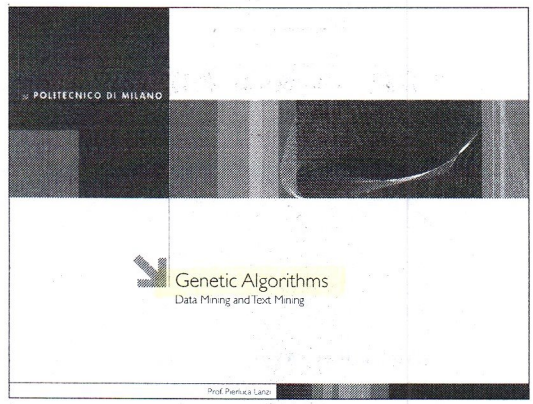

Genetic Algorithms

Data Mining and Text Mining

Syllabus

- A.E. Eiben & J.E. Smith Introduction to Evolutionary Computing (Natural Computing Series) 2nd ed. 2015
- Sean Luke Essentials of Metaheuristics https://cs.gmu.edu/~sean/book/metaheuristics/
- David E. Goldberg "The Design of Innovation" Springer 2002
- Martin Pelikan "Hierarchical Bayesian optimization algorithm: Toward a new generation of evolutionary algorithms", Springer 2005
- Zbigniew Michalewicz "Genetic Algorithms + Data Structures = Evolution Programs" Springer 1998

What's the problem we are trying to solve?

Given a certain problem and a target function over the domain find the maximum/minimum

(we're not looking for the prediction)

e.g. in linear regression with Lasso we want to find the best α param., or we want to find the best set of initial centroids which leads to the best clustering results, or we want to find the best subset of original variables which allows to have the highest performance with the least number of variables

If we knew the analytic form, ...

Algorithm 1 *Gradient Ascent*

1: $\vec{x} \leftarrow$ random initial vector
2: **repeat**
3: $\quad \vec{x} \leftarrow \vec{x} + \alpha \nabla f(\vec{x})$
4: **until** $\vec{x}$ is the ideal solution or we have run out of time
5: **return** $\vec{x}$

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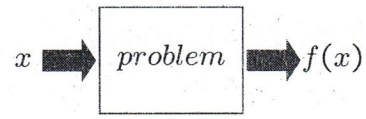

we give some inputs to the problem and the problem gives us a result
trial and error: best α? we try several α's and we take the best based on the performance of the model (black-box procedure))

Basic Black Box Optimization

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- Random search
- Hill Climbing
- Tabu Search
- Simulated Annealing
- ...

we try some values at random and we keep the best (w.r.t. performance)

we have a value and we try similar ones to see if they lead to an improvement

Genetic Algorithms

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Basic Idea
Evolve a population (multiset) of candidate solutions using the concepts of survival of the fitness, variation, and inheritance

Genetic Algorithm
Generate an initial population
Repeat
  Select promising solutions from the population
  Create new solutions by applying variation
  Incorporate new solutions into original population
Until stop criterion met

A Simple Genetic Algorithm for Binary Strings

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```
Genetic algorithm(n,N,f,pm,pc)
  P = generate(n,N);
  while (!done())
    fv = evaluate(P,f,n,N);
    S = selection(P,fv,n,N);
    O = variation(S,n,N,pm,pc);
    P = replacement(O,P,n,N);
```

Parameters

`n`	The number of bits
`N`	The population size
`f`	The objective function
`pm`	Probability of mutation
`pc`	Probability of crossover

(n: number of variables on which the solutions depend)

Common Terminology in Genetic Algorithms

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- Solution String
- String position
- Bit, feature value
- Objective Function
- Selected solutions
- New candidate solutions
- Iteration
- Structure
- Decoded structure
- Nonlinearity
- Individual, chromosome
- Locus
- Allele
- Fitness function, fitness
- Parents
- Offspring
- Generation
- Genotype
- Phenotype
- Epistasis

Operators

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Initialization	Randomly generates the initial population of strings.
Evaluation	Evaluates the population of strings using the given fitness function.
Selection	Selects promising solutions from the current population by making more copies of better solutions at the expense of the worse ones.
Variation	Processes selected solutions to generate new candidate solutions that share similarities with selected solutions but are novel in some way.
Replacement	Incorporates new candidate solutions into the original population.

Generating the Initial Population

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```
generate(n,N)
  P = new population of size N;
  for i=1 to N
    P[i] = generate_random(n);
  return P;
```

n = # parameters (variables)
N = population size

Evaluation

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```
evaluate(P,f,n,N)
  fv = new array of N real numbers;
  for i=1 to N
    fv[i]=f(P[i],n);
  return fv;
```

f = fitness function

How do we select the best ones?

Tournament selection

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Parameters
Tournament size k

Procedure
To select each candidate solution, select a random subset of k solutions from the original population and then select the best solution out of this subset.

Comments
- Tournament selection is among the most popular selection methods in genetic algorithms.
- Binary tournament selection (k = 2) is probably most popular.

Binary Tournament Selection

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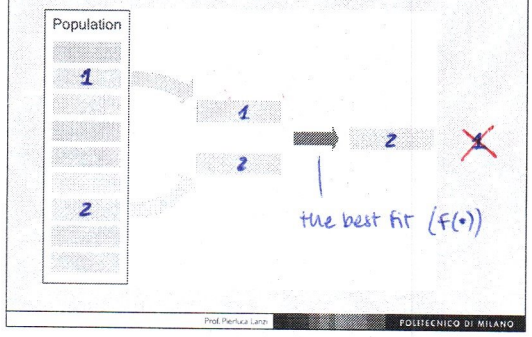


Binary Tournament Selection

