a)] \geq \frac{\epsilon}{|A|} T \rightarrow L_T \geq \frac{\epsilon}{|A|} T \sum_a (V^* - Q(a))$

**Hoeffding Inequality:** Let  $x_1, \dots, x_n$  random variables in  $(0,1)$ , let  $\bar{x}_t = \frac{1}{t} \sum_{k=1}^t x_k \Rightarrow P(|\mathbb{E}[X] - \bar{x}_t| \geq u) \leq e^{-2tu^2} \quad \forall u \geq 0$

(UCB) **Upper Confidence Bound** → rewards in  $(0,1)$  Call the upper bound on  $Q(a) \rightarrow \hat{Q}_t(a) \Rightarrow P[Q(a) > \hat{Q}_t(a) + \hat{U}_t(a)] \leq e^{-2N_t(a)\hat{Q}_t(a)^2} - p$

→  $\hat{U}_t(a) = \sqrt{\frac{-\log p}{2N_t(a)}} \rightarrow$  less time chosen greater the uncertainty

**OPTIMISM** Between all the high probable  $(1-p)$  models choose the most optimistic to improve the policy  $\hat{Q}_t(a) + \hat{U}_t(a)$

• If we reduce  $p_t = t^{-\alpha}$  (fixed  $\alpha > 0$ ) we have a **sublinear policy**  $a = \operatorname{argmax}_a [\hat{Q}_t(a) + \sqrt{\frac{\alpha \log t}{2N_t(a)}}] = \pi_t(S_t)$

→ Guarantees asymptotic convergence to optimal action

- It has sublinear regret → because it doesn't use random exploration but it's based on uncertain actions that could be optimal

increases with uncertainty and time

# STATE OF THE ART MODELS

## PROXIMAL POLICY GRADIENT

We want to limit the variation of  $\pi$  across weight updates

Is heavy to put a constraint on  $D_{KL}$  or to compute  $G_{\theta}$

To keep  $D_{KL}$  small at every step we can:

1) PPO-Penalty (proximal policy optimization)

$$\mathcal{L}(\theta) = \mathbb{E}_t \left[ \frac{\pi_{\theta}(a_t | s_t) \hat{A}_w(a_t, s_t) - \beta_n D_{KL}(\pi_{\theta} \| \pi_{\theta_{t-1}})}{\pi_{\theta_{t-1}}(a_t | s_t)} \right]$$

$\hat{A}_w(a_t, s_t)$ : how much P of taking  $a_t | s_t$  would increase with  $\theta_t$   
 $\beta_n D_{KL}$ : penalty big  $D_{KL}$   
 $(a_t, s_t)$  were collected via  $\pi_{\theta_{t-1}}$  → importance sampling

$$\beta_{n+1} = \begin{cases} \frac{\beta_n}{2} & \text{if } d < \frac{2}{3} \bar{d} \\ 2\beta_n & \text{if } d > \frac{3}{2} \bar{d} \\ \beta_n & \text{otherwise} \end{cases}$$

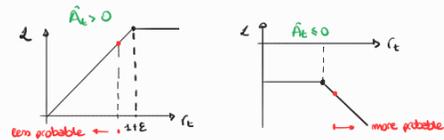
$\bar{d}$ : user-defined th.

2) PPO-Clipping  $\mathcal{L}(\theta) = \mathbb{E}_t \left[ \min \left\{ \frac{\pi_{\theta}(a_t | s_t)}{\pi_{\theta_{t-1}}(a_t | s_t)}, g(\epsilon, A_t) \right\} \hat{A}_w(a_t, s_t) \right]$

$$g(\epsilon, A_t) = \begin{cases} 1+\epsilon & \text{if } \hat{A}_t > 0 \\ 1-\epsilon & \text{otherwise} \end{cases}$$

We are clipping  $\epsilon$ :  
 1) if  $\hat{A}_t$  is good ( $\hat{A}_t > 0$ ) by  $1+\epsilon$   
 2) if  $\hat{A}_t$  is bad by  $1-\epsilon$

→ prevents too big changes ( $\epsilon$  really high)



