Inference: Integer Linear Programs

CS 6355: Structured Prediction



So far in the class

- Thinking about structures
 - A graph, a collection of parts that are labeled jointly, a collection of decisions
- Algorithms for learning
 - Local learning
 - Learn parameters for individual components independently
 - Learning algorithm not aware of the full structure
 - Global learning
 - Learn parameters for the full structure
 - Learning algorithm "knows" about the full structure
- This section: Prediction
 - Sets structured prediction apart from binary/multiclass

Inference

- What is inference?
 - An overview of what we have seen before
 - Combinatorial optimization
 - Different views of inference
- Graph algorithms
 - Dynamic programming, greedy algorithms, search
- Integer programming
- Heuristics for inference
 - Sampling
- Learning to search

The big picture

- MAP Inference is combinatorial optimization
- Combinatorial optimization problems can be written as integer linear programs (ILP)
 - The conversion is not always trivial
 - Allows injection of "knowledge" into the inference in the form of constraints
- Different ways of solving ILPs
 - Commercial solvers: CPLEX, Gurobi, etc
 - Specialized solvers if you know something about your problem
 - Incremental ILP, Lagrangian relaxation, etc.
 - Can approximate to linear programs and hope for the best
- Integer linear programs are NP hard in general
 - No free lunch

Today's Agenda

- Linear and integer linear programming
 - What are they?
 - The geometric perspective
- ILPs for inference
 - Simple example: Multiclass classification
 - More general structures

Detour: Linear programming

- Minimizing a linear objective function subject to a finite number of linear constraints (equality or inequality)
- Very widely applicable
 - Operations research, micro-economics, management
- Historical note/anecdote
 - Developed during world war 2 to optimize army expenditure
 - Nobel Prize in Economics 1975
 - "Programming" not the same as computer programming
 - "Program" referred to military schedules and programming referred to optimizing the program

A student wants to spend as little money on food while getting sufficient amount of vitamin Z and nutrient X. Her options are:

Item	Cost/100g	Vitamin Z	Nutrient X
Carrots	2	4	0.4
Sunflower seeds	6	10	4
Double cheeseburger	0.3	0.01	2

How should she spend her money to get at least 5 units of vitamin Z and 3 units of nutrient X?

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Let c, s and d denote how much of each item is purchased

Minimize total cost

such that

At least 5 units of vitamin Z,

At least 3 units of nutrient X,

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$$2c + 6s + 0.3d$$

Minimize total cost

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$$4c + 10s + 0.01d \ge 5$$

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$$\min \ 2c+6s+0.3d \qquad \qquad \text{Minimize total cost}$$
 such that
$$4c+10s+0.01d \geq 5 \qquad \qquad \text{At least 5 units of vitamin Z,} \\ 0.4c+4s+2d \geq 3 \qquad \qquad \text{At least 3 units of nutrient X,}$$

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How should she spend her money to get at least 5 units of vitamin Z and 3 units of nutrient X?

Let c, s and d denote how much of each item is purchased

$$\begin{array}{ll} \min & 2c+6s+0.3d \\ \text{such that} \\ & 4c+10s+0.01d \geq 5 \\ & 0.4c+4s+2d \geq 3 \\ & c \geq 0, s \geq 0, d \geq 0. \end{array} \qquad \begin{array}{ll} \text{Minimize total cost} \\ \text{At least 5 units of vitamin Z,} \\ \text{At least 3 units of nutrient X,} \\ & c \geq 0, s \geq 0, d \geq 0. \end{array}$$

In general

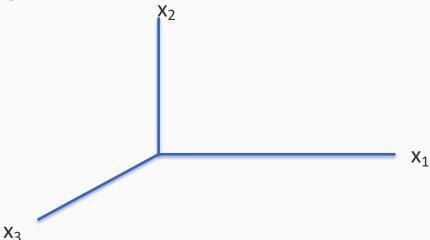
$$\begin{array}{lll} \max & \mathbf{c}^T\mathbf{x} & --- & \text{linear} \\ \text{subject to} & A\mathbf{x} \leq \mathbf{b}_{\longleftarrow} --- & \text{linear} \\ & \mathbf{x} \geq 0. \end{array}$$

