Elective Course
Course Code: CS4103
Autumn 2025-26

Lecture #51

Artificial Intelligence for Data Science

Week-14:

Concluding Session

Problem Solving, A Few Applications, Doubt Clearing

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SVM Example Problem

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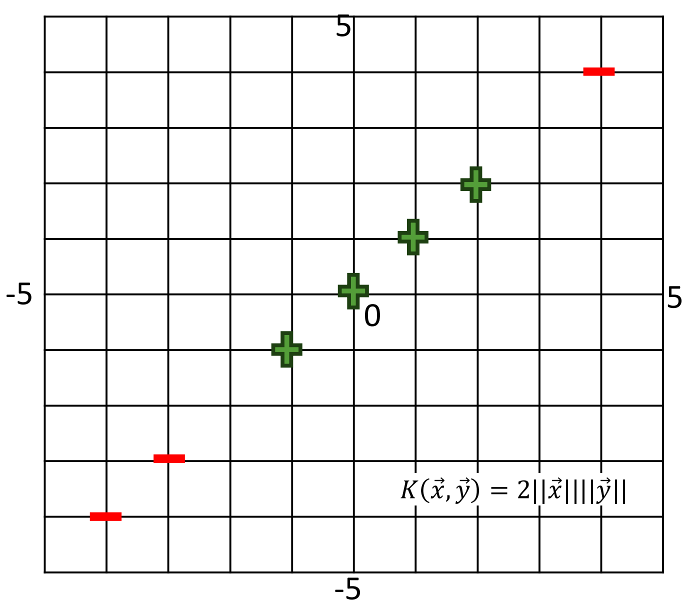

$K(\vec{x},\vec{y}) = 2||\vec{x}||||\vec{y}||$

Data Point	Class
(-1,1)	+
(-1,2)	+
(-2,1)	+
(0,0)	-
(1,1)	-
(0,-1)	-

$$-x_1 - 0.5 = 0$$
$$x_2 - x_1 - 1 = 0$$

Doubt Clearing

FOL: Homework

- **[Homework]** Convert the following sentence to clause form

  $$(\forall x)(P(x) \;=>\; ((\forall y)(P(y) \;=>\; P(f(x,y))) \land \sim(\forall y)(Q(x,y) \;=>\; P(y))))$$

  Ans.: $\{\sim P(x) \lor \sim P(y) \lor P\big(f(x,y)\big),\ \sim P(x) \lor Q\big(x, g(x)\big),\ \sim P(x) \lor \sim P(g(x))\}$

- **[Homework]** Consider the following axioms:
  1. All hounds howl at night. ∀x(Hound(x) → Howl(x))
  2. Anyone who has any cat will not have any mice.
     ∀x∀y(Has(x, y) ∧ Cat(y) → ¬∃z(Has(x, z) ∧ Mouse(z)))
  3. Light sleepers do not have anything which howls at night. ∀x(LS(x) → ¬∃y(Has(x, y) ∧ Howl(y)))
  4. John has either a cat or a hound. ∃x(Has(John, x) ∧ (Cat(x) ∨ Hound(x)))
  5. (Conclusion) If John is a light sleeper, then John does not have any mice.
     LS(John) → ¬∃z(Has(John, z) ∧ Mouse(z))

  Now, prove the conclusion using Resolution

Street Puzzle

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1 2 3 4 5

N_i = {English, Spaniard, Japanese, Italian, Norwegian}
C_i = {Red, Green, White, Yellow, Blue}
D_i = {Tea, Coffee, Milk, Fruit-juice, Water}
J_i = {Painter, Sculptor, Diplomat, Violinist, Doctor}
A_i = {Dog, Snails, Fox, Horse, Zebra}

The Englishman lives in the Red house
The Spaniard has a Dog
The Japanese is a Painter
The Italian drinks Tea
The Norwegian lives in the first house on the left
The owner of the Green house drinks Coffee
The Green house is on the right of the White house
The Sculptor breeds Snails
The Diplomat lives in the Yellow house
The owner of the middle house drinks Milk
The Norwegian lives next door to the Blue house
The Violinist drinks Fruit juice
The Fox is in the house next to the Doctor's
The Horse is next to the Diplomat's

Who owns the Zebra?
Who drinks Water?

