Data Structures for Efficient Inference and Optimization

in Expressive Continuous Domains

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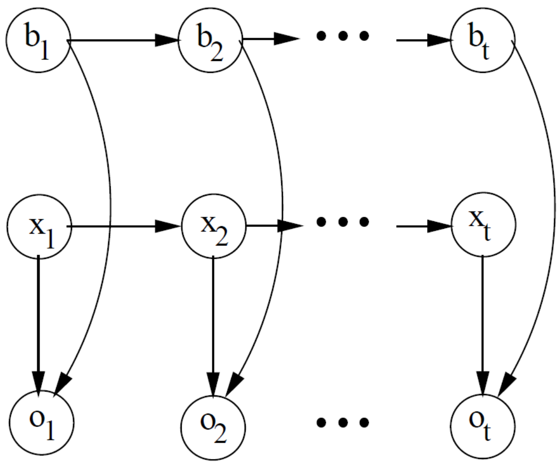
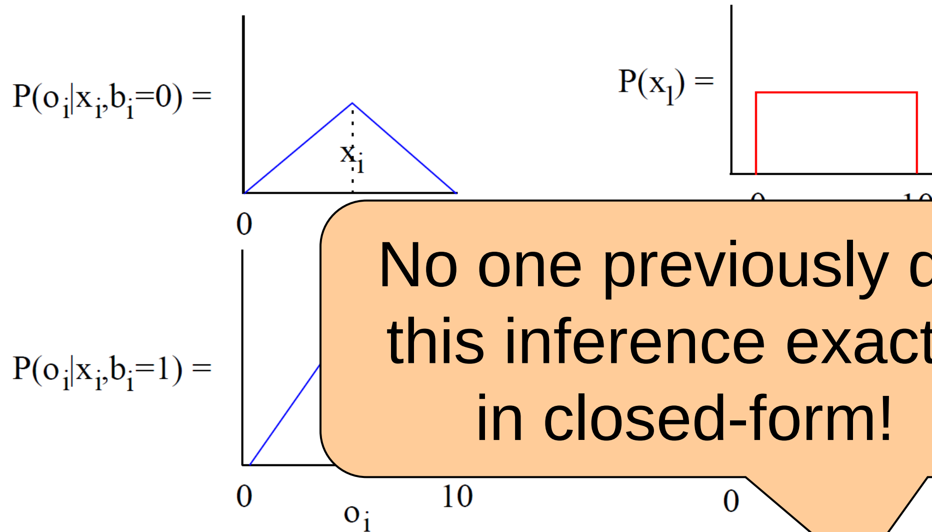
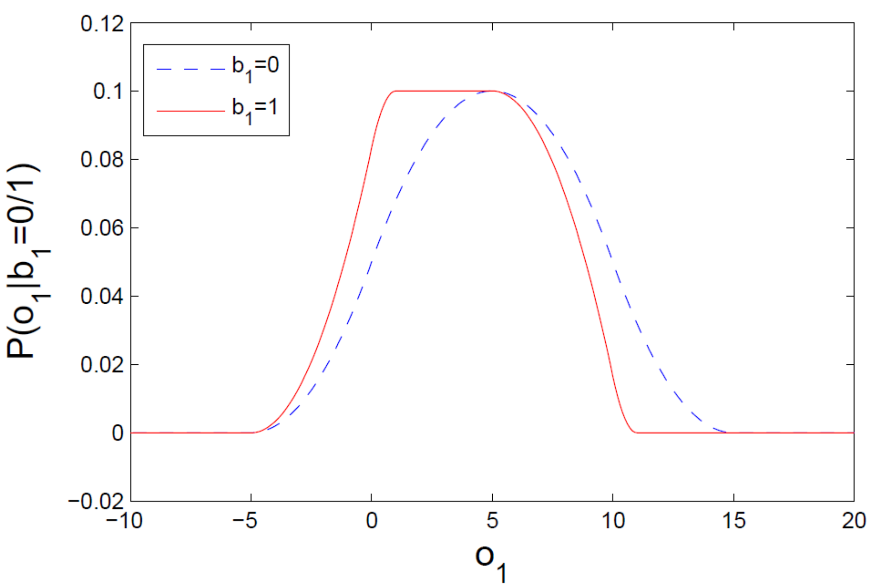
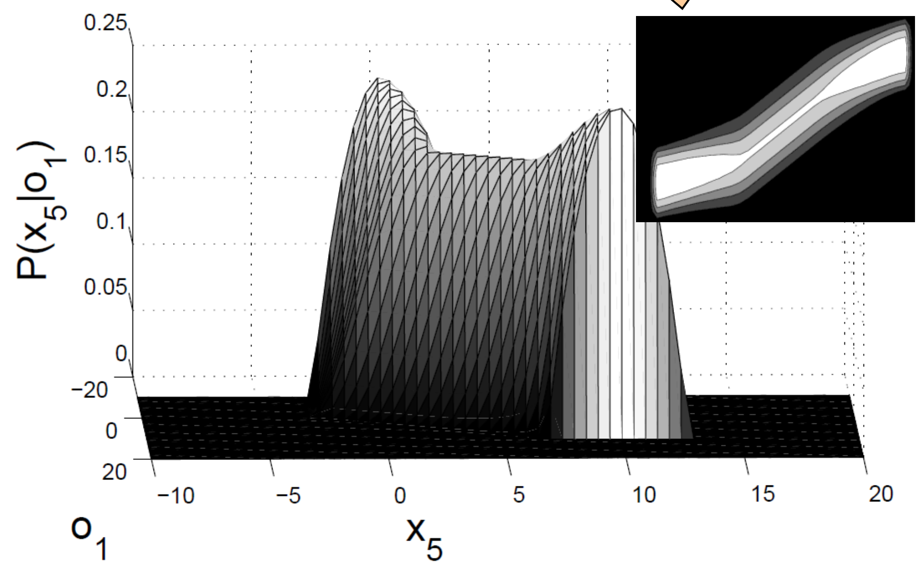
Discrete & Continuous HMMs





No one previously did this inference exactly in closed-form!





Exact Closed-form Continuous Inference

- Fully Gaussian
  - Most inference including conditional
- Fully Uniform
  - 1D, n-D hyperrectangular cases
  - General Uniform
- Piecewise, Asymmetrical, Multimodal
  - Exact (conditional) inference possible in closed-form?

Yes, but not a solution you can write on 1 sheet of paper

What has everyone been missing?

Symbolic representations and operations on piecewise functions

Piecewise Functions (Cases)

$$z = f(x,y) = \begin{cases} (x > 3) \wedge (y \cdot \; x) : & x + y \\ (x \cdot \; 3) \vee (y > x) : & x^2 + xy^3 \end{cases}$$

Partition

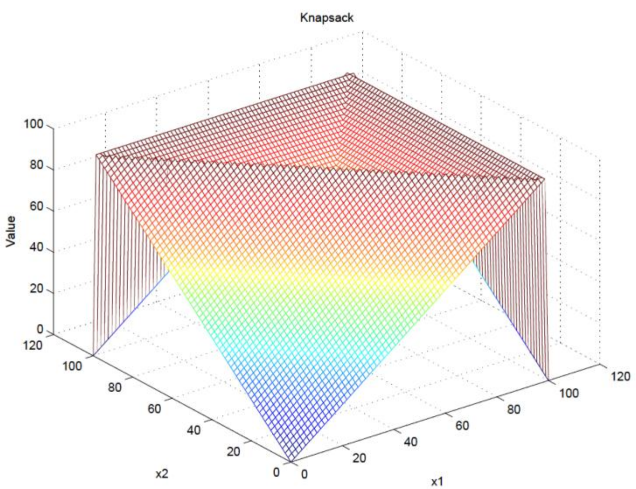
Constraint

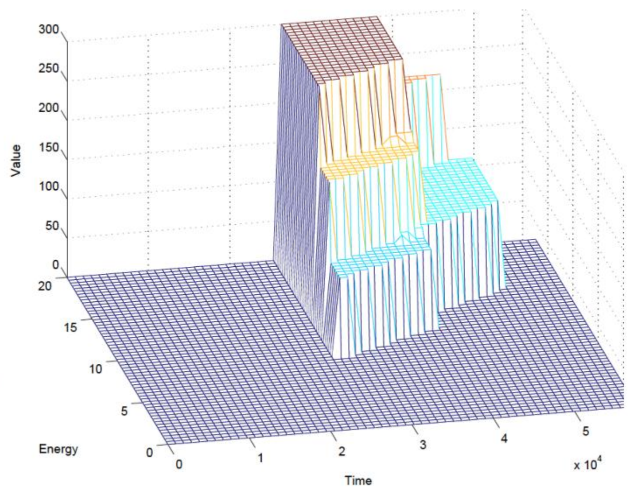
Value

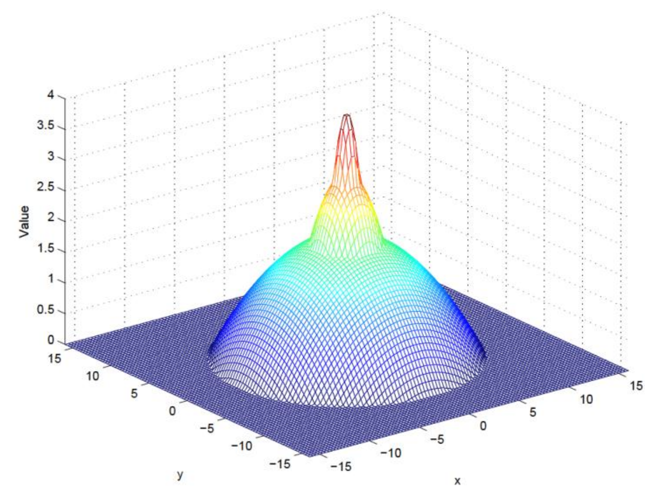
Linear constraints and value

Linear constraints, constant value

Quadratic constraints and value







Formal Problem Statement

- General continuous graphical models represented by piecewise functions (cases)

$$f = \begin{cases} \phi_1 : & f_1 \\ \vdots & \vdots \\ \phi_k : & f_k \end{cases}$$

- Exact closed-form solution inferred via the following piecewise calculus:
  - $f_1 \oplus f_2$, $f_1 \otimes f_2$
  - $\max(f_1, f_2)$, $\min(f_1, f_2)$
  - $\int_x f(x)$
  - $\max_x f(x)$, $\min_x f(x)$

Question: how do we perform these operations in closed-form?

Polynomial Case Operations: ⊕, ⊗

$$\begin{cases} \phi_1 : & f_1 \\ \phi_2 : & f_2 \end{cases} \oplus \begin{cases} \psi_1 : & g_1 \\ \psi_2 : & g_2 \end{cases} = \qquad ?$$

Polynomial Case Operations: ⊕, ⊗

$$\begin{cases} \phi_1 : & f_1 \\ \phi_2 : & f_2 \end{cases} \oplus \begin{cases} \psi_1 : & g_1 \\ \psi_2 : & g_2 \end{cases} = \begin{cases} \phi_1 \wedge \psi_1 : & f_1 + g_1 \\ \phi_1 \wedge \psi_2 : & f_1 + g_2 \\ \phi_2 \wedge \psi_1 : & f_2 + g_1 \\ \phi_2 \wedge \psi_2 : & f_2 + g_2 \end{cases}$$

- Similarly for ⊗
  - Polynomials closed under +, *
- What about max?
  - Max of polynomials is not a polynomial ☹

Polynomial Case Operations: max

$$\max\left(\begin{cases} \phi_1 : & f_1 \\ \phi_2 : & f_2 \end{cases}, \begin{cases} \psi_1 : & g_1 \\ \psi_2 : & g_2 \end{cases} \right) =$$

?