In general

$$\begin{array}{ll}
\max & \mathbf{c}^T \mathbf{x} \\
\text{subject to} & A\mathbf{x} \leq \mathbf{b} \\
\mathbf{x} \geq 0.
\end{array}$$

This is a continuous optimization problem

- And yet, there are only a finite set of possible solutions
- For example:

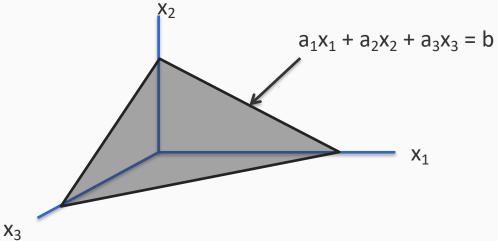


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 X_3

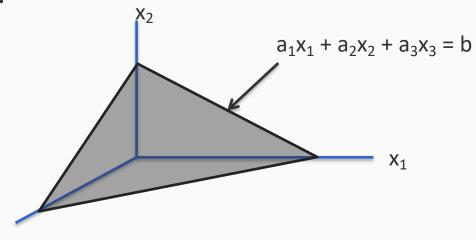
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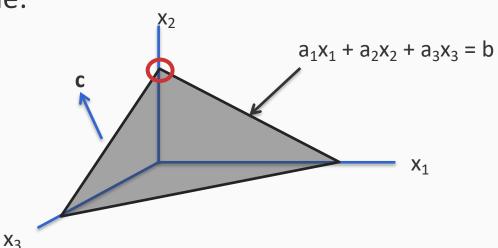
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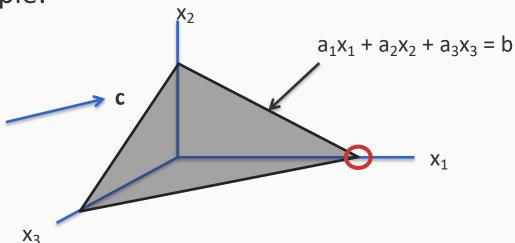


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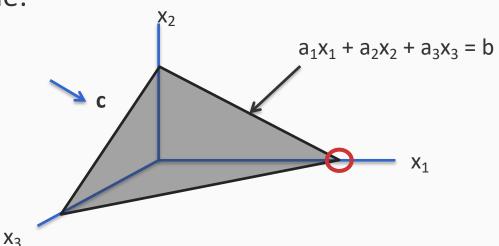


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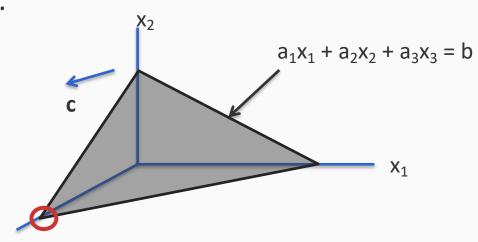


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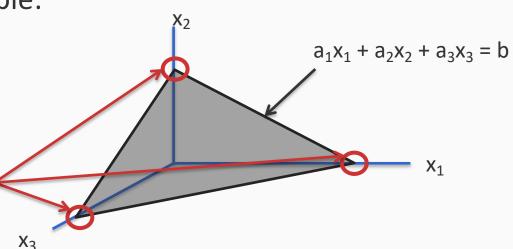
This is a continuous optimization problem

And yet, there are only a finite set of possible solutions

– For example:

Suppose we had to maximize any $\mathbf{c}^{\mathsf{T}}\mathbf{x}$ on this region

These three vertices are the only possible solutions!



