Seminar on Constraint Solving Meets Data Mining and Machine Learning
Spring 2013

Matti Järvisalo

Practical Arrangements, introduction.

Course Information

Instructor:	Dr. Matti Järvisalo `matti.jarvisalo@cs.helsinki.fi`
Reception:	Contact instructor by email for an appointment
Credit units:	3 ECTS
Language:	English (by default)
WWW:	`http://www.cs.helsinki.fi/u/mjarvisa/teaching/seminar13/`

Course Requirements

- Choose a topic (scientific article) to study
- Write a 10-15 page (plus references) report n the topic
- Give a 30-min presentation on the topic
- Give constructive feedback on another student's report (and draft)
- Act as the opponent of another student's presentation
- Attend the seminar 1-2 workshop day(s) in May

Choosing a Topic

- List of topics available on the seminar webpage
- If you have not reserved a topic, do this *by this Friday March 15*
- Each topic consists of one scientific article
- *Can suggest a topic outside the list!*
- The article provides a starting-point for your work
- You may need to read additional articles for necessary background
- Synthesis of multiple related articles is a major plus

Deadlines

- All deadlines are strict — you will fail the course if you do not meet a deadline
- March 15: vote on the workshop dates, choose topic
- April 13: at least 5-page draft report (send to teacher)
- April 20: feedback on another student's report draft
  (send to teacher and your opponent)
- One week before the workshop: Full-length report and preliminary presentation slides
  (send to teacher and your opponent)
- At the workshop: act as an opponent
- One week after the workshop: Final report

Report and Presentation

- A seminar report is a short review paper: you explain some interesting results in your own words.
- A typical seminar report will consist of the following parts:
  - an informal introduction,
  - a formally precise definition of the problem that is studied,
  - a brief overview of very closely related work— here you might cite approx. 3–10 papers and explain their main contributions,
  - a more detailed explanation of one or two interesting results, with examples
  - conclusions.
- Superficially, your report should look like a typical scientific article.
  - However, it will not contain any new scientific results, just a survey of previously published work.
- The presentation is an overview of the report
  - You should understand what you are saying
  - Everyone should understand you
  - The abstraction level should be right
  - Examples are always good to communicate ideas

Agreeing on the workshop day(s)

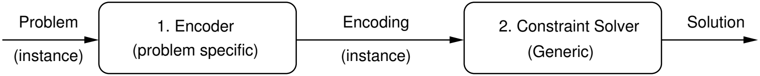
- We need to agree on two full workshop days during May 6–14
- All presentations take place during the workshop days
- Go to `http://www.doodle.com/xwbnvtvabiftmr7c`
- Attendance mandatory at least *on the day you are scheduled for*

What This Course is about

- Interplay between onstraint solving and data analysis
- How to use constraint satisfaction and optimization techniques to solve data analysis task
  - Providing optimal solutions?
  - Addressing more general problems that classical approaches?
  - Example: Clustering: from k-means style local search to *guaranteed optimal clustering*?
- How to use machine learning to speed-up constraint solving in practice?
  - Learning to select the best algorithm for solving a given problem instance as input

Declarative Programming and Constraint Solving

- Two-step approach to solving hard combinatorial problems:



1. **Encoding**: *Domain-specific* declarative formulation of problem using chosen *(constraint) modelling language*
   - ★ Given any problem instance,
     formulate the instance in terms of *mathematical constraints*
2. **Solving**: A *generic* solver—a search algorithm—for the chosen modelling language, which can find a *solution* (or determine that none exist) to any formulation in the modelling language
   - ★ Found solution mapped back to a solution of the original problem instance

Various approaches based on *different modelling languages*:
integer programming, linear programming, constraint programming, Boolean satistiability, Boolean optimization (MaxSAT), . . .

Constraints: A general view

- A set of variables $X = \{x_1, \ldots, x_n\}$
- Each variable x_i has domain D_i
- A *constraint* C over X is a subset of $D_1 \times \cdots \times D_n$

Example. Let $D_1 = D_2 = \{1, 2, 3\}$. The constraint $\neq$ over x_1, x_2 is $\{(d_1, d_2) \mid d_1 \in D_1, d_2 \in D_2, d_1 \neq d_2\}$

$$= \{(1,2),(1,3),(2,1),(2,3),(3,1),(3,2)\} \subset D_1 \times D_2.$$

- The above is an example of a *finite-domain* constraint, where the domain of each variable is a finite set of values
  - A special case are *Boolean constraints* that are defined over *Boolean variables*, i.e., variables with domain $\mathbb{B} = \{0, 1\}$.
  - 1 is the value *true*, 0 is the value *false*
- Depending on the constraint language, the variables may also have infinite domains.
  - Examples: $\mathbb{R}$ (real domains), $\mathbb{Z}$ (integer domains)

Constraint Satisfaction Problems (CSPs)