Polynomial Case Operations: max

$$\max\left(\begin{cases}\phi_1 : & f_1 \\ \phi_2 : & f_2\end{cases}, \begin{cases}\psi_1 : & g_1 \\ \psi_2 : & g_2\end{cases}\right) = \begin{cases}\phi_1 \wedge \psi_1 \wedge f_1 > g_1 : & f_1 \\ \phi_1 \wedge \psi_1 \wedge f_1 \cdot g_1 : & g_1 \\ \phi_1 \wedge \psi_2 \wedge f_1 > g_2 : & f_1 \\ \phi_1 \wedge \psi_2 \wedge f_1 \cdot g_2 : & g_2 \\ \phi_2 \wedge \psi_1 \wedge f_2 > g_1 : & f_2 \\ \phi_2 \wedge \psi_1 \wedge f_2 \cdot g_1 : & g_1 \\ \phi_2 \wedge \psi_2 \wedge f_2 > g_2 : & f_2 \\ \phi_2 \wedge \psi_2 \wedge f_2 \cdot g_2 : & g_2\end{cases}$$

- Still a piecewise polynomial!

Size blowup?
We'll get to that…

Integration: $\int_x$

- $\int_x$ closed for polynomials
  - But how to compute for case?

$$\int_x \begin{cases} \phi_1 : & f_1 \\ \vdots & \vdots \\ \phi_k : & f_k \end{cases} dx = \int_x \sum_{i=1}^{k} [\phi_i] \cdot f_i \, dx$$

$$= \sum_i \int_x [\phi_i] \cdot f_i \, dx$$

  - Just integrate case partitions, ⊕ results!

Partition Integral

1. Determine integration bounds

$$\int_x [\phi_1] \cdot f_1 \, dx$$

$$\phi_1 := [x > -1] \wedge [x > y - 1] \wedge [x \cdot \quad z] \wedge [x \cdot \quad y + 1] \wedge [y > 0]$$

$$f_1 := x^2 - xy$$

$$LB := \begin{cases} y - 1 > -1 : & y - 1 \\ y - 1 \cdot \quad -1 : & -1 \end{cases} \qquad UB := \begin{cases} z < y + 1 : & z \\ z \geq y + 1 : & y + 1 \end{cases}$$

$$[\phi_{cons}] \int_{x = LB}^{UB} f_1 \, dx$$

UB and LB are symbolic!

How to evaluate?

What constraints here?

- independent of x
- pairwise UB > LB

Definite Integral Evaluation

- How to evaluate integral bounds?

$$\int_{x=LB}^{UB} x^2 - xy \; = \; \frac{1}{3}x^3 - \frac{1}{2}x^2 y \Big|_{LB}^{UB}$$

$$LB := \begin{cases} y - 1 > -1 : & y - 1 \\ y - 1 \cdot \; -1 : & -1 \end{cases} \qquad UB := \begin{cases} z < y + 1 : & z \\ z \geq y + 1 : & y + 1 \end{cases}$$

- Can do polynomial operations on cases!

$$f_1 \Big|_{LB}^{UB} = \left[\frac{1}{3} UB \quad UB \quad UB \ominus \frac{1}{2} UB \quad UB \quad (y) \right]$$

$$\ominus \left[\frac{1}{3} LB \quad LB \quad LB \ominus \frac{1}{2} LB \quad LB \quad (y) \right]$$

Symbolically, exactly evaluated!

Exact Graphical Model Inference!

(directed and undirected)

- Can do general probabilistic inference

$$p(x_2|x_1) = \frac{\int_{x_3} \cdots \int_{x_n} \bigotimes_{i=1}^{k} case_i \; dx_n \cdots dx_3}{\int_{x_2} \cdots \int_{x_n} \bigotimes_{i=1}^{k} case_i \; dx_n \cdots dx_2}$$

- Or an exact expectation of *any* polynomial

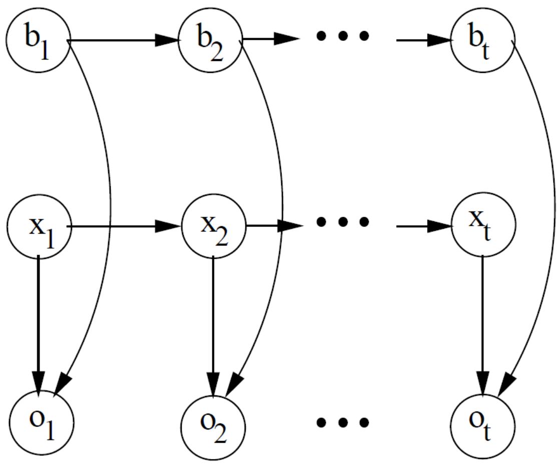
$$\mathbb{E}_{\mathbf{x} \sim p(\mathbf{x}|\mathbf{o})}[poly(\mathbf{x})|\mathbf{o}] = \int_{\mathbf{x}} p(\mathbf{x}|\mathbf{o}) poly(\mathbf{x}) d\mathbf{x}$$

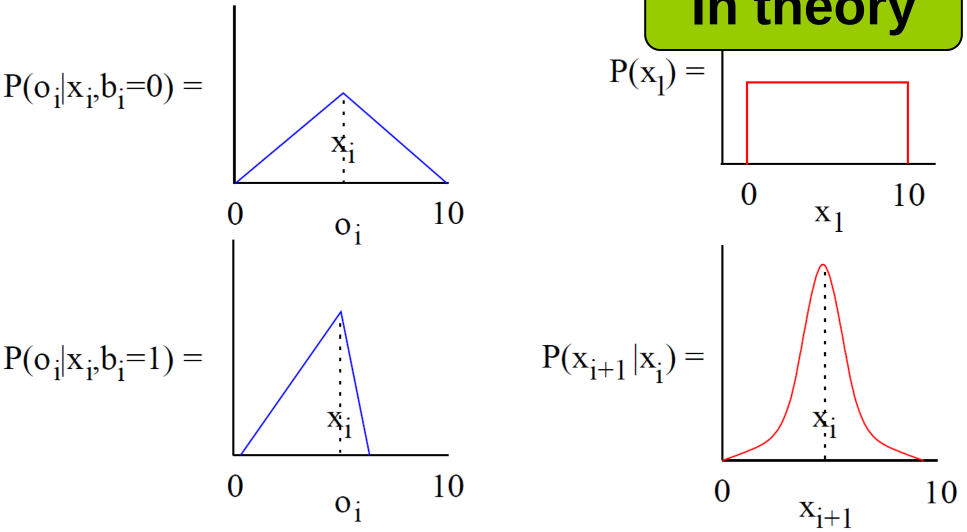
  – *poly*: mean, variance, skew, curtosis, …, x^2+y^2+xy

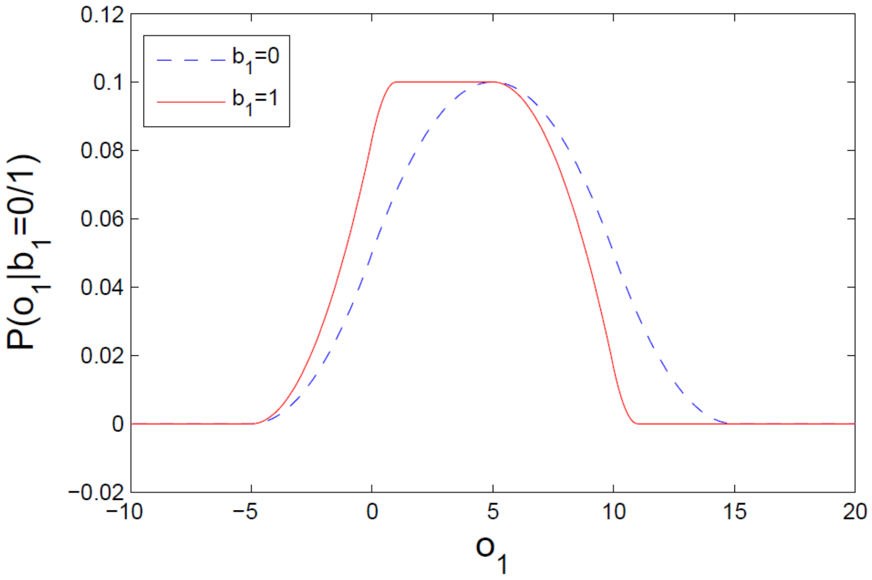
All computed by
Symbolic Variable Elimination (SVE)

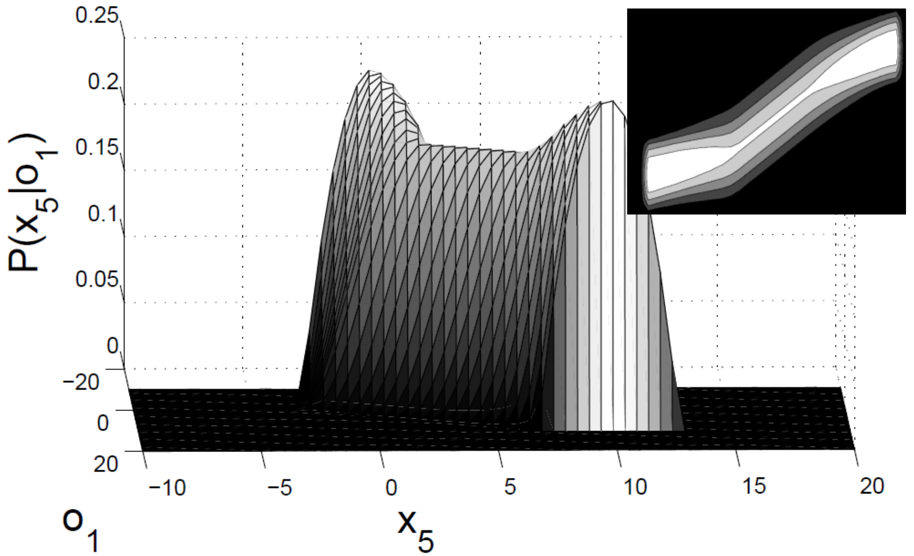
Voila: Closed-form Exact Inference via SVE!