In general
$$\begin{aligned} \max & \mathbf{c}^T \mathbf{x} \\ \text{subject to} & A\mathbf{x} \leq \mathbf{b} \\ \mathbf{x} \geq 0. \end{aligned}$$

This is a continuous optimization problem

- And yet, there are only a finite set of possible solutions
- The constraint matrix defines a convex polytope
- Only the vertices or faces of the polytope can be solutions

The constraint matrix defines a polytope that contains allowed solutions (possibly not closed)

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One of the constraints: $A_i^T \mathbf{x} \leq b_i$

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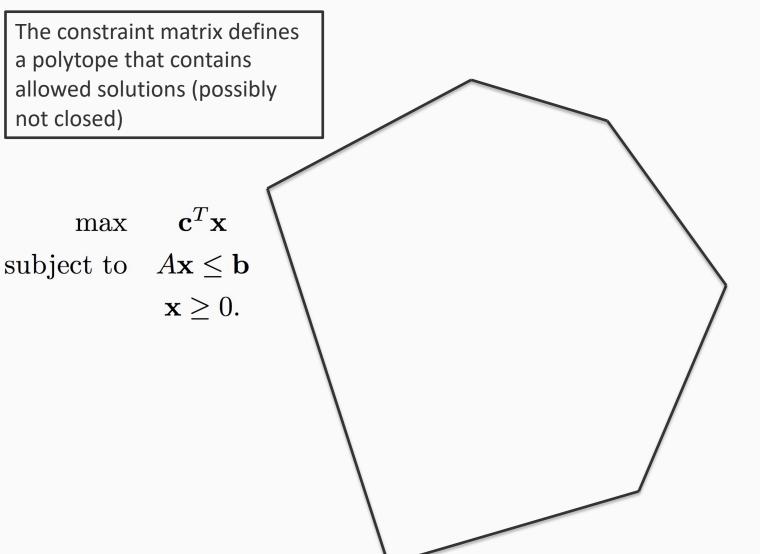
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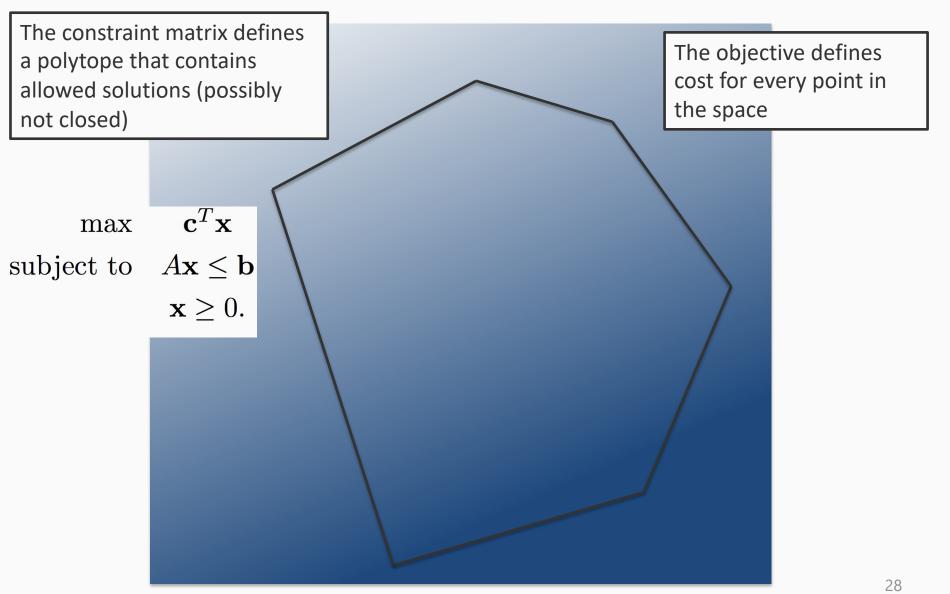
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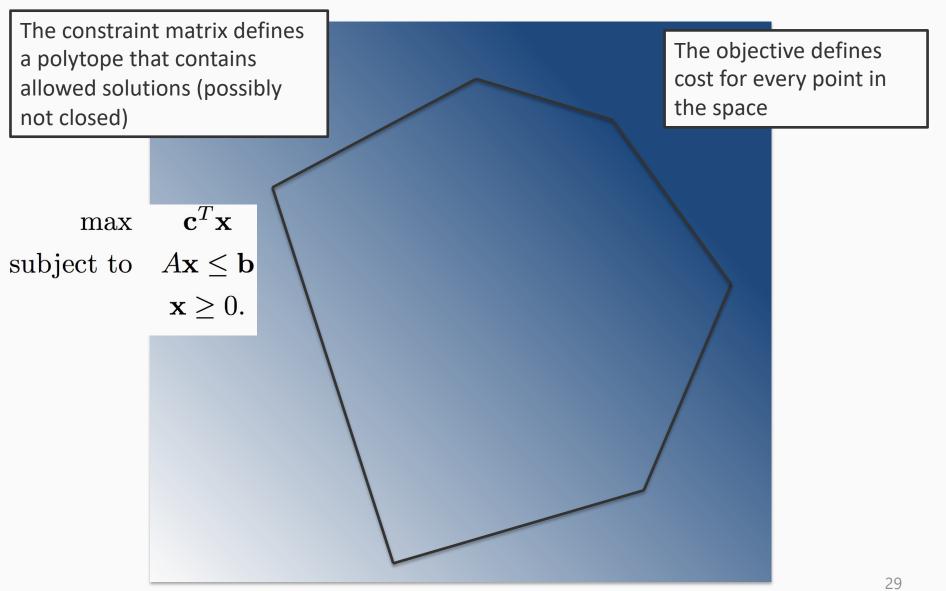
Points in the shaded region can are not allowed by this constraint