• There is no reward of having  $\epsilon \notin [1-\epsilon, 1+\epsilon]$

## DEEP DETERMINISTIC POLICY GRADIENT

DPG Theorem: Let  $\mathcal{L}(\theta) = \mathbb{E}_{s \sim d(s)} [R(s, \pi_{\theta}(s))]$  with  $\pi_{\theta}, R, P \in C^1 \rightarrow \nabla_{\theta} \mathcal{L}(\theta) = \mathbb{E}_{s \sim d(s)} [\nabla_{\theta} \pi_{\theta}(s) \nabla_a Q(s, a) |_{a=\pi_{\theta}(s)}]$

more efficient especially in continuous-action space

Deterministic compatible Value Approximation Theorem: If we use  $\hat{Q}_w(s, a) \in C^1$  a parametrized version of  $Q(s, a) \rightarrow$  DPG theorem holds  $\Leftrightarrow$

- 1)  $\nabla_a \hat{Q}_w(s, a) |_{a=\pi_{\theta}(s)} = \nabla_a Q(s, a) |_{a=\pi_{\theta}(s)}$
  - 2)  $\mathbb{E}_{s \sim d(s)} [(\nabla_a \hat{Q}_w(s, a) - \nabla_a Q(s, a)) |_{a=\pi_{\theta}(s)}] \xrightarrow{t \rightarrow \infty} 0$
- guarantee to have no bias substituting  $Q$  with  $\hat{Q}_w$

From 1) deduce that  $Q_w(s, a) = \alpha^T \nabla_{\theta} \pi_{\theta}(s)^T w$

$$\rightarrow \delta_t = r_t + \gamma Q_w(s_{t+1}, \pi_{\theta}(s_{t+1})) - Q_w(s_t, a_t) \rightarrow TD(0) \text{ error}$$

$$\textcircled{1} \theta_{t+1} = \theta_t + \lambda_{\theta} \nabla_{\theta} \mathcal{L} = \theta_t + \lambda_{\theta} \nabla_{\theta} \pi_{\theta}(s) \nabla_a Q(s, a) |_{a=\pi_{\theta}(s)} \Rightarrow \theta_{t+1} = \theta_t + \lambda_{\theta} \nabla_{\theta} \pi_{\theta}(s) \nabla_a \pi_{\theta}(s)^T w_t$$

$$\textcircled{2} w_{t+1} = w_t + \lambda_w \delta_t \nabla_a Q(s_t, a_t) \Rightarrow w_{t+1} = w_t + \lambda_w \delta_t \nabla_a \pi_{\theta}(s) \alpha$$

Natural Policy Modification:  $\theta_{t+1} = \theta_t + \lambda_{\theta} w_t$  when we use the Fisher matrix to weight  $\nabla_{\theta} \mathcal{L}(\theta)$

TWIN DELAYED DDPG (TD3) → DDPG is sensitive to hyperparameters and tends to overestimate  $Q$

① TARGET POLICY SMOOTHING → add noise to  $\pi$ , making it difficult to exploit  $Q$  errors (smoothing)  
 $\tilde{\alpha} = \text{clip}[\pi_{\theta}(s) + \text{clip}(\epsilon, -c, +c), a_{\min}, a_{\max}]$  with  $a_{\min}, a_{\max} \in \mathbb{R}$ ,  $c \in \mathbb{R}^+$ ,  $\epsilon \sim N(0, \sigma)$

② CLIPPED DOUBLE-Q LEARNING Uses two  $Q_w, Q_{w'}$  trained independently → difficult to have the same overestimation

$$y(r, s') = r + \gamma \min_{i=1,2} Q_{w_i}(s', a_i(s'))$$

$$\mathcal{L}(w_i) = \mathbb{E}_b \left[ (Q_{w_i}(s, a) - y(r, s'))^2 \right] \rightarrow \text{same for } w_2 \text{ (start from different } \tilde{w}_1 \neq \tilde{w}_2)$$

$$\pi_{\theta'} = \arg \max_{\pi} \mathbb{E}_b \left[ Q_{w_i}(s, \pi_{\theta}(s)) \right] \rightarrow \text{uses DPG to update } \theta, \text{ but not computationally } \Rightarrow \text{BIAS}$$

③ DELAYED POLICY UPDATES → updates policy  $\pi_{\theta}$  once every  $d$  critic update ( $w_1, w_2$ )  
 typically  $d=2$