In theory









An Expressive Conjugate Prior for Bayesian Inference

- General Bayesian Inference

$$p(\vec{\theta}|D_{n+1}) \propto p(d_{n+1}|\vec{\theta})p(\vec{\theta}|D_n)$$

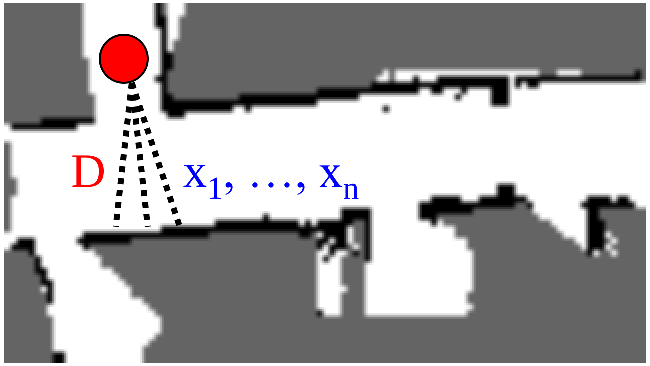
case

case

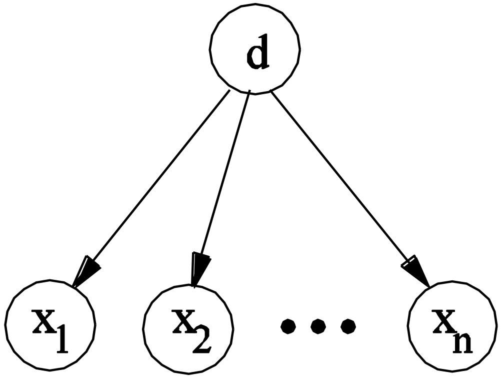
case

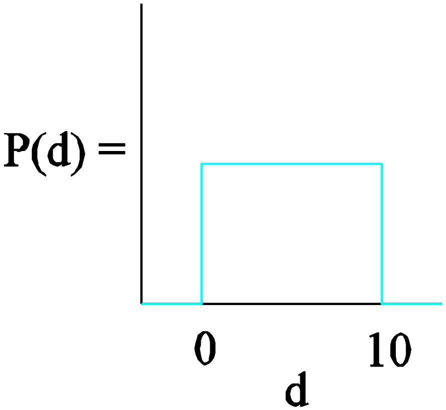
- Prior & likelihood for computational convenience?
  - No, choose as appropriate for your problem!

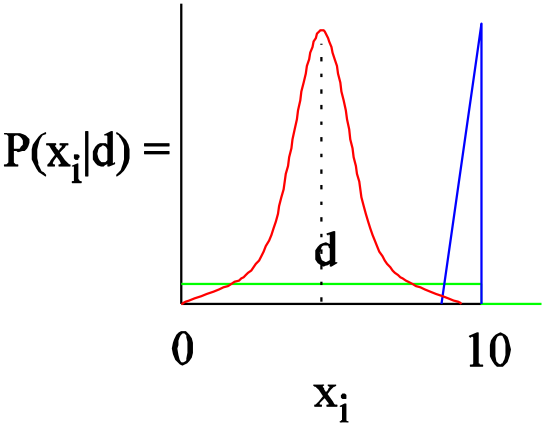
Bayesian Robotics



- D: true distance to wall
- $x_1, \ldots, x_n$: measurements
- want: $E[D \mid x_1, \ldots, x_n]$

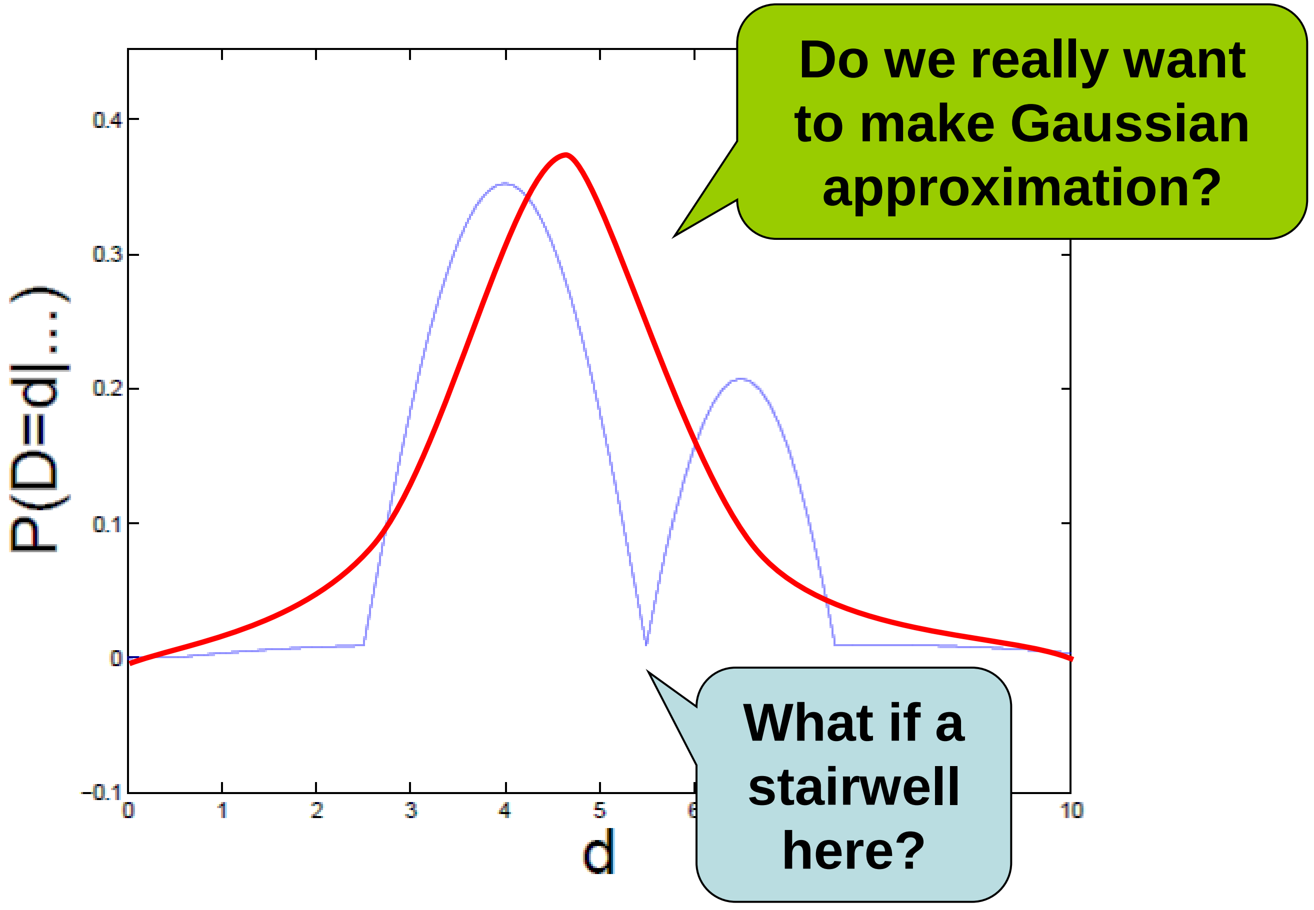






Bayesian Robotics: Results

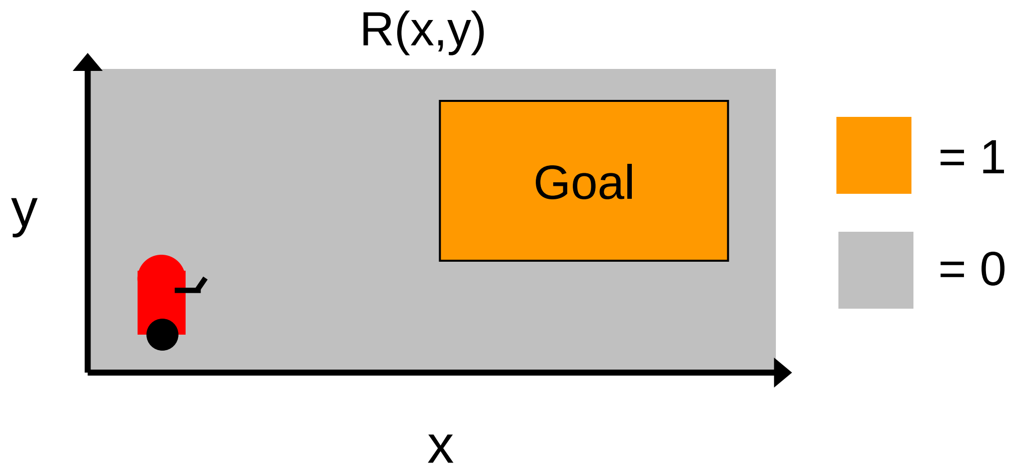
- Example posterior given measurements {3,5,8}:



Symbolic Sequential Decision Optimization?

Continuous State MDPs

- 2-D Navigation
- State: (x,y) $\in \mathbb{R}^2$
- Actions:
  - move-x-2
    - x' = x + 2
    - y' = y
  - move-y-2
    - x' = x
    - y' = y + 2
- Reward:
  - R(x,y) = I[(x > 5) ^ (x < 10) ^ (y > 2) ^ (y < 5)]

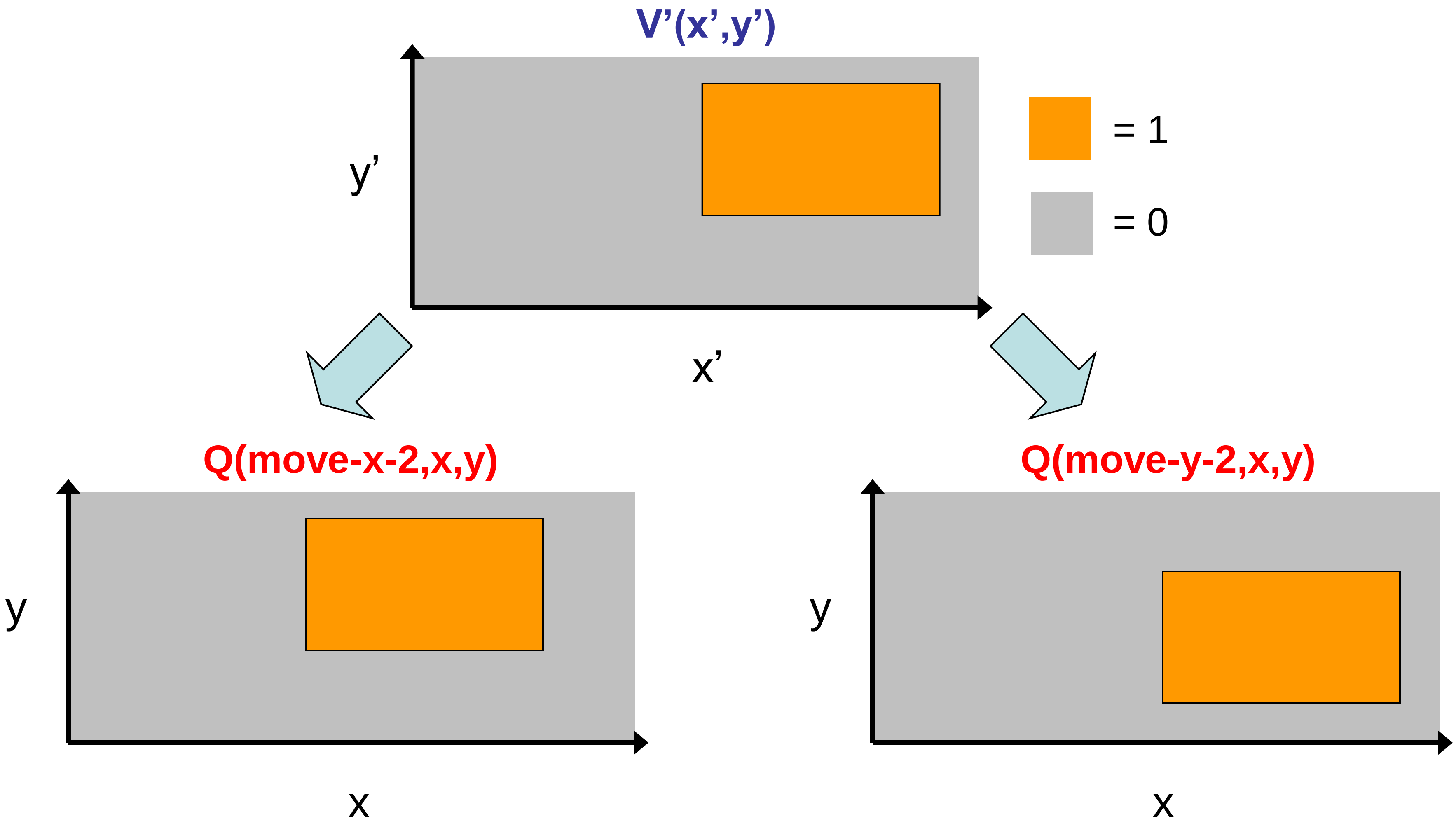


Feng *et al* (UAI-04) Assumptions:

1. Continuous transitions are deterministic and linear
2. Discrete transitions can be stochastic
3. Reward is piecewise rectilinear convex

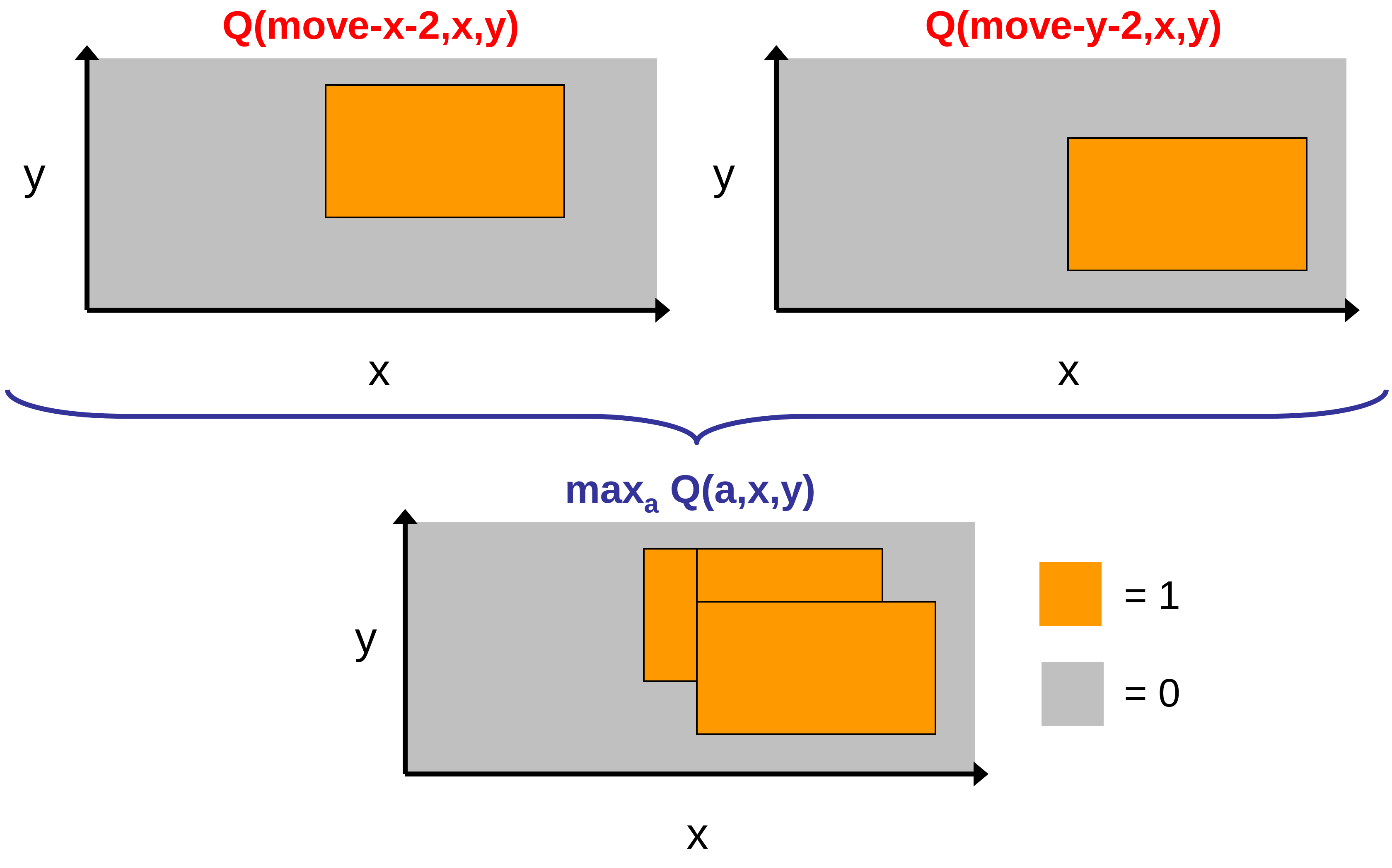
Exact Solutions to DC-MDPs: Regression

- Continuous regression is just translation of “pieces”



Exact Solutions to DC-MDPs: Maximization

- Q-value maximization yields piecewise rectilinear solution



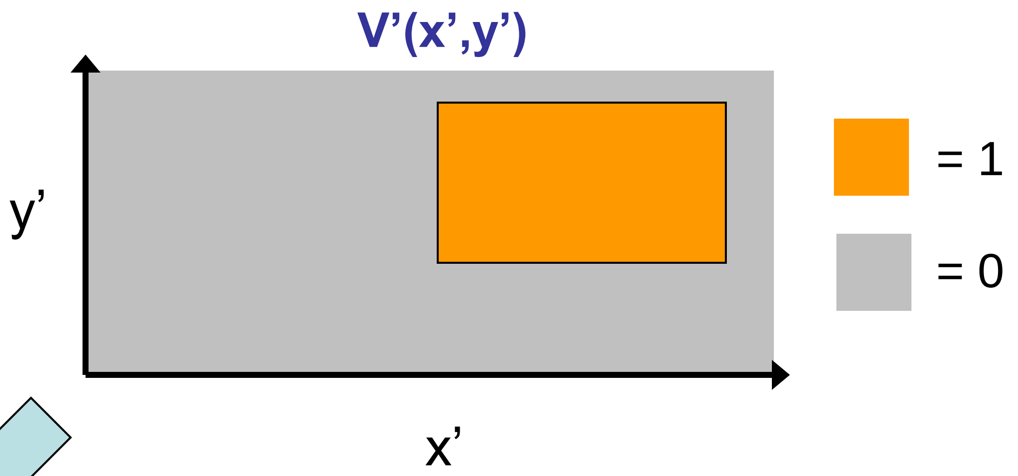
Previous Work Limitations I

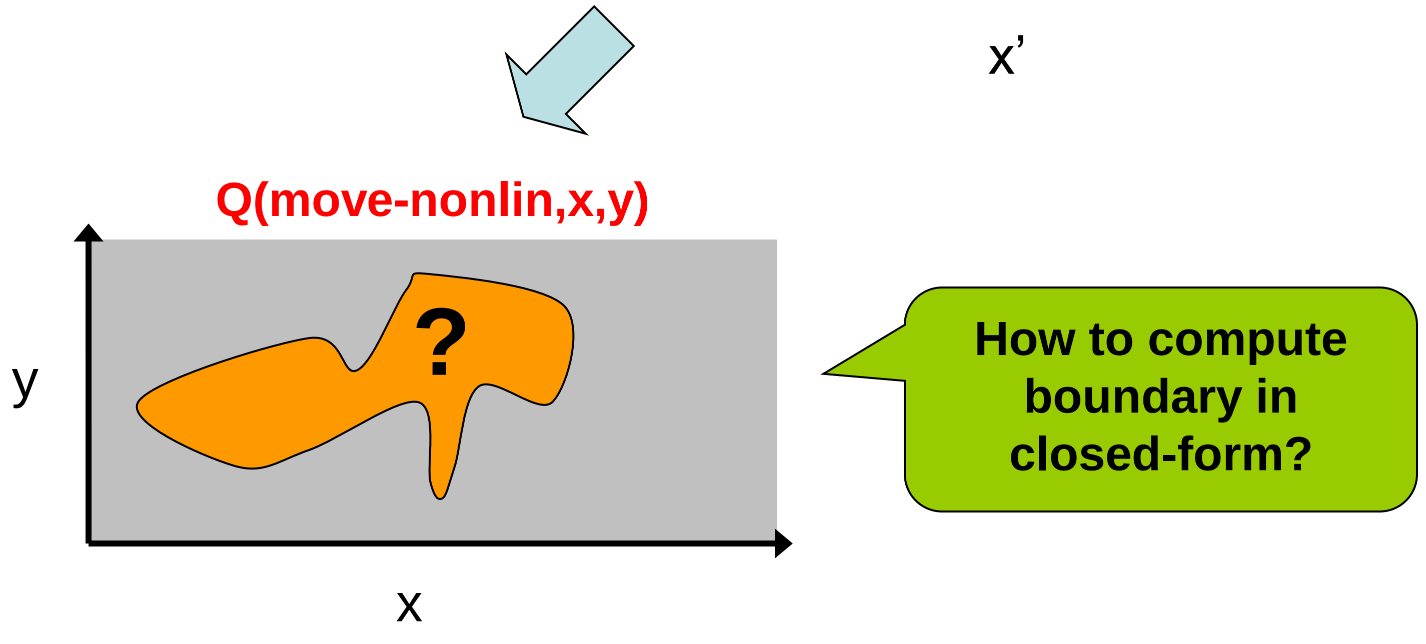
- Exact regression when transitions nonlinear?

Action move-nonlin:

– $x' = x^3y + y^2$

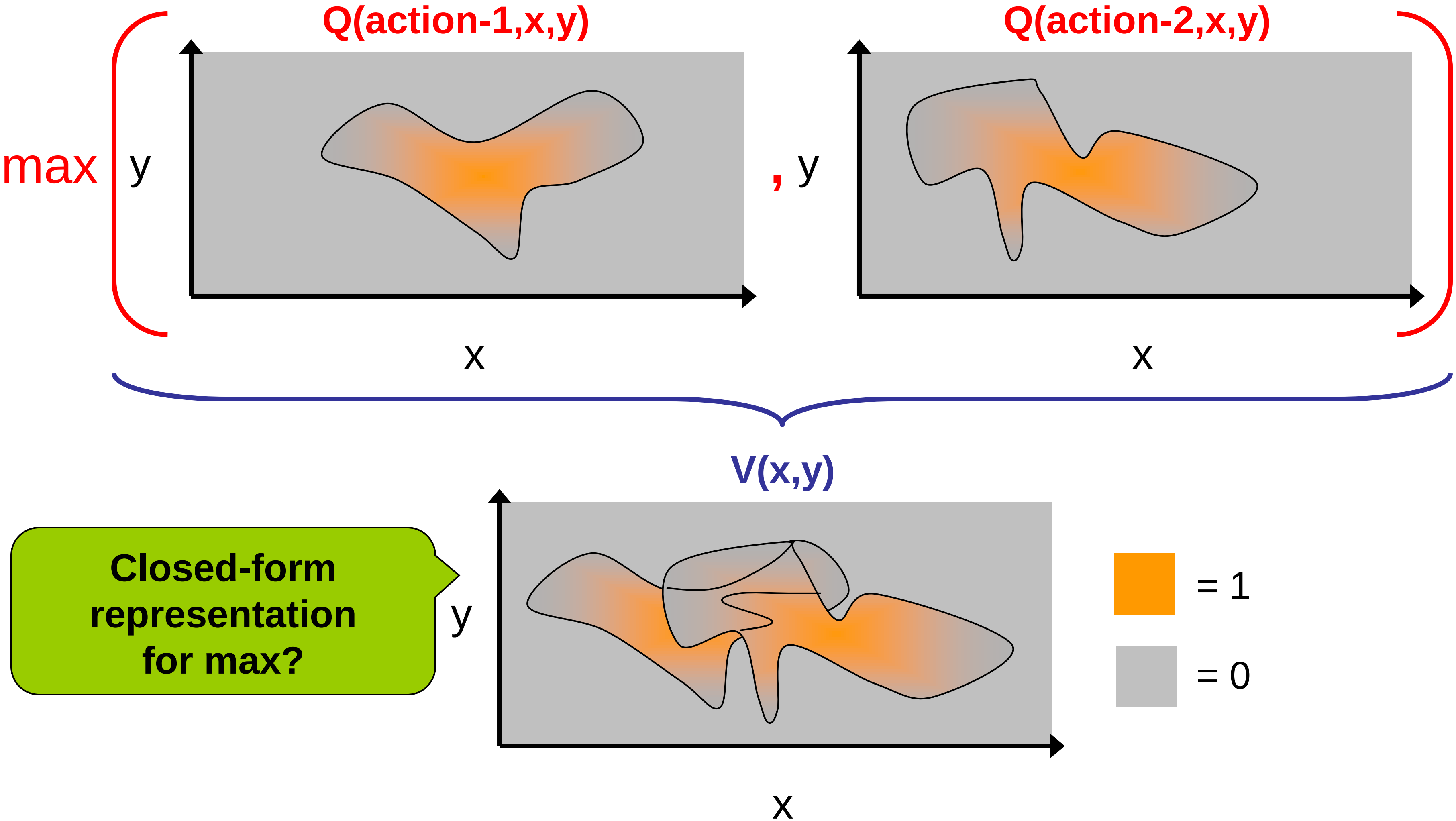
– $y' = y * \log(x^2y)$





Previous Work Limitations II

- max(.,.) when reward/value arbitrary piecewise?



Continuous Actions?

If we can solve this, can solve **multivariate inventory control** – closed-form policy unknown for 50+ years!

Continuous Actions

- Inventory control
  - Reorder based on stock, future demand
  - Action: $a(\vec{\Delta});\ \vec{\Delta} \in \mathbb{R}^{|a|}$

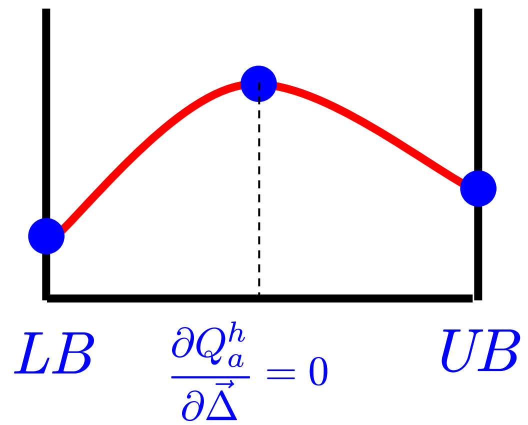
- Need $\max_{\Delta}$ in Bellman backup

$$V_{h+1} = \max_{a \in A} \max_{\vec{\Delta}} Q_a^{h+1}(\vec{\Delta})$$

- $\max_x$ case(x) similar to $\int_x$ case(x)
  - Track maximizing Δ substitutions to recover π

Max-out Case Operation

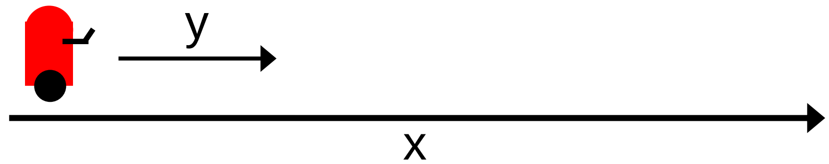
- Like $\int_x$ case(x), reduce to single partition max
  - In a *single* case partition …*max* w.r.t. critical points
    - LB, UB
    - Derivative is zero (Der0)
    - max(case(x/LB),
      case(x/UB),
      case(x/Der0))

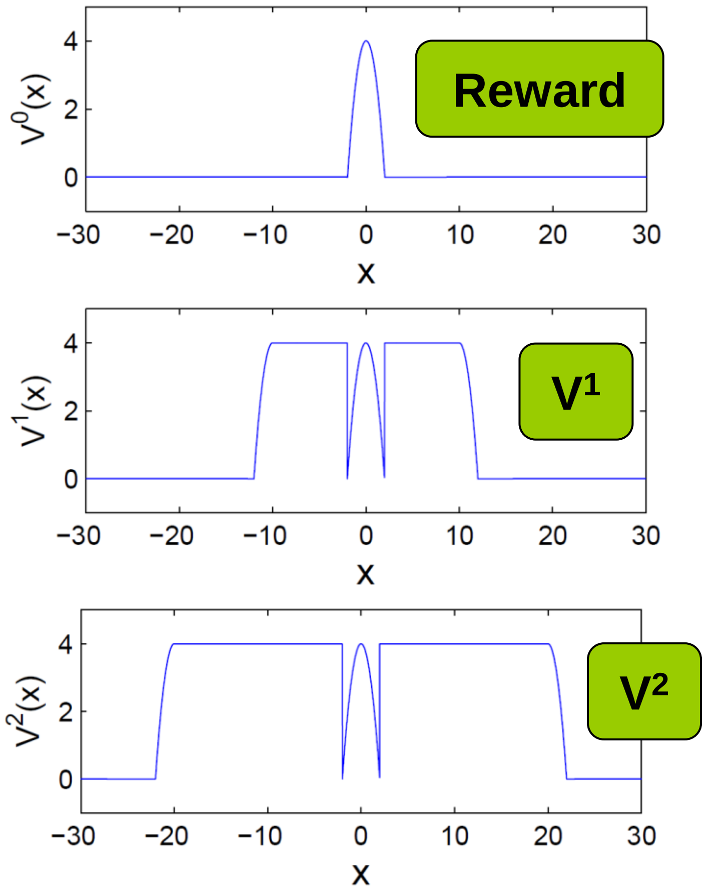


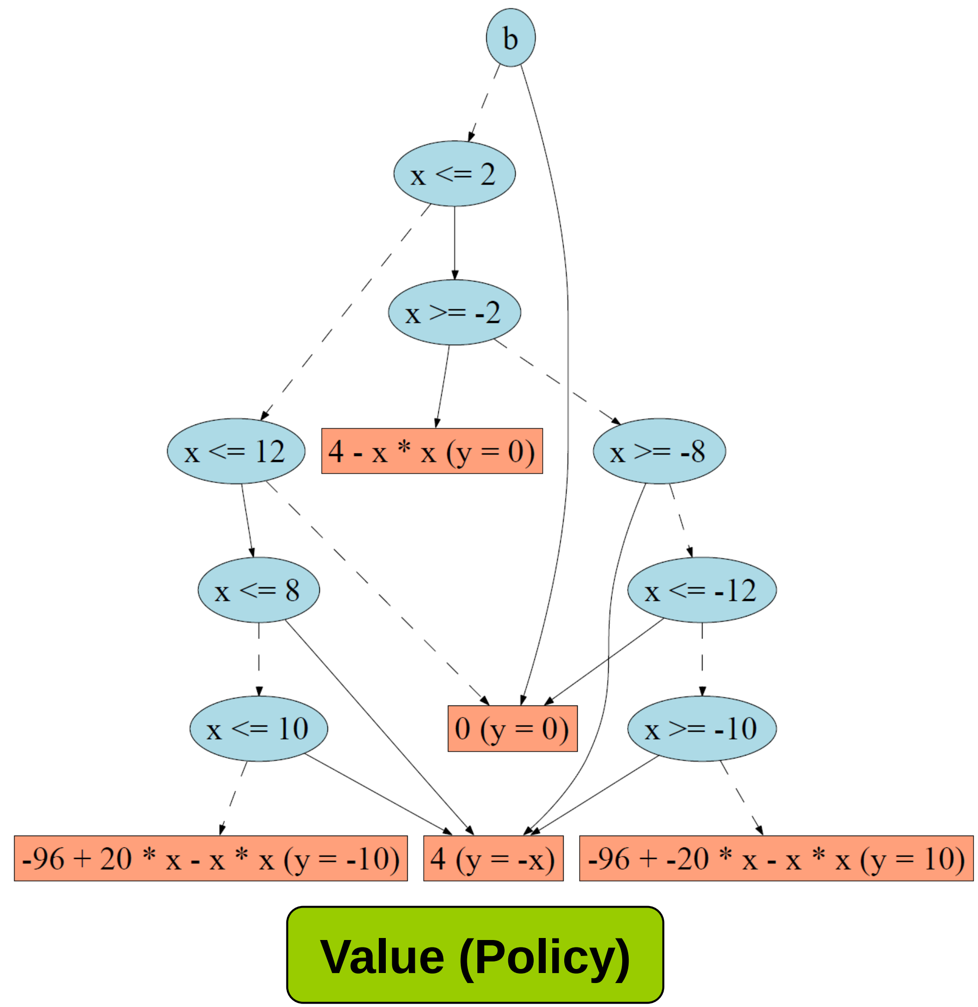
See UAI 2011, AAAI 2012 papers for more details

  - Can even track substitutions through max to recover function of maximizing assignments!

Illustrative Value and Policy







Sequential Control Summary

- Continuous state, action, observation (PO)MDPs
  - Discrete action MDPs **UAI-11**
  - Continuous action MDPs (incl. exact policy) **AAAI-12b**
  - Continuous observation POMDPs **NIPS-12**
  - Extensions to general continuous noise **In progress**

Symbolic Constrained Optimization

$\max_x$ case(x) = Constrained Optimization!

- Conditional constraints
  - E.g., if $(x > y)$ then $(y < z)$
  - 0-1 MILP, MIQP equivalent

- Factored / sparse constraints
  - Constraints may be sparse!

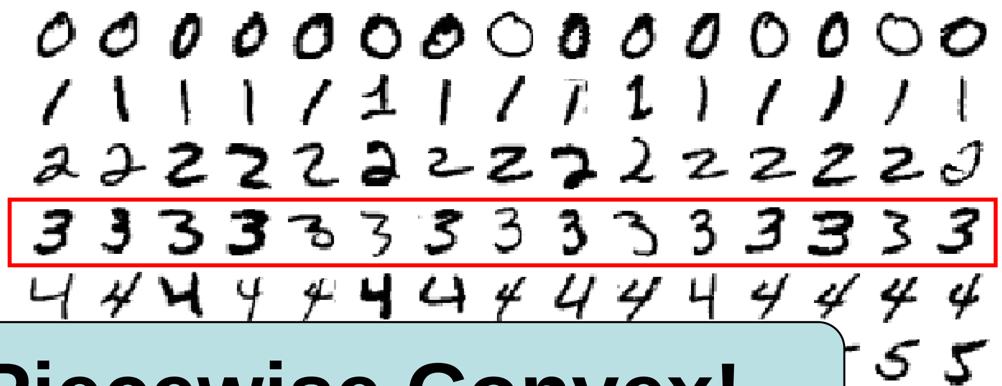
    $x_1 > x_2, \quad x_2 > x_3, \quad \ldots, \quad x_{n-1} > x_n$
  - Dynamic programming for continuous optimization!