```
binary_tournament_selection(P,fv,n,N)
  S = new population of size N;
  for i=1 to n
    a=rand(1,n);
    b=rand(1,n-1);
    if (b>=a) b++;
    if (fv[a]>fv[b])
      S[i]=P[a];
    else
      S[i]=P[b];
  return S;
```


Variation

Purpose
- Process selected promising solutions.
- Create new solutions that share features with selected solutions but are new in some way.
- Two basic principles:
  - variation (introducing novelty), and
  - inheritance (reusing the old).

Variation in genetic algorithms
Two components
- Crossover: Combines bits and pieces of promising solutions.
- Mutation: Makes small perturbations to promising solutions.

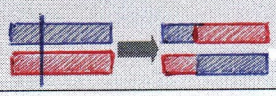
Variation: Basic Procedure


```
variation(S,n,N,pm,pc)
  O = new population of size N;
  shuffle(S,n,N);
  for i=1 to N with step 2
    O[i] = mutation(S[i],n,pm);
    O[i+1] = mutation(S[i+1],n,pm);
    if (rand01()<pc)
      crossover(O[i],O[i+1],n);
  return O;
```

Comments
- The call shuffle(S,n,N) randomly reorders strings in the population P

One-point Crossover

Basic idea
- Randomly select one string position called crossing point.
- Exchange all bits after this position.

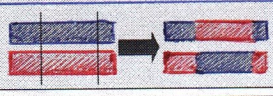


Pseudocode

```
onepoint_crossover(x,y,n)
  cp=random(2,n);
  for i=cp to n
    exchange(x[i],y[i]);
```


Two-point Crossover

Basic idea
- Exchange all bits between two randomly chosen points



Pseudocode

```
twopoint_crossover(x,y,n)
  cp1=random(1,n);
  cp2=random(1,n);
  if (cp1>cp2)
    exchange(cp1,cp2);
  for i=cp1 to cp2
    exchange(x[i],y[i]);
```

Uniform Crossover

Basic idea
- Exchange every bit with probability 0.5

Pseudocode

```
uniform_crossover(x,y,n)
  for i=1 to n
    if (rand01()<0.5)
      exchange(x[i],y[i]);
```


Bit-Flip Mutation

Basic idea
- Flip every bit with a specified probability
- Usually one or only few bits should be mutated
- Typically pm=1/n

Pseudocode

```
mutation(x,n)
  y=new binary string of n bits;
  for i=1 to n
    if (rand01()<pm)
      y[i]=1-x[i];
    else
      y[i]=x[i];
```


When we're done iterating we call:

Replace All

Basic idea
- Assume that the offspring population is of the same size as the original population.
- Replace the entire original population with offspring.

Pseudocode

```
replace_all(O,P,n,N)
  new_P = new population of N strings;
  for i=1 to N
    new_P[i]=O[i];
  return new_P;
```


Replace Worst (Elitism)

Basic idea
- Assume that the offspring population is smaller than the original population.
- Replace worst strings in the original population by new offspring.

Elitism
Elitist genetic algorithms preserve best solutions found so far. This is one of elitist schemes.

Real-Coded Genetic Algorithms

Real-Valued Operators

- Candidate solutions are vectors of real values.
- Random initialization generates a random number from an interval for each variable.
- Operators must deal with real-valued parameters.
- There are many ways to do this.
- We only look at some simple methods.

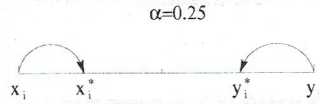
Arithmetic Crossover

- Two real-valued parents
  - $x = (x_1, \ldots, x_n)$
  - $y = (y_1, \ldots, y_n)$
- Choose random variable $i \in \{1, 2, \ldots, n\}$.
- Randomly generate $\alpha \in [0, 1]$.
- The first child is
  - $o_1 = (x_1, \ldots, x_{i-1}, \alpha y_i + (1-\alpha)x_i, x_{i+1}, \ldots, x_n)$
- The second child is
  - $o_2 = (y_1, \ldots, y_{i-1}, \alpha x_i + (1-\alpha)y_i, y_{i+1}, \ldots, y_n)$

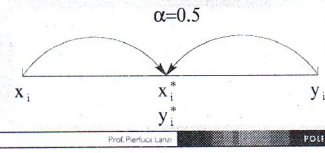
numerical combinations between the parents

Arithmetic Crossover: Example

- Example 1



- Example 2



Simple Mutation

- **Simple mutation**
  - Change each variable with a fixed probability.
  - To change a variable, start by generating a random number from $[-\delta, \delta]$ where $\delta > 0$ is a small number.
  - Add the generated number to the variable.
- **Gaussian mutation**
  - The change is generated according to the Gaussian distribution $N(0, \sigma^2)$ where σ^2 is the variance of the mutation steps, which is a small number.
- **Another idea**
  - Choose a random variable for each solution and mutate that one.