• this allows to train  $\pi_{\theta}$  with a lower variance value estimate → more stable

**SOFT ACTOR CRITIC (SAC)** → We can use entropy regularization to enforce exploration

Given a density function  $p$  and a random variable  $x \sim p \rightarrow H(p) \doteq -\mathbb{E}_x[\ln(p(x))]$

Define a new loss with exploratory bonus:  $\pi^* = \operatorname{argmax}_{\pi} \mathbb{E}_p \left[ \underbrace{\sum_{t=0}^{\infty} \delta^t (R(s_t, a_t))}_{G_t} + \underbrace{v H(\pi(s_t))}_{\text{entropy bonus} \rightarrow \text{more exploration}} \right] \quad v > 0$

Approximate  $G_t = \min_{i=1,2} \hat{Q}_{w_i}(a_t, s_t)$  →  $\operatorname{argmax}_{\pi_0} \mathbb{E}_{s \sim \Delta, a \sim \pi_0} \left[ \min_{j=1,2} Q_{w_j}(s, a) - v \ln \pi_0(a|s) \right]$   
not used in TD3  
typically decreased over time  $v$

reparameterization trick since is difficult to compute directly  $\pi_0^*$  I could divide it in two:

$a_0(s, \epsilon) = \tanh(\mu_0(s) + \sigma_0(s) \circ \epsilon) \in [-1, +1]$  with  $\epsilon \sim \mathcal{N}(0, 1)$  now  $\pi_0 \approx \mathcal{N}(\mu_0, \sigma_0)$

decoupled randomness of  $\pi_0(a|s)$  from model parameters

⇒  $\pi^* = \operatorname{argmax}_{\theta} \mathbb{E}_{s \sim \Delta, \epsilon \sim \mathcal{N}} \left[ \min_{j=1,2} Q_{w_j}(s, a_0(s, \epsilon)) - v \ln \pi_{\theta}(a_0(s, \epsilon) | s) \right] \Rightarrow \pi_{\theta} \sim \mathcal{N}(\mu_{\theta}, \sigma_{\theta})$

Can be written the entropy bellman equation in order to learn  $Q$

$Q_{\pi}(s, a) = \mathbb{E}_{s' \sim p, a' \sim \pi(s')} \left[ R(s, a) + \gamma (Q_{\pi}(s', a') - v \ln(\pi(a'|s))) \mid s, a \right]$

⇒  $\mathcal{L}(w_i) = \mathbb{E}_{\pi} \left[ \delta_t^2 \right] \rightarrow$  similar to TD3 but with entropy correction

- Differences
- 1) TD3 uses a deterministic policy
  - 2) SAC uses entropy regularization
  - 3) SAC doesn't use policy smoothing

# ALPHA THEORY

Mathematical field in which the Axiom of Archimede holds

let  $F$  be a totally ordered field  $\rightarrow \forall x, y \in F, 0 < x < y, \exists n \in \mathbb{N} : y < nx$   
 $\nexists n \in \mathbb{N} : \alpha < nx \quad \forall x \in \mathbb{R} \subseteq E$

Axiom 1 (existence):  $\exists$  an ordered field  $E \supset \mathbb{R}$  whose numbers are called **algebraic numbers**

(and a **function**  $\lim_{n \rightarrow \alpha} \mathbb{R}^{\mathbb{N}} \rightarrow E$ : axiom 3)  
sequence

DEF: given  $E \in E$  then:

- 1)  $E$  is infinite  $\Leftrightarrow \forall n \in \mathbb{N}, |E| > n$
- 2)  $E$  is finite  $\Leftrightarrow \exists n \in \mathbb{N} : \frac{1}{n} < |E| < n$
- 3)  $E$  is infinitesimal  $\Leftrightarrow \forall n \in \mathbb{N}, |E| < \frac{1}{n}$

Axiom 2:  $\exists$  a function  $\text{num} : \mathcal{U} \rightarrow E$   
set of sets

- $\text{num}(A) = |A|$  if  $A$  is finite
- $\text{num}(A) < \text{num}(B)$  if  $A \subset B$
- $\text{num}(A \cup B) = \text{num}(A) + \text{num}(B) - \text{num}(A \cap B)$
- $\text{num}(A \times B) = \text{num}(A) \cdot \text{num}(B) \rightarrow$  **coherent with Cantor's**  $\text{num}(\mathbb{N} \times \mathbb{N}) = \alpha^2$  but  $|\mathbb{N} \times \mathbb{N}| = |\mathbb{N}|$