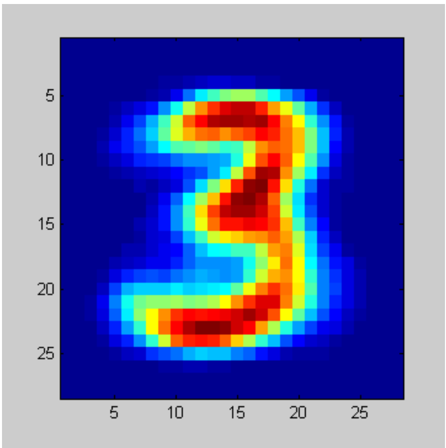
- Parameterized optimization
  - $f(y) = \max_x f(x,y)$
  - Maximum value, substitution as a **function of y**

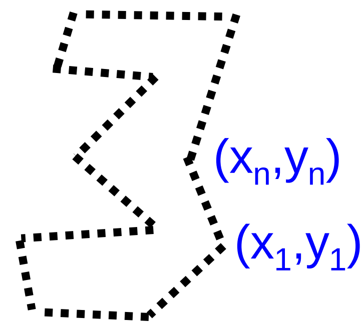
Symbolic Machine Learning

Geometric Models: Piecewise Regression

- How to learn geometric models of objects?





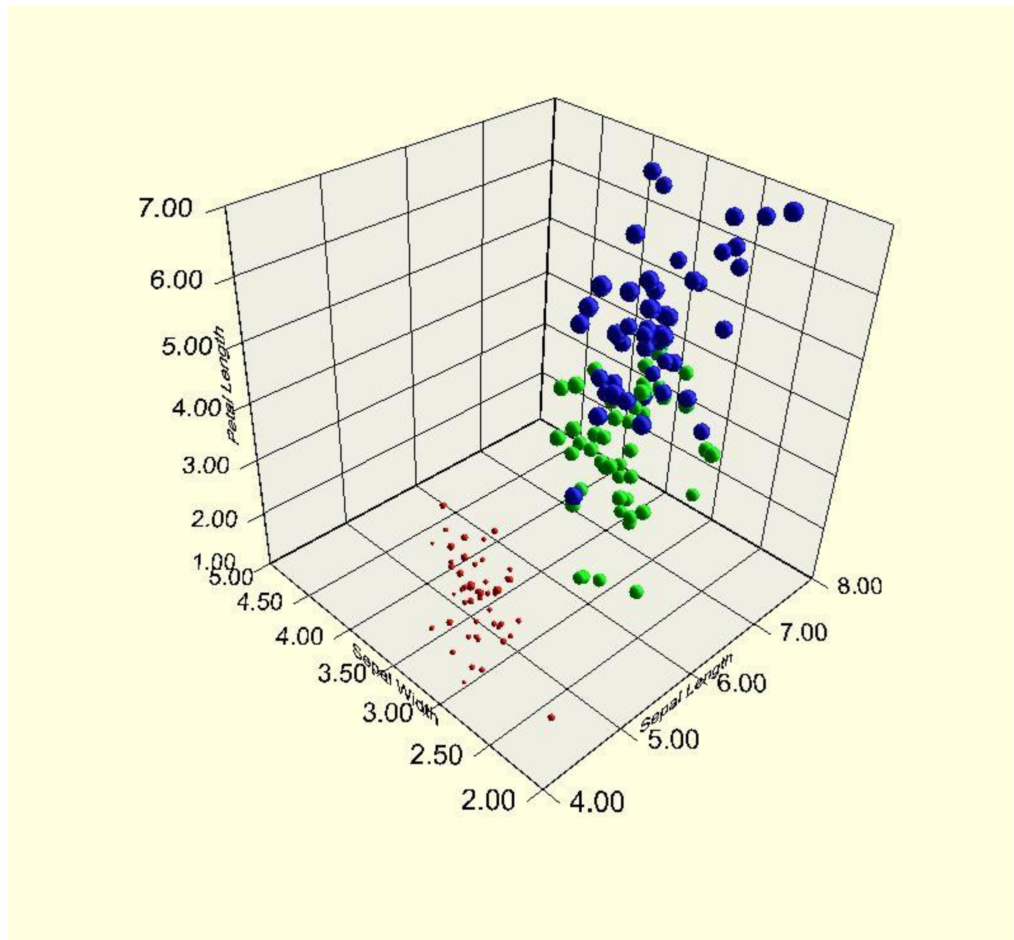


Piecewise Convex!

$$\arg\min_{x_1,y_1,\ldots,x_n,y_n} \sum_{(x,y)\to z^* \in Images} \left| z^* - \begin{cases} x \geq x_1 \wedge y \geq y_1 \wedge \cdots : & 1 \\ x \cdot \;\; x_1 \wedge y \cdot \;\; y_1 \wedge \cdots : & 0 \end{cases} \right|$$

Optimal Clustering?

- Use min to make any point “snap to” nearest center
  - Minimize sum of min distances
- Piecewise convex!
- No latent variables



What has everyone been missing?

Symbolic algebra / calculus?

No, they weren't Computer Scientists.

"case" representation blows up… need a data structure: XADD.

BDD / ADDs

Quick Introduction

Function Representation (Tables)

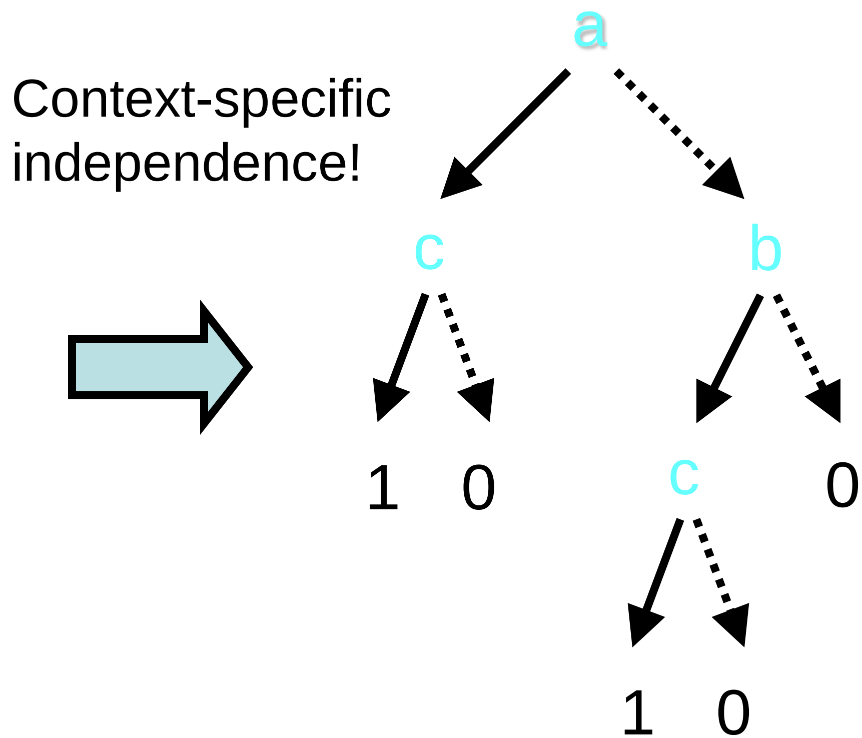
- How to represent functions: $B^n \rightarrow R$?
- How about a fully enumerated table…
- …OK, but can we be more compact?

a	b	c	F(a,b,c)
0	0	0	0.00
0	0	1	0.00
0	1	0	0.00
0	1	1	1.00
1	0	0	0.00
1	0	1	1.00
1	1	0	0.00
1	1	1	1.00

Function Representation (Trees)

- How about a tree? Sure, can simplify.

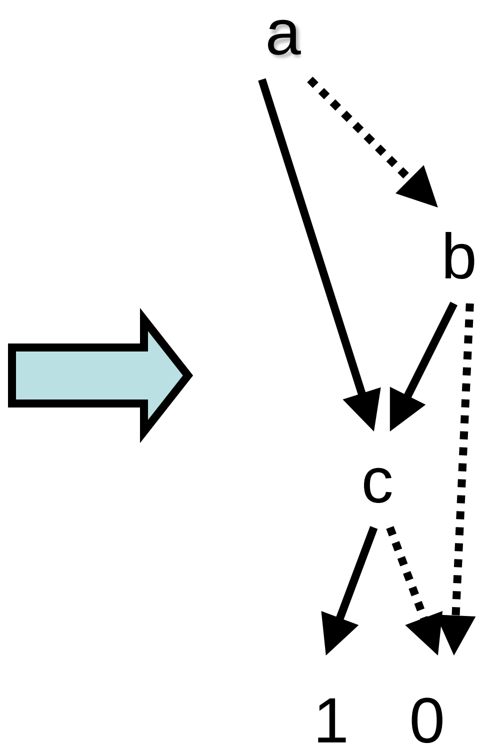
a	b	c	F(a,b,c)
0	0	0	0.00
0	0	1	0.00
0	1	0	0.00
0	1	1	1.00
1	0	0	0.00
1	0	1	1.00
1	1	0	0.00
1	1	1	1.00



Function Representation (ADDs)

- Why not a directed acyclic graph (DAG)?

a	b	c	F(a,b,c)
0	0	0	0.00
0	0	1	0.00
0	1	0	0.00
0	1	1	1.00
1	0	0	0.00
1	0	1	1.00
1	1	0	0.00
1	1	1	1.00