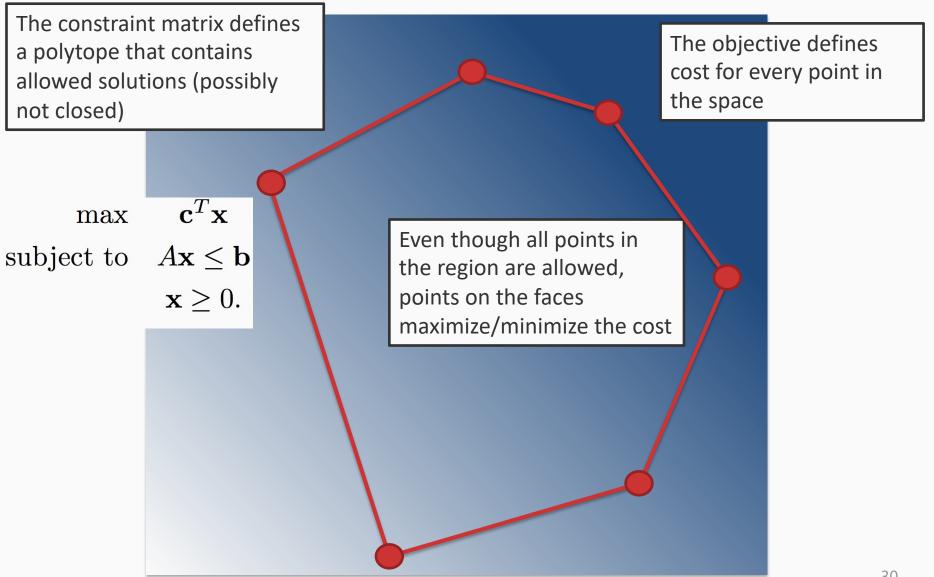
The constraint matrix defines a polytope that contains allowed solutions (possibly not closed)

Every constraint forbids a half-space The points that are allowed form the feasible region