DEF:  $\alpha \hat{=} \text{num}(\mathbb{N})$

$\eta = \alpha^{-1} \quad \lim_{n \rightarrow \alpha} \frac{1}{n} = \eta$

Axiom 3: every sequence  $\psi, \varphi : \mathbb{N} \rightarrow \mathbb{R}$  has a **unique**  $\alpha$  limit which satisfy the following properties

- $\lim_{n \rightarrow \alpha} \varphi(n) = \alpha \quad \forall n \in \mathbb{N} \Rightarrow \lim_{n \rightarrow \alpha} \varphi(n) = \alpha$
- $\lim_{n \rightarrow \alpha} \varphi(n) = r \quad \forall n \in \mathbb{N} \Rightarrow \lim_{n \rightarrow \alpha} \varphi(n) = r$
- $\lim_{n \rightarrow \alpha} \varphi(n) + \lim_{n \rightarrow \alpha} \psi(n) = \lim_{n \rightarrow \alpha} (\varphi(n) + \psi(n))$
- $\lim_{n \rightarrow \alpha} \varphi(n) \lim_{n \rightarrow \alpha} \psi(n) = \lim_{n \rightarrow \alpha} (\varphi(n) \cdot \psi(n))$

IMPLICATIONS:

- 1) if  $\varphi(n) \in \mathcal{P}(n) \Rightarrow \varphi(x) \in \mathcal{P}(x) \quad E$  operator precedence
- 2) Given  $A$  non empty:  $A^* = \{ \varphi(x) \mid \varphi : \mathbb{N} \rightarrow A \}$  eg  $f^* : A^* \rightarrow B^*$
- 3) Given  $\mathbb{R}^* = \{ \varphi(x) \mid \varphi : \mathbb{N} \rightarrow \mathbb{R} \}$

sequence that picks on elements  $n \in \mathbb{N}$  from  $\mathcal{P}$   
 eg  $\mathcal{P}(n) = \{0, \frac{1}{n}\}$  then  $\varphi(n) = \frac{1}{n} \in \mathcal{P}(n)$

Axiom (Internal set): If  $\mathcal{P}(n)$  is a sequence of non-empty set  $\Rightarrow \lim_{n \rightarrow \alpha} \mathcal{P}(n) = \{ \lim_{n \rightarrow \alpha} \varphi(n) \mid \varphi(n) \in \mathcal{P}(n) \forall n \}$   
internal set

Axiom (Extension): let  $\varphi : \mathbb{N} \rightarrow \mathbb{R}$  and  $f : \mathbb{R} \rightarrow \mathbb{R}$  be a function for which  $f \circ \varphi$  is defined  $\Rightarrow f$  can be **uniquely extended** at  $\Sigma = \lim_{n \rightarrow \alpha} \varphi(n)$  as follows:  
 $f^*(x) = f(x) \quad \forall x \in \mathbb{R}$

$f^*(\Sigma) = \lim_{n \rightarrow \alpha} f(\varphi(n)) \quad f^* : E \rightarrow E$   
can be demonstrated that it doesn't depend on  $\varphi$  definition

define  $\varphi(n) = x \quad \forall x \in \mathbb{R} \Rightarrow f^*(x) = \lim_{n \rightarrow \alpha} f(x) = f(x)$   
constant sequence  $\varphi(n) = f(x)$

DEF An elementary formula is a finite string of symbols in first order logic (alphabet,  $\neg, \wedge, \vee, \Rightarrow, \Leftrightarrow, \exists, \forall, =, \epsilon$ )  
logic connectives, quantifier

Th (Transfer Principle) let  $\sigma(x_1, \dots, x_n)$  an elementary formula and let  $\varphi_1, \dots, \varphi_n$  be arbitrary sequences

$\sigma(\varphi_1(n), \dots, \varphi_n(n))$  holds almost every where  $\Leftrightarrow \sigma(\lim_{n \rightarrow \alpha} \varphi_1(n), \dots, \lim_{n \rightarrow \alpha} \varphi_n(n))$   
does not hold in a measure zero set  
 $\exists n \in \mathbb{N} : \forall n > n^* \sigma(\varphi_1(n), \dots, \varphi_n(n))$  holds

$\rightarrow$  guarantees that some properties are preserved by the  $\alpha$ -limit eg continuity, differentiability, ...