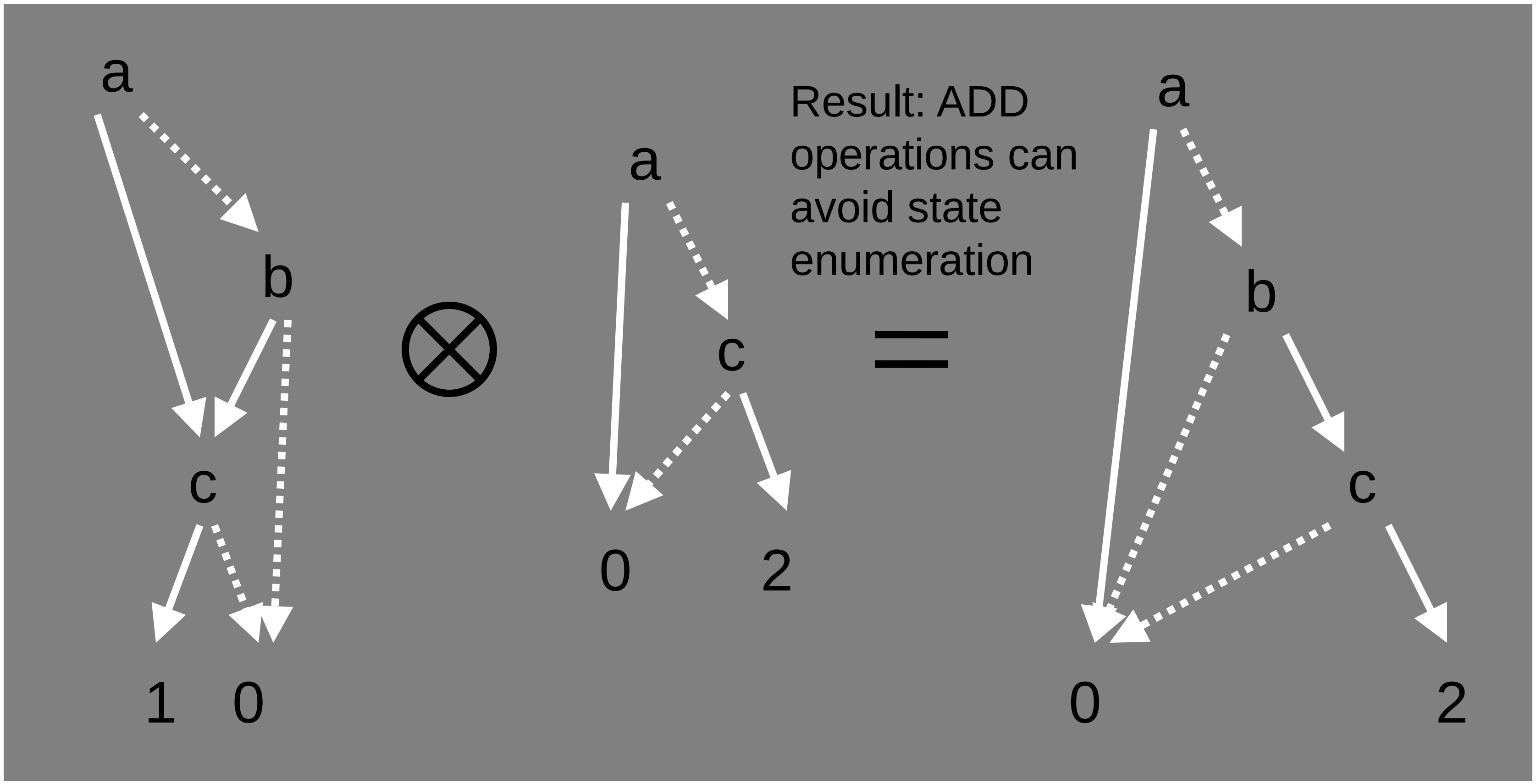


Algebraic Decision Diagram (ADD)

Think of BDDs as {0,1} subset of ADD range

Binary Operations (ADDs)

- Why do we order variable tests?
- Enables us to do efficient binary operations…



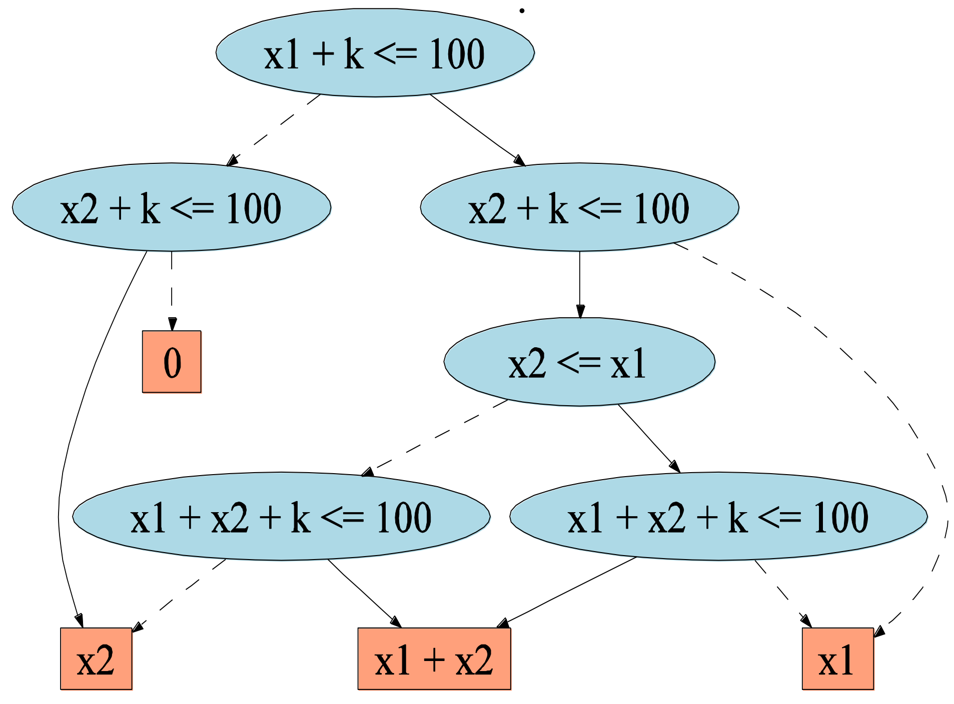
Case $\rightarrow$ XADD

XADD = continuous variable e**x**tension
of **a**lgebraic **d**ecision **d**iagram

- ➔ compact, minimal case representation
- ➔ efficient case operations

Case → XADD

$$V = \begin{cases} x_1 + k > 100 \wedge x_2 + k > 100 : & 0 \\ x_1 + k > 100 \wedge x_2 + k \leq 100 : & x_2 \\ x_1 + k \leq 100 \wedge x_2 + k > 100 : & x_1 \\ x_1 + x_2 + k > 100 \wedge x_1 + k \leq 100 \wedge x_2 + k \leq 100 \wedge x_2 > x_1 : & x_2 \\ x_1 + x_2 + k > 100 \wedge x_1 + k \leq 100 \wedge x_2 + k \leq 100 \wedge x_2 \leq x_1 : & x_1 \\ x_1 + x_2 + k \leq 100 : & x_1 + x_2 \\ \vdots & \vdots \end{cases}$$

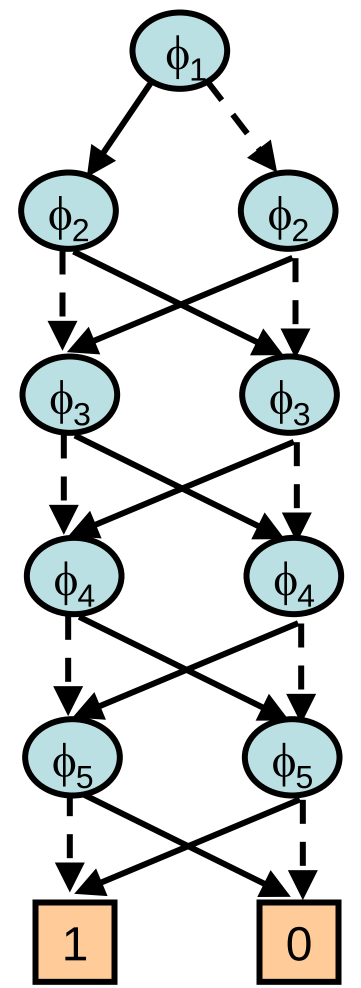


*With non-trivial extensions over ADD, can reduce to a minimal canonical form!

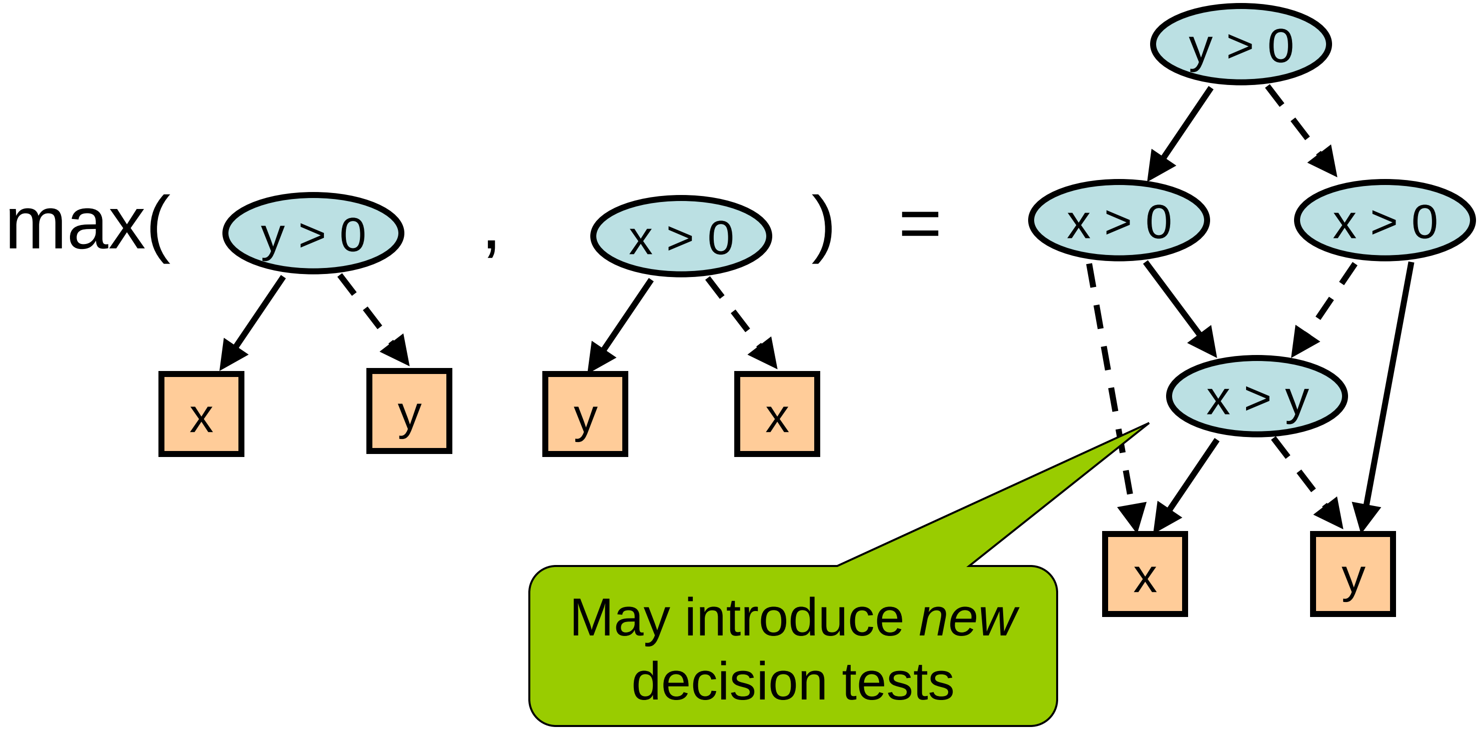
Compactness of (X)ADDs

- Linear in number of decisions ϕ_i

- Case version has exponential number of partitions!