- Given: a set of variables $X = \{x_1, \ldots, x_n\}$ with domains $D_1, \ldots, D_n$
- a *constraint satisfaction problem* (CSP) is a set of constraints $\mathbf{C} = \{C_1, \ldots, C_m\}$
  - each constraint C is defined over some subset of X.
- *Value assignment* for $x_1, \ldots, x_n$ is a function T that assigns for each x_i a value from the domain D_i.
- T *satisfies* a constraint C over variables $x_{i_1}, \ldots, x_{i_k} \subseteq X$ iff $(T(x_{i_1}), \ldots, T(x_{i_m})) \in C$.
- T is a *solution to* **C** iff T satisfies every constraint in **C**.
- If **C** has a solution, then **C** is *satisfiable*, and otherwise *unsatisfiable*

CSPs: Example

Quasigroup Completion problem:

- $n \times n$ matrix
- Some cells have been pre-filled
- Fill each of the cells with integers $1, \ldots, n$ so that: each $1..n$ appears *exactly once in each column and row*

	3			
3	4			
4	5			
5				

A CSP encoding:

- Let $\text{AllDiff}(x_1, \ldots, x_k) = \{(v_1, \ldots, v_k) \mid v_1 \in D_1, \ldots, v_k \in D_k, v_i \neq v_j \; \forall i \neq j, i, j \in \{1, \ldots, k\}\}$
- Introduce variable x_{ij} for each cell in the $n \times n$ matrix: x_{ij} represents the value in cell on row i, column j
- Domains:
  - $D_{ij} = \{1, \ldots, n\}$ for each ij such that the cell ij is empty
  - $D_{ij} = \{v_{ij}\}$ for each ij with a pre-filled value v_{ij}
- Constraints:
  - For each row i: $\text{AllDiff}(x_{i1}, \ldots, x_{in})$
  - For each column j: $\text{AllDiff}(x_{1j}, \ldots, x_{nj})$

Boolean Satisfiability

- An important special case of CSPs is the *Boolean satisfiability problem* SAT
- In general, SAT the question of whether a given *propositional logic formula is satisfiable*
- Typically SAT refers to CNF SAT
  - The satisfiability problem of propositional (Boolean) formulas in *conjunctive normal form*, CNF formulas
- Despite its simplicity, SAT is an often used constraint language that provides a highly efficient approach to solving various hard computational problems

CNF SAT

- A *literal* is a Boolean variable x, or the *negation* $\neg x$ of x
  - $\neg x$ is the *negative literal* of x, x the positive literal
- A *clause* is the constraint $\bigvee_{i=1}^{n} l_k$ (i.e., $l_1 \vee \cdots \vee l_k$) over distinct literals l_i
  - $\vee$ is called *disjunction*, i.e., logical OR
- A CNF formula is a set of clauses
  - In other words:
    a CNF formula is a constraint of the form $\bigwedge_{C \in \mathbf{C}} C$,
    where each $C \in \mathbf{C}$ is a clause
- A value assignment T over Boolean variables is a *truth assignment*
- T satisfies a literal l iff
  - l is a positive literal x and $T(x) = 1$, or
  - l is a negative literal $\neg x$ and $T(x) = 0$
- T satisfies a clause $C = l_1 \vee \cdots \vee l_k$ iff
  there is a literal $l \in \{l_1, \ldots, l_k\}$ such that $T(l) = 1$.

CNF: Example

A CNF encoding of the Quasigroup Completion problem:

- Boolean variables x_{ijk}, where $i, j, k = 1, \ldots, n$:
  x_{ijk} means "cell at row i, column j has value k"
- Use clauses to enforce that for each cell ij, *exactly one* of $x_{ij1}, \ldots, x_{ijn}$ is assigned to 1:
  - At least one: $(x_{ij1} \vee \cdots \vee x_{ijn})$
  - At most one: $(\neg x_{ijk} \vee \neg x_{ijk'})\ \forall i, j \in \{1, \ldots, n\}$, where $i \neq j$
- Similarly, enforce that
  - for each row i, *exactly one* of $x_{i1k}, \ldots, x_{ink}$ is assigned to 1 for each k (all cells in row i have different values)
  - for each column i, *exactly one* of $x_{1jk}, \ldots, x_{njk}$ is assigned to 1 for each k (all cells in column i have different values)
  - SAT encodings of AllDiff!

Constraint Optimization Problems (COPs)

- A CSP has some set S of solutions (possible *infinite*).
- An *objective* (or *cost*) *function* f is a mapping from S to some set of values (can be reals, integers, etc).
- A *constraint optimization problem* (COP) consists of a set of constraints and a cost function
- Each element in S is a *feasible* solution
- An *optimal solution*:
  - as a *minimization problem*:
    any $s \in S$ such that $f(s') \geq f(s)$ for each $s' \in S$.
  - as a *maximization problem*:
    any $s \in S$ such that $f(s') \leq f(s)$ for each $s' \in S$.
- Search task: find an optimal solution
- Different paradigms:
  - Maximum Boolean satisfiability (MaxSAT): maximize the number of satisfied CNF clauses
  - Integer/Linear programming (ILP, MIP)
  - Some CP solvers can also cope with optimization