DEF (completeness)  $X$  is complete  $\Leftrightarrow$  every non-empty subset of  $X$  having an upper-bound must have a supremum in  $X$

- Transfer principle doesn't transfer  $\mathbb{R}$  completeness
- eg  $\mu(\alpha) = \{ y \in E \mid y \text{ is infinitesimal} \}$  is bounded by 1 but doesn't have a sup in  $E$

$\mathbb{R}$  is too large to fit in computers

**Algorithmic Field** is the set of all numbers that can be represented exactly in a machine (also number not present in the original field it approximate like  $\pi, \ln, e, \dots$ )  $(\hat{\mathbb{R}}, \hat{E})$

- 1) **Fixed length representation**
  - faster code with probability of hardware accelerators
  - deterministic time consumption
- 2) **Symbolic representation**
  - variable size with 'infinite' precision  $\rightarrow$  programs will be slower

**Algorithmic Number** (AN):  $\mathbb{Z} \in \mathbb{E}$  is an AN  $\iff$  can be represented by a finite sum  $\mathbb{Z} = \sum_{k=0}^{\infty} r_k \alpha^k$  with  $r_k \in \mathbb{B}$ ,  $s_k \in \mathbb{Q}$ ,  $s_k > s_{k+1}$

The (AN normal form): Any AN  $\mathbb{Z}$  can be represented by  $\mathbb{Z} = \alpha^p P(\eta^{\pm})$  with  $p \in \mathbb{Z}$ ,  $m \in \mathbb{N}$ ,  $P(x)$  is a polynomial with real coefficients:  $P(x) \neq 0$

parallelism:  $1.37 \cdot 10^3$   $10^3$  is  $\alpha^p$  and  $1.37 = 1 \cdot 10^0 + 3 \cdot 10^{-1} + 7 \cdot 10^{-2}$  is  $P(\eta^{\pm})$  polynomial with negative coefficients in  $\alpha$

Two problems arise with AN:

- 1) The inverse of an AN is not always an AN (not closed under inversion) eg.  $(1+\alpha)^{-1} \notin \mathbb{E}$   $\frac{1}{1+\alpha} = \frac{1}{\alpha(1+\eta)} \stackrel{\text{long}}{=} \eta [1 - \eta + \eta^2 - \dots]$   $\frac{1}{1-x} = 1+x+x^2+\dots$
- 2) They have variable length coding:  $3^i$  has infinite # of digits

To solve those we need **truncation** of  $P(x)$ :  $P(x) = p_0 x^0 + \dots + p_m x^m \rightarrow t_n(P(x)) = \begin{cases} P(x) & n \geq m \\ p_0 x^0 + \dots + p_n x^n & n < m \end{cases}$

**Bounded AN (BAN)**:  $\mathbb{Z} \in \mathbb{E}$  is a BAN  $\iff$  can be represented by  $\mathbb{Z} = \alpha^p P_m(\eta)$  [BAN  $\subset$  AN]  $10^p P(10^{-1})$  notation scientific  
 ensures closure under basic operations  
 integer polynomial  $\alpha^2 [1 + 0.7\eta + 3.4\eta^2]$

- sufficient for elementary operations (needed in Ex) but not for non-linear ones eg.  $x^2 = x \rightarrow x = \sqrt{x} \notin \text{BAN}$
- $m=1$  because operation between BANs are a lot easier than ANs

**LHOP (lexicographic M.O problems)**

$$\begin{cases} \text{lex min } f_1, \dots, f_n \\ x \in D \end{cases} \quad \begin{matrix} D \subseteq \mathbb{R}^n \\ f_i: \mathbb{R}^n \rightarrow \mathbb{R} \end{matrix}$$

$$\begin{aligned} \Omega &= D \\ \text{for } i=1, \dots, n \text{ do} \\ &\text{if } \Omega = \{b\} \vee |\Omega| = 1 \text{ then} \\ &\quad \text{break} \\ \Omega &= \{x \mid \text{argmin}_{x \in \Omega} f_i(x)\} \\ \text{return } \Omega \end{aligned}$$