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Street Puzzle (Solution)

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1 2 3 4 5

N_i = {English, Spaniard, Japanese, Italian, Norwegian}
C_i = {Red, Green, White, Yellow, Blue}
D_i = {Tea, Coffee, Milk, Fruit-juice, Water}
J_i = {Painter, Sculptor, Diplomat, Violinist, Doctor}
A_i = {Dog, Snails, Fox, Horse, Zebra}

1) The Englishman lives in the Red house → N1=C1
2) The Spaniard has a Dog → N2=A1
3) The Japanese is a Painter → N3=J1
4) The Italian drinks Tea → N4=D1
5) The Norwegian lives in the first house on the left → N5=H1
6) The owner of the Green house drinks Coffee → C2=D2
7) The Green house is on the right of the White house → C3=Hx ; C2=Hx+1
8) The Sculptor breeds Snails → J2=A2
9) The Diplomat lives in the Yellow house → J3=C4
10) The owner of the middle house drinks Milk → D3=H3
11) The Norwegian lives next door to the Blue house → C5=Hx ; N5=Hx$\pm$1
12) The Violinist drinks Fruit juice → J4=D4
13) The Fox is in the house next to the Doctor's → A3=Hx ; J5=Hx$\pm$1
14) The Horse is next to the Diplomat's → A4=Hx ; J3=Hx$\pm$1

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Street Puzzle (Solution)

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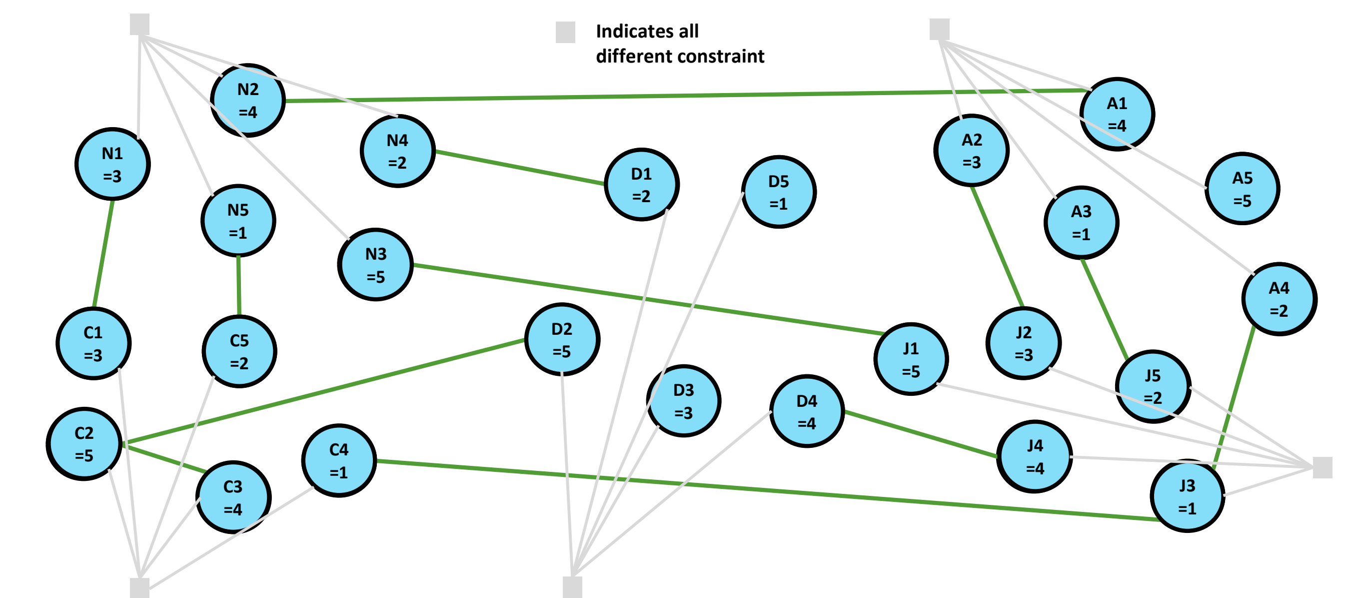

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A Few More Applications of AI