XADD Maximization



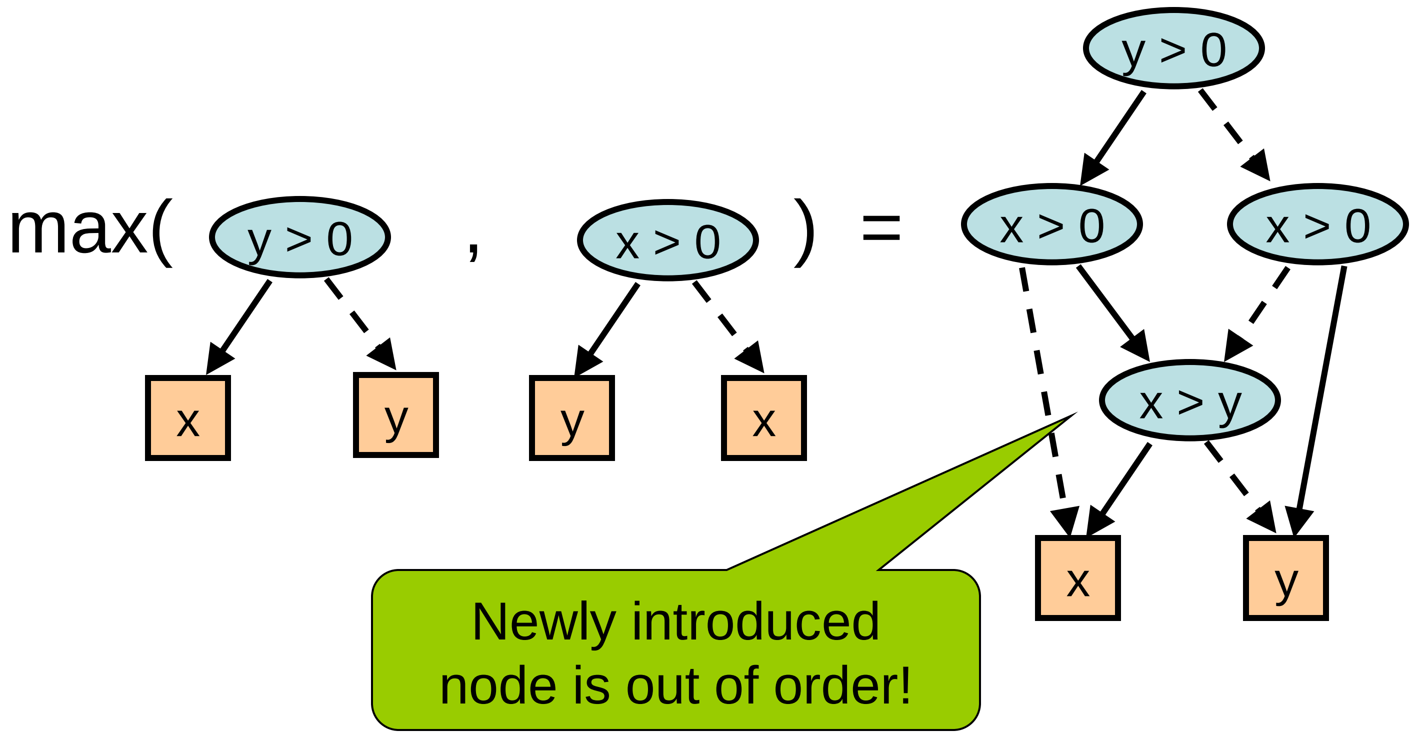
Operations exploit structure: O(|f||g|)

Maintaining XADD Orderings

- Max may get decisions out of order

Decision ordering (root→leaf)

- x > y
- y > 0
- x > 0

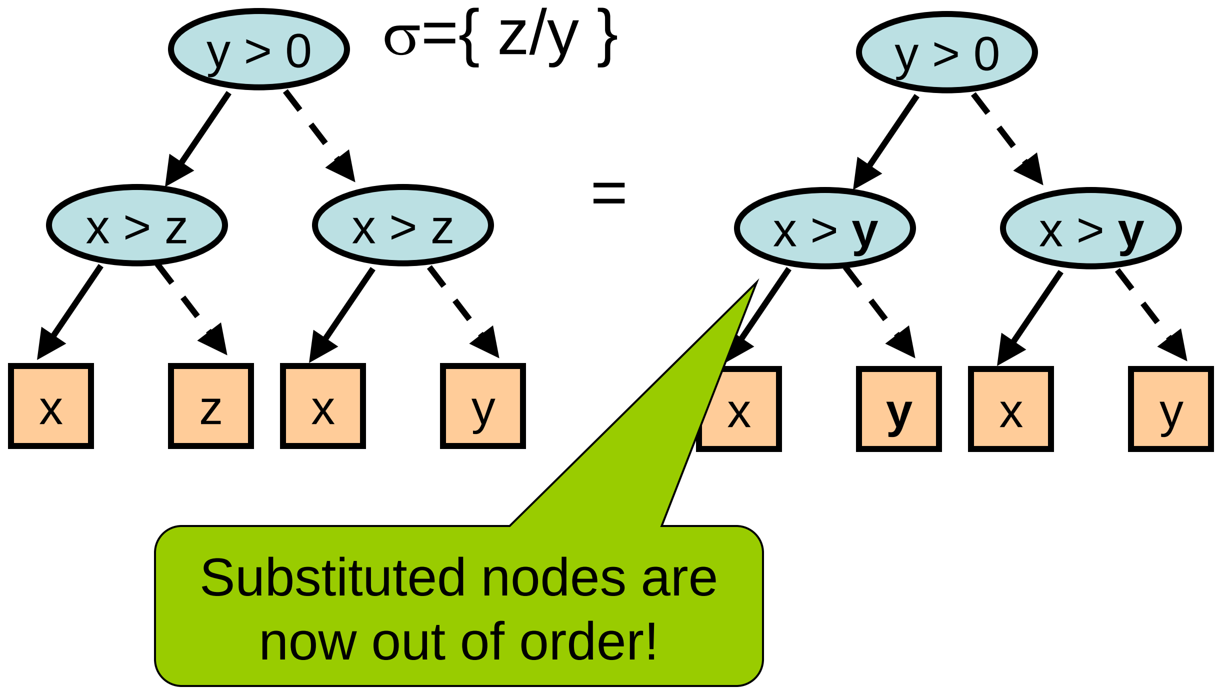


Maintaining XADD Orderings

- Substitution may get decisions out of order

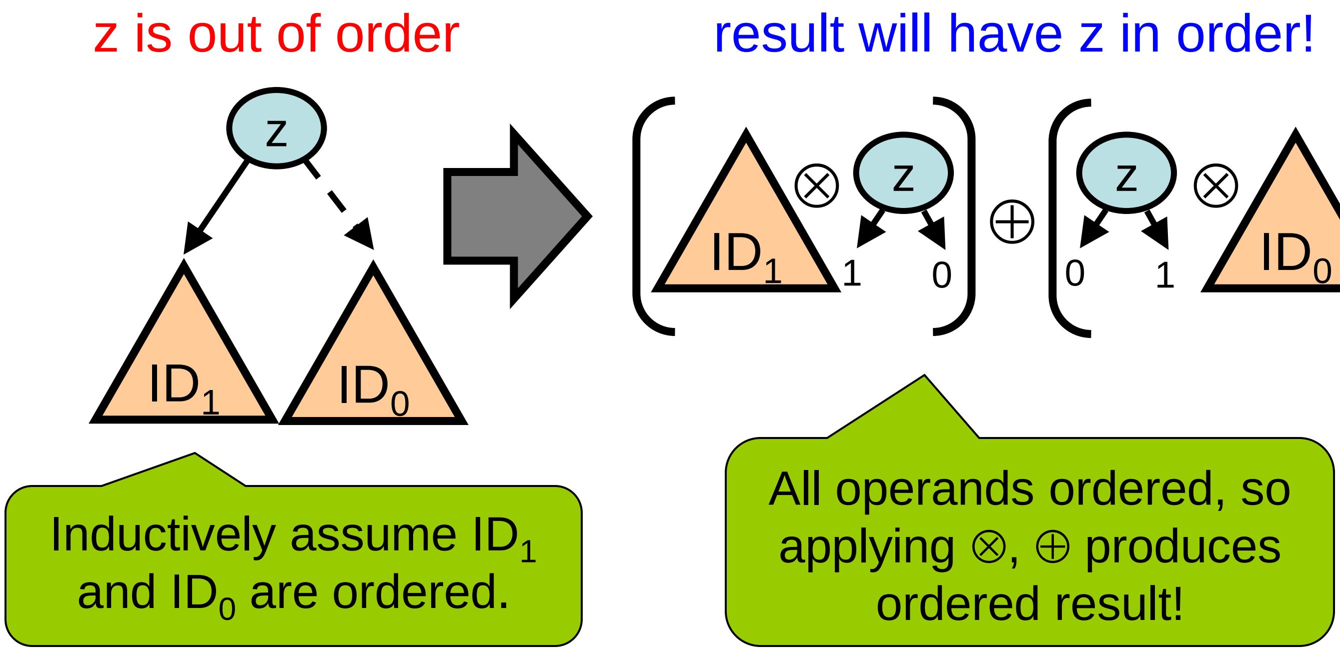
Decision ordering (root→leaf):

- x > y
- y > 0
- x > z

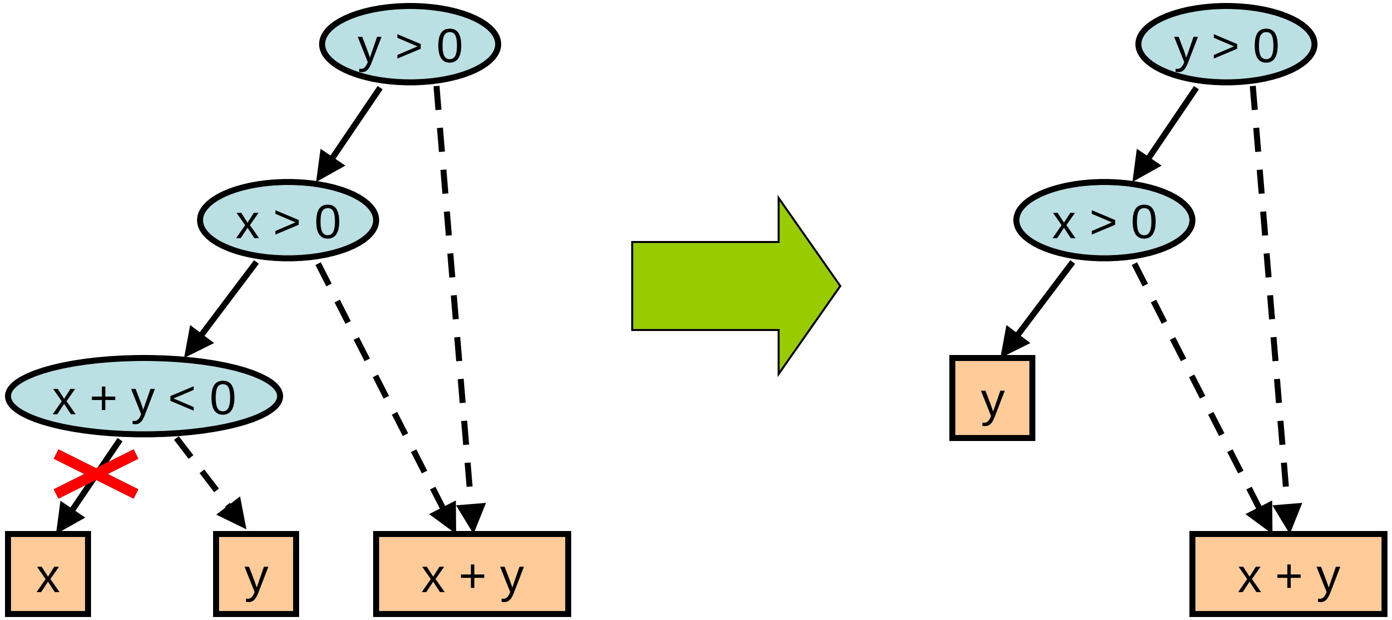


Correcting XADD Ordering

- Obtain *ordered* XADD from *unordered* XADD
  - key idea: binary operations maintain orderings



Maintaining Minimality



Node unreachable – x + y < 0 always false if x > 0 & y > 0

If **linear**, can detect with feasibility checker of LP solver & prune

More subtle prunings as well.

XADD Makes Possible all Previous Inference