It can be reformulated with  $n$  optimization problems  
**PRE-EMPTIVE APPROACH**

$$\begin{cases} \min_x f_i(x) \\ f_j(x) = \min_{x \in D} f_j(x) \quad \forall j = \{1, \dots, i-1\} \\ x \in D \end{cases}$$

- $\rightarrow$  after each run a constraint is added
- it gets more and more complex
  - bad use of hardware (cache) and software (unless the warm start)
  - nature of the problem may change eg. convex to non-convex with new constraints

**SCALARIZATION**  $\{w_i\}_{i=1}^n$  :  $\frac{w_{i+1}}{w_i} \ll 1$

$$\begin{cases} \min_x \sum_{i=1}^n w_i f_i(x) \\ x \in D \end{cases}$$

- no guarantee of problem equivalence
- choice of weights are error-prone and arbitrary  $\rightarrow$  may induce numeric instabilities

**NON-STANDARD SCALARIZATION**  $w_i = \alpha^{-i} \rightarrow$  the choice is not unique, it is sufficient to have infinitesimal  $\frac{w_{i+1}}{w_i}$

$$\begin{cases} \min_x \sum_{i=1}^n \alpha^{-i} f_i(x) \\ x \in D \end{cases}$$

- the problems are equivalent and here we use a single objective
- the transfer principle guarantees the equivalence between optimal solutions of the original LHOP and its scalarization

**The (Equivalence)** Given a LHOP with  $f_1, \dots, f_n$  real functions, with priority induced by natural order

$\Rightarrow \exists$  an equivalent scalar program over the same domain, whose objective is non-standard with the following form:  $F(x) = \beta_1 f_1(x) + \dots + \beta_n f_n(x)$   
 with  $\beta_1, \dots, \beta_n \in \mathbb{E}$  :  $\frac{\beta_{i+1}}{\beta_i} \approx 0 \quad \forall i = \{1, \dots, n-1\}$

**Proof:** Let  $\Omega$  be the domain of the two problems, and  $w \in \Omega$  be a global maximum of LHOP

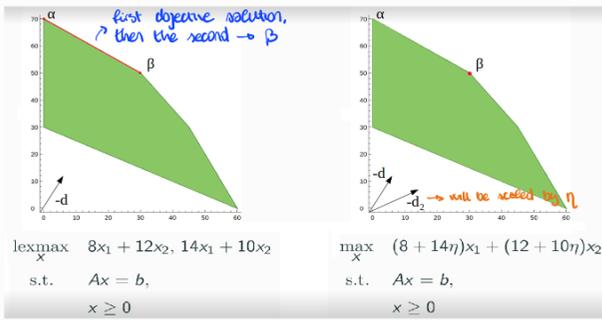
$$\Rightarrow \forall w' \in \Omega : f_i(w') > f_i(w) \vee \left[ \exists i \in \{2, \dots, n\} : f_j(w') > f_j(w) \quad \forall j = \{1, \dots, i-1\} \wedge f_i(w') > f_i(w) \right]$$

This is true  $\iff \forall w' \in \Omega : F(w') > F(w)$  by the definition of  $F$  itself

**LHOP (linear)**

$$\begin{cases} \text{lex min } c^T x, \dots, c_0^T x \\ Ax = b \\ x \geq 0 \end{cases} \iff \begin{cases} \min_x \sum_{i=1}^n c_i^T x \alpha^{-i} \\ Ax = b \\ x \geq 0 \end{cases}$$

- could use the **NA-c-Simplex** algorithm
- $\rightarrow$  simplex with non-standard cost function (same property eg. big M)
- $\rightarrow$  transfer principle guarantees all the property of LP



**SIMPLEX PROBLEM** What if a starting feasible solution is unknown

$Ax = b \rightarrow \begin{matrix} \text{AUXILIARY PROBLEM} \\ \text{min} \\ \text{max} \end{matrix} Ax + I\delta = b \rightarrow \begin{matrix} \text{min} \\ \text{max} \end{matrix} [A | I] \begin{pmatrix} x \\ \delta \end{pmatrix} = b$