• In general $\begin{aligned} \max & \mathbf{c}^T \mathbf{x} \\ \text{subject to} & A\mathbf{x} \leq \mathbf{b} \\ \mathbf{x} \geq 0. \end{aligned}$

- This is a continuous optimization problem
 - And yet, there are only a finite set of possible solutions
 - The constraint matrix defines a convex polytope
 - Only the vertices or faces of the polytope can be solutions
- Linear programs can be solved in polynomial time

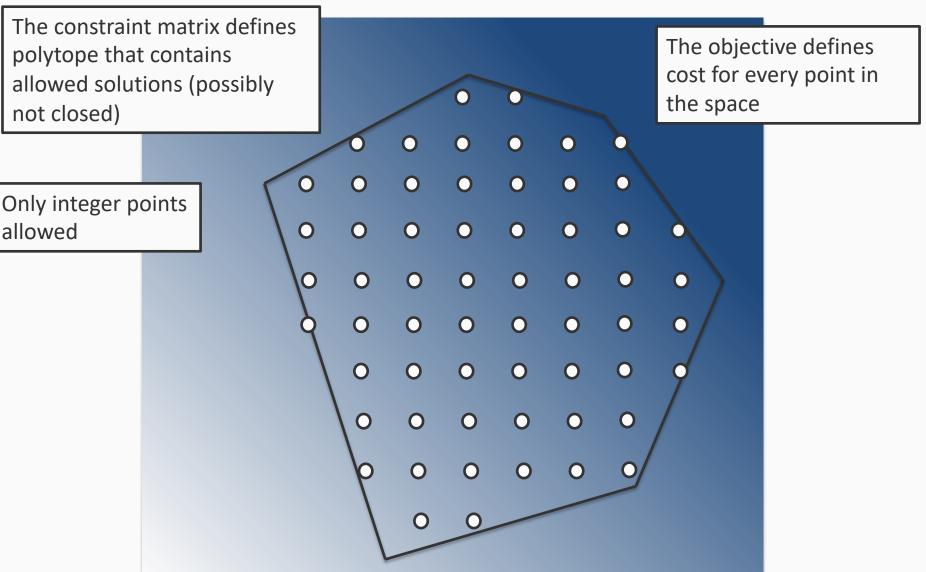
Integer linear programming

In general

max
$$\mathbf{c}^T \mathbf{x}$$
 subject to $A\mathbf{x} \leq \mathbf{b}$ $\mathbf{x} \geq 0$

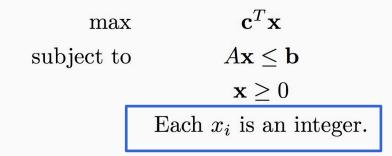
Each x_i is an integer.

Geometry of integer linear programming



Integer linear programming

In general



 Solving integer linear programs in general can be NPhard!

 LP-relaxation: Drop the integer constraints and hope for the best

0-1 integer linear programming

In general

$$\begin{array}{ll}
\max & \mathbf{c}^T \mathbf{x} \\
\text{subject to} & A\mathbf{x} \leq \mathbf{b} \\
& \mathbf{x} \geq 0 \\
& \mathbf{x} \in \{0, 1\}^n
\end{array}$$

- An instance of integer linear programs
 - Still NP-hard
- Geometry: We are only considering points that are vertices of the Boolean hypercube

0-1 integer linear programming

In general

$$\begin{array}{ll}
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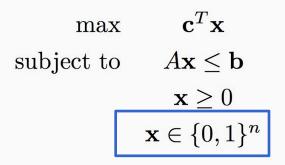
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Constraints prohibit certain vertices

Eg: Only points within this region are allowed

0-1 integer linear programming

In general



Solution can be an interior point of the constraint set defined by $Ax \le b$

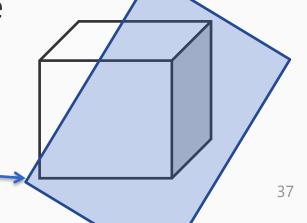
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Back to structured prediction