Application of CSP in Real Systems

A TOY PROBLEM SETTING THE SATELITE

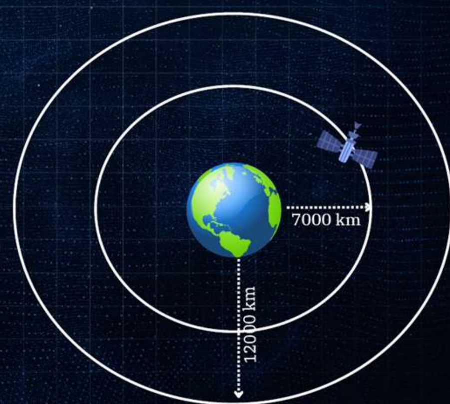
Question

A satellite is currently in a circular orbit of radius
r1 = 7000 km
It must reach a higher circular orbit of radius
r2 = 12000 km.
The Hohmann-like transfer (the fuel-efficient way to move a spacecraft from one orbit to another) requires a change of velocity let's say,

$$\Delta v_{required} = 3.2 \text{ km/s}$$

However due to communication constraints, the spacecraft is allowed to fire its engine only in three burn windows (firing the engine for a short period)

Burn Window	Maximum allowed Δv
W1	0-2.0 km/s
W2	0-2.0 km/s
W3	0-2.0 km/s



The Spacecraft has a total fuel budget equivalent to $\Delta v_{budget} = 3.40$ km/s

Credit: Suvradip Maity

Task

- Formulate this as a constraint satisfaction problem by choosing variables, domains and constraints.
- Use CSP logic to determine if there is a feasible set of burns that achieves the transfer

Credit: Suvradip Maity

Application of CSP in Real Systems

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SOLUTION

Variables

Let d1,d2,d3 be the Δv used in burn windows W1,W2,W3

Domains

Since each burn is limited to 0-2.0 km/s,

Constraints

Total required Δv : $d_1 + d_2 + d_3 \geq 3.20$

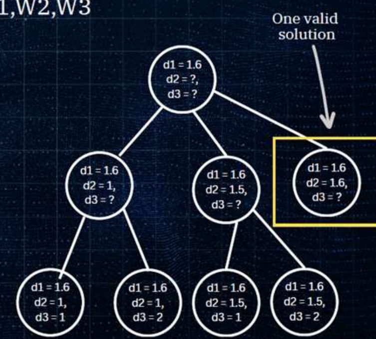
Fuel budget: $d_1 + d_2 + d_3 \leq 3.40$

Window limit: $0 \leq d_i \leq 2.0$

A Valid Solution

To satisfy $3.20 \leq d_1 + d_2 + d_3 \leq 3.40$

One valid solution would be , d1 = 1.6, d2 = 1.6 and d3 = 0, try finding out other 2 solutions.



Some papers where CSP has been used to solve spacecraft problems :

1. https://ai.jpl.nasa.gov/public/documents/papers/wac00-pfmd.pdf
2. https://ntrs.nasa.gov/api/citations/19950017340/downloads/19950017340.pdf

Credit: Suvradip Maity

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Application of FOL in Chemical Science

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```
import pytholog as pl
# Creating knowledge base
kb = pl.KnowledgeBase("chemical_reactions")
kb([
#Reagents
"acid(hbr)",
"acid(hcl)",
"acid(h2so4)",
"strong_base(naoh)",
"strong_base(lda)",
"strong_base(nanh2)",
"nucleophile(oh_minus)",
"nucleophile(cn_minus)",
"nucleophile(rmgx)",
"peroxide(roor)",
"hydride_donor(nabh4)",
"hydride_donor(lialh4)",
"electrophile(br_plus)",
"electrophile(no2_plus)",
"base(naoh)",
"base(ro_minus)",
```

```
#Substrate features
"double_bond(alkene)",
"acidic_hydrogen(alpha_h)",
"carbonyl(aldehyde)",
"carbonyl(ketone)",
"leaving_group(br)",
"leaving_group(cl)",
"leaving_group(i)",
"unhindered(primary_carbon)",
"beta_hydrogen(secondary_carbon)",
"aromatic_ring(benzene)",
"epoxide(epoxide_ring)",
"heat(heat_condition)",
```

Credit: Sreya Gain

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Application of FOL in Chemical Science

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```
#RULES
#1. Acid + Alkene → Protonation
"first_step(X,Y,protonation) :- acid(X), double_bond(Y)",
#2. Strong Base + α-H → Deprotonation
"first_step(X,Y,deprotonation) :-strong_base(X), acidic_hydrogen(Y)",
#3. Nucleophile + Carbonyl → Nucleophilic Attack
"first_step(X,Y,nucleophilic_attack) :- nucleophile(X), carbonyl(Y)",
#4. Peroxide → Radical Initiation
"first_step(X,radical_initiation) :- peroxide(X)",
#5. Nucleophile + Leaving Group + Unhindered → SN2
"first_step(X,Y,sn2) :- nucleophile(X), leaving_group(Y), unhindered(Y)",
#6. Strong Base + Leaving Group + β-H → E2
"first_step(X,Y,e2) :- strong_base(X), leaving_group(Y), beta_hydrogen(Y)",
#7. Aromatic Ring + Electrophile → Sigma Complex
"first_step(X,Y,eas_sigma_complex) :- aromatic_ring(Y), electrophile(X)",
#8. Heat → Pericyclic Rearrangement
"first_step(pericyclic_rearrangement) :- heat(heat_condition)",
#9. Base + Epoxide → Epoxide Opening (Less Substituted)
"first_step(X,Y,epoxide_open_less_substituted) :-   epoxide(Y), base(X)",
#10. Acid + Epoxide → Protonation then Opening
"first_step(X,Y,epoxide_protonation_then_attack) :-epoxide(Y), acid(X)"])
```