Linear and Integer Programs

- A *linear function* is of the form $c_1x_1 + \cdots + c_nx_n$
- *Linear constraints* over variables $x_1, \ldots, x_n$ are of the form

  $$a_1x_1 + \cdots + a_nx_n \;\Box\; b,$$

  where $a_1, \ldots, a_n$ and b are constants, and $\Box$ is
  - $=$ (linear equality/equation), or
  - $\geq$ or $\leq$ (linear inequality)
- A *linear program* (LP) is a COP such that
  - each constraint in the problem is linear,
  - the objective function in the problem is linear, and
  - the variable domains are real-valued ranges $[l_i, u_i]$, i.e., $l_i \leq x_i \leq u_i$.
  - Solvable in polynomial-time.
- *Integer programs* (IPs) are like linear programs, except that *the variables can only take integer values*. Capture NP.
- *Mixed integer programs* (MIPs) have both integer and real-valued variables.

Integer Programming: Example

Knapsack problem:

- Given: A knapsack of size S (an integer), items $1, \ldots, n$, and the size s_i (integers) and value v_i (integers) of each item i.
- Find a subset of the n items that fits into the knapsack and maximizes the total value of the objects in the knapsack.

IP formulation:

- Take a binary variable x_i for each item i.
  - $x_i = 1$ ($x_i = 0$) means that item i is (not) included in the knapsack.

$$\max \sum_{i=1}^{n} v_i x_i$$

$$\sum_{i=1}^{n} s_i x_i \leq S$$
$$x_i \in \{0, 1\} \ \forall i \in \{1, \ldots, n\}$$

- The above formulation is a *0-1 integer program*: all variables have binary domains

Different paradigms

- Different constraint solving paradigms have different strengths and weaknesses
  - Deciding whether a given finite-domain CSPs, Boolean formula (SAT), or (M)IP has a solution is NP-hard
  - LPs can be solved in polynomial time
  - Tradeoffs between expressiveness (high-level constraints, CP) and fast solver techniques (low-level, SAT)
  - Satisfaction vs optimization:
    SAT vs MaxSAT, CP, MIP
  - Variable domains (binary, integer, real, ...)
- CP / SAT / MIP solvers are algorithmically different

Topics

- A: Data Mining using constraint solvers / knowledge compilation
- B: Using machine learning to configure / speed-up constraint solving
- C: Clustering with constraints
- D: Learning Bayesian networks using constraint solvers / heuristic search
- E: Learning causal models using constraint solving
- F: Model counting and probabilistic inference
- G: *miscellaneous* — ask me for further ones if necessary

Background: Propositional logic

Propositional formulas

- Syntax based on:
  Boolean variables $X = \{x_1, x_2, \ldots\}$
  Boolean connectives $\lor, \land, \neg$
- The set of (propositional) formulas is the smallest set such that all Boolean variables are formulas and if ϕ_1 and ϕ_2 are formulas, so are $\neg\phi_1$, $(\phi_1 \land \phi_2)$, and $(\phi_1 \lor \phi_2)$.
  For example, $((x_1 \lor x_2) \land \neg x_3)$ is a formula but $((x_1 \lor x_2)\neg x_3)$ is not.
- A formula of the form x_i or $\neg x_i$ is called a *literal* where x_i is a Boolean variable.
- Usual shorthands:
  $\phi_1 \rightarrow \phi_2$: $\neg\phi_1 \lor \phi_2$
  $\phi_1 \leftrightarrow \phi_2$: $(\neg\phi_1 \lor \phi_2) \land (\neg\phi_2 \lor \phi_1)$
  $\phi_1 \oplus \phi_2$: $(\neg\phi_1 \land \phi_2) \lor (\phi_1 \land \neg\phi_2)$

Semantics

- Boolean variables are either true or false
- A truth assignment T is mapping from a finite subset $X' \subset X$ to the set of truth values $\{1, 0\}$.
- Consider a truth assignment $T : X' \longrightarrow \{1, 0\}$ which is appropriate to ϕ, i.e., $X(\phi) \subseteq X'$ where $X(\phi)$ be the set of Boolean *variables appearing in* ϕ.
- $T \models \phi$ (T *satisfies* ϕ) is defined inductively as follows:
  If ϕ is a variable, then $T \models \phi$ iff $T(\phi) = 1$.
  If $\phi = \neg\phi_1$, then $T \models \phi$ iff $T \not\models \phi_1$
  If $\phi = \phi_1 \wedge \phi_2$, then $T \models \phi$ iff $T \models \phi_1$ and $T \models \phi_2$
  If $\phi = \phi_1 \vee \phi_2$, then $T \models \phi$ iff $T \models \phi_1$ or $T \models \phi_2$

Example. Let $T(x_1) = 1$, $T(x_2) = 0$.
Then $T \models x_1 \vee x_2$, and $T \not\models (x_1 \vee \neg x_2) \wedge (\neg x_1 \wedge x_2)$