- Recall that we are solving $argmax_{\mathbf{y}} w^T \phi(x, \mathbf{y})$
 - The goal is to produce a graph
- The set of possible values that y can take is finite, but large

- General idea: Frame the argmax problem as a 0-1 integer linear program
 - Allows addition of arbitrary constraints

Let's start with multi-class classification

$$\underset{y \in \{A,B,C\}}{\operatorname{argmax}} w^{T} \phi(x,y) = \underset{y \in \{A,B,C\}}{\operatorname{argmax}} \operatorname{score}(y)$$

Introduce decision variables for each label

- $z_A = 1$ if output = A, 0 otherwise
- $z_B = 1$ if output = B, 0 otherwise
- $z_C = 1$ if output = C, 0 otherwise

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$$\max_{\mathbf{z}} \quad z_A \mathbf{score}(A) + z_B \mathbf{score}(B) + z_C \mathbf{score}(C) \quad \text{Maximize the score}$$
 s.t.
$$\text{Pick exactly one label}$$

$$z_A, z_B, z_C \in \{0, 1\}.$$

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Maximize the score

Pick exactly one label

An assignment to the **z** vector gives us a **y**

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Intr

We have taken a trivial problem (finding a highest scoring element of a list) and converted it into a representation that is NP-hard in the worst case!

Lesson: Don't solve multiclass classification with an ILP solver

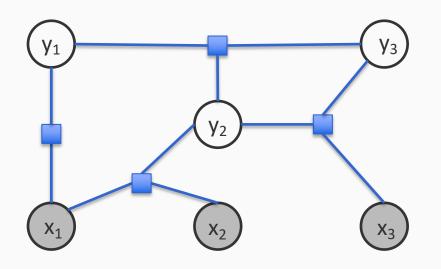
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Maximize the score

Pick exactly one label

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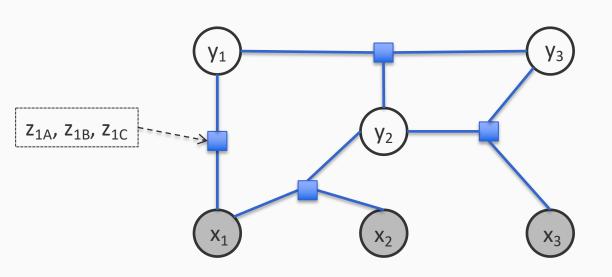


Suppose each y_i can be A, B or C

Introduce one decision variable for each part being assigned labels

Our goal

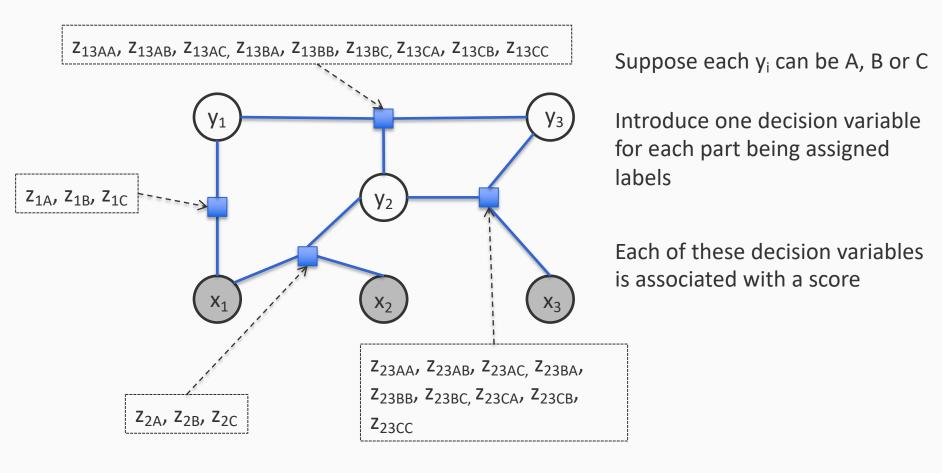
$$\max_{y_1, y_2, y_3} \mathbf{w}^T \phi(x_1, y_1) + w^T \phi(y_1, y_2, y_3) + w^T \phi(x_3, y_1, y_3) + w^T \phi(x_1, x_2, y_2)$$