$(0, b)$  is feasible of the new problem

Setting  $\bar{x} = \bar{0}$  we have that  $B' = \{n_1, \dots, n_m\}$  is a valid base (column indexes of  $[A|I]$  to get a  $m \times m$  invertible matrix)

In fact  $I^{-1} \cdot I \rightarrow \delta = b$

such that with other variables = 0  $A_0 x_0 = b$

Two methods to make the original and auxiliary problem the same:

1) Two-Phase Method  $\rightarrow$  I need to get  $\bar{s} = \bar{0}$  to be feasible in the first problem

**First-Phase:**  $\begin{cases} \min_{x, s} \sum_{i=1}^m s_i \\ Ax + I\delta = b \\ x, s \geq 0 \end{cases}$

If  $s^* = \bar{0}$  move to phase 2, otherwise P is infeasible  
 - The starting base will be  $B'$

**Second-Phase:** solve P starting from previous  $x^*$ .  $B = B'[1:n] \rightarrow$  original variables

2) Big-M Method  $\rightarrow$  try to make the two things at once

$\begin{cases} \min_{x, s} d^T x + M \sum_{i=1}^m s_i \\ Ax + I\delta = b \\ x, s \geq 0 \end{cases}$

Th:  $\exists M > 0$  sufficiently large:  $\bar{x}' = [\bar{x}, 0]$  is the solution to the larger problem  $\Leftrightarrow \bar{x}$  is solution to the original one

3) Infinite Big-M method (I-Big-M)

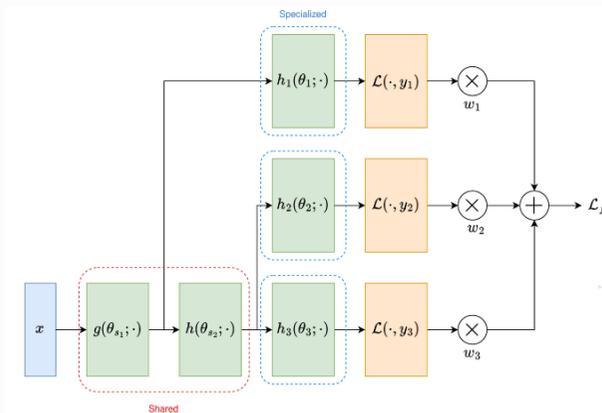
M prioritize the zeroing of s over the minimization of  $d^T x$   
 $\rightarrow$  similar to lexicographic problem

Set  $M = \alpha$

- M is always large enough for equivalence  $\rightarrow$  do not need to retry
- No numerical instabilities by very large M

**HIERARCHICAL CLASSIFICATION**  $\rightarrow$  classification based on trees (hierarchy)

1) Branching DNN

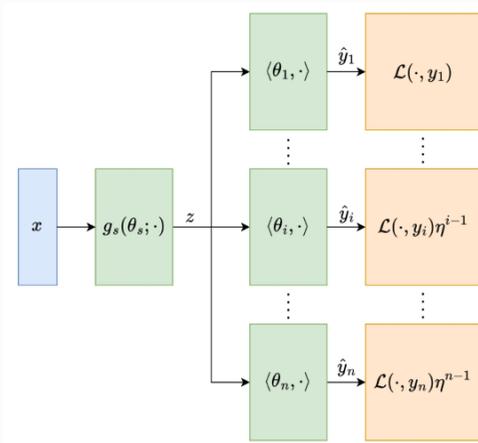


$L_{D-DNN}(\theta) = \sum_{i=1}^3 w_i(t) L(f_i(\theta, x), y_i)$

$(w_1, w_2, w_3) |_{t=0} = [1, 0, 0]$

$(w_1, w_2, w_3) |_{t=\beta_{max}} = [0, 0, 1]$

## 2) Lexicographic DNN



$$\text{exmin } \mathcal{L}(f_1(\theta_1, x), y_1), \dots, \mathcal{L}(f_n(\theta_n, x), y_n)$$

$$\Leftrightarrow \min \sum_{i=1}^n \mathcal{L}(f_i(\theta_i, x), y_i) \eta^{i-1}$$

→ Cannot directly backpropagate otherwise updates of less important losses may worsen more important one

- perform a particular projection on gradient step to avoid it

Differences

- 1) Different depth setting
- 2) Different losses

→ allows a NN to obtain a classification if unseen data

→ prioritized learning