Credit: Sreya Gain

Application of FOL in Chemical Science

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```
# Queries
print("\nWhat will be the first step when lda and α-H are present?")
print([item['What'] for item in kb.query(pl.Expr("first_step(lda,alpha_h,What)"))])
```

```
What will be the first step when lda and α-H are present?
['deprotonation']
```

```
print("\nWhat will be the first step when br_plus and benzene are present?")
print([item['What'] for item in kb.query(pl.Expr("first_step(br_plus,benzene,What)"))])
```

```
What will be the first step when br_plus and benzene are present?
['eas_sigma_complex']
```

```
print("\nIf the first step is eas_sigma_complex in the presence of Benzene, then what can be the
possible electrophiles?")
print([item['What'] for item in kb.query(pl.Expr("first_step(What,benzene,eas_sigma_complex)"))])
```

```
If the first step is eas_sigma_complex in the presence of Benzene, then what can be the possible electrophiles?
['br_plus', 'no2_plus']
```

```
print("\nIf the first step is protonation, then what can be the possible reagent and substrate?")
print(kb.query(pl.Expr("first_step(Reagent,Substrate,protonation)")))
```

```
If the first step is protonation, then what can be the possible reagent and substrate?
[{'Reagent': 'h2so4', 'Substrate': 'alkene'}, {'Reagent': 'hbr', 'Substrate': 'alkene'}, {'Reagent': 'hcl', 'Substrate': 'alkene'}]
```

Application of FOL in Chemical Science

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```
print("\nIf the first step is deprotonation, then what can be the possible reagent and
substrate?")
print(kb.query(pl.Expr("first_step(Reagent,Substrate,deprotonation)")))
```

```
If the first step is deprotonation, then what can be the possible reagent and substrate?
[{'Reagent': 'lda', 'Substrate': 'alpha_h'}, {'Reagent': 'nanh2', 'Substrate': 'alpha_h'}, {'Reagent': 'naoh', 'Substrate': 'alpha_h'}]
```

```
print("\nIf the first step is nucleophilic_attack, then what can be the possible reagent and
substrate?")
```

```
If the first step is nucleophilic_attack, then what can be the possible reagent and substrate?
[{'Reagent': 'cn_minus', 'Substrate': 'aldehyde'}, {'Reagent': 'cn_minus', 'Substrate': 'ketone'}, {'Reagent': 'oh_minus', 'Substrate': 'aldehyde'},
{'Reagent': 'oh_minus', 'Substrate': 'ketone'}, {'Reagent': 'rmgx', 'Substrate': 'aldehyde'}, {'Reagent': 'rmgx', 'Substrate': 'ketone'}]
```

```
print("\nIf the first step is eas_sigma_complex, then what can be the possible reagent and
substrate?")
print(kb.query(pl.Expr("first_step(Reagent,Substrate,eas_sigma_complex)")))
```

```
If the first step is eas_sigma_complex, then what can be the possible reagent and substrate?
[{'Reagent': 'br_plus', 'Substrate': 'benzene'}, {'Reagent': 'no2_plus', 'Substrate': 'benzene'}]
```

```
print("\nIf the first step is epoxide_open_less_substituted, then what can be the possible
reagent and substrate?")
print(kb.query(pl.Expr("first_step(Reagent,Substrate,epoxide_open_less_substituted)")))
```

```
If the first step is epoxide_open_less_substituted, then what can be the possible reagent and substrate?
[{'Reagent': 'naoh', 'Substrate': 'epoxide_ring'}, {'Reagent': 'ro_minus', 'Substrate': 'epoxide_ring'}]
```


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Questions?