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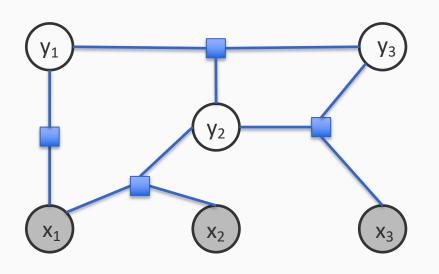
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Our goal

$$\max_{y_1, y_2, y_3} \mathbf{w}^T \phi(x_1, y_1) + w^T \phi(y_1, y_2, y_3) + w^T \phi(x_3, y_1, y_3) + w^T \phi(x_1, x_2, y_2)$$
Questions?

45



Suppose each y_i can be A, B or C

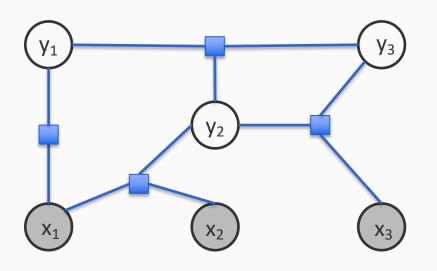
Introduce one decision variable for each part being assigned labels

Each of these decision variables is associated with a score

$$\sum_{l} z_{1l} s_{1l} + \sum_{l} z_{2l} s_{2l} + \sum_{l,l'} z_{13ll'} s_{13ll'} + \sum_{l,l'} z_{23ll'} s_{23ll'}$$

Our goal

$$\max_{y_1, y_2, y_3} \mathbf{w}^T \phi(x_1, y_1) + w^T \phi(y_1, y_2, y_3) + w^T \phi(x_3, y_1, y_3) + w^T \phi(x_1, x_2, y_2)$$



$$\begin{array}{ll} \max & \sum_{l} z_{1l} s_{1l} + \sum_{l} z_{2l} s_{2l} + \sum_{l,l'} z_{13ll'} s_{13ll'} + \sum_{l,l'} z_{23ll'} s_{23ll'} \\ \text{s.t} & \text{Only valid output allowed} \end{array}$$

Suppose each y_i can be A, B or C

Introduce one decision variable for each part being assigned labels

Each of these decision variables is associated with a score

Not all decisions can exist together.

Eg: z_{13AB} implies z_{1A} and z_{3B}

Our goal

$$\max_{y_1, y_2, y_3} \mathbf{w}^T \phi(x_1, y_1) + w^T \phi(y_1, y_2, y_3) + w^T \phi(x_3, y_1, y_3) + w^T \phi(x_1, x_2, y_2)$$

Writing constraints as linear inequalities

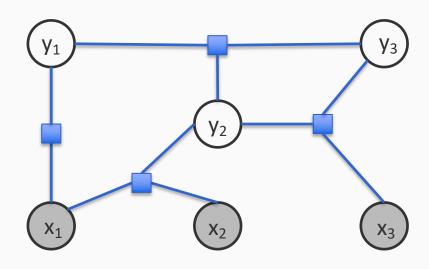
- Exactly one of z_A , z_B , z_C can be true $z_A + z_B + z_C = 1$
- At least m of z_A , z_B , z_C should be true $z_A + z_B + z_C$, m
- At most m of z_A , z_B , z_C should be true $z_A + z_B + z_C \cdot m$
- Implication: z_i) z_i
 - Convert to disjunction: : z_i Ç z_j
 - At least one of "not z_i" or z_i
 - $1 z_i + z_j$, 1 (i.e.) z_i , z_i

Writing constraints as linear inequalities

- Exactly one of z_A , z_B , z_C can be true $z_A + z_B + z_C = 1$
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 - $1 z_i + z_j$, 1 (i.e.) z_i , z_i

Generally: All Boolean formulas can be converted to constraints

Exercise: Convert the toy conditional model below to an ILP by hand



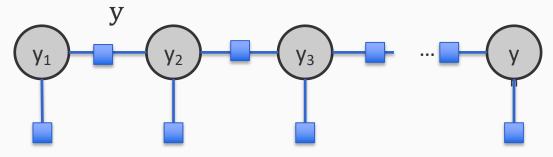
Integer linear programming for inference

- Easy to add additional knowledge
 - Specify them as Boolean formulas
 - Examples
 - "If y₁ is an A, then y₂ or y₃ should be a B or C"
 - "No more than two A's allowed in the output"
- Many inference problems have "standard" mappings to ILPs
 - Sequences, parsing, dependency parsing
- Encoding of the problem makes a difference in solving time
 - The mechanical encoding may not be efficient to solve
- Generally: more complex constraints make solving harder

Exercise 1: Sequence labeling

Goal: Find argmax $w^T \phi(x, y)$

$$\mathbf{y} = (y_1, y_2, \dots, y_n)$$



$$\mathbf{w}^T \phi(\mathbf{x}, \mathbf{y}) = \sum_i \left(\mathbf{w}^T \phi_T(y_i, y_{i+1}) + \mathbf{w}^T \phi_E(\mathbf{x}, y_i) \right)$$

How can this be written as an ILP?

Exercise 2: Alignment

Suppose we have two sequences

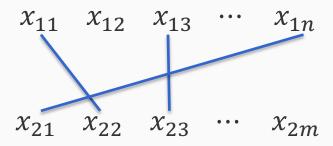
$$x_{11}$$
 x_{12} x_{13} \cdots x_{1n}

$$x_{21}$$
 x_{22} x_{23} \cdots x_{2m}

Each pair x_{1i} , x_{2j} is assigned a score s_{ij} .

Exercise 2: Alignment

Suppose we have two sequences



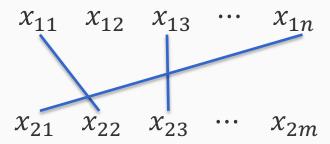
Each pair x_{1i} , x_{2j} is assigned a score s_{ij} .

The goal is to find edges between the two sequences such that the following conditions hold:

- 1. The total score of the selected edges is maximized
- No more than one edge should be connected to any element of the second sequence.

Exercise 2: Alignment

Suppose we have two sequences



Each pair x_{1i} , x_{2j} is assigned a score s_{ij} .

The goal is to find edges between the two sequences such that the following conditions hold:

- 1. The total score of the selected edges is maximized
- No more than one edge should be connected to any element of the second sequence.

How can this be written as an ILP?

ILP for inference: Remarks

- Any combinatorial optimization problem can be written as an ILP
 - Even the "easy"/polynomial ones
 - Given an ILP, checking whether it represents a polynomial problem is intractable in general
- ILPs are a general language for thinking about combinatorial optimization
 - The representation allows us to make general statements about inference
 - Important: Framing/writing down the inference problem is separate from solving it
- Off-the-shelf solvers for ILPs are quite good
 - Gurobi, CPLEX
 - Use an off the shelf solver only if you can't solve your inference problem otherwise

The big picture

- MAP Inference is combinatorial optimization
- Combinatorial optimization problems can be written as 0-1 integer linear programs
 - The conversion is not always trivial
 - Allows injection of "knowledge" into the inference in the form of constraints
- Different ways of solving ILPs
 - Commercial solvers: CPLEX, Gurobi, etc
 - Specialized solvers if you know something about your problem
 - Incremental ILP, Lagrangian relaxation, etc
 - Can relax to linear programs and hope for the best
- Integer linear programs are NP hard in general
 - No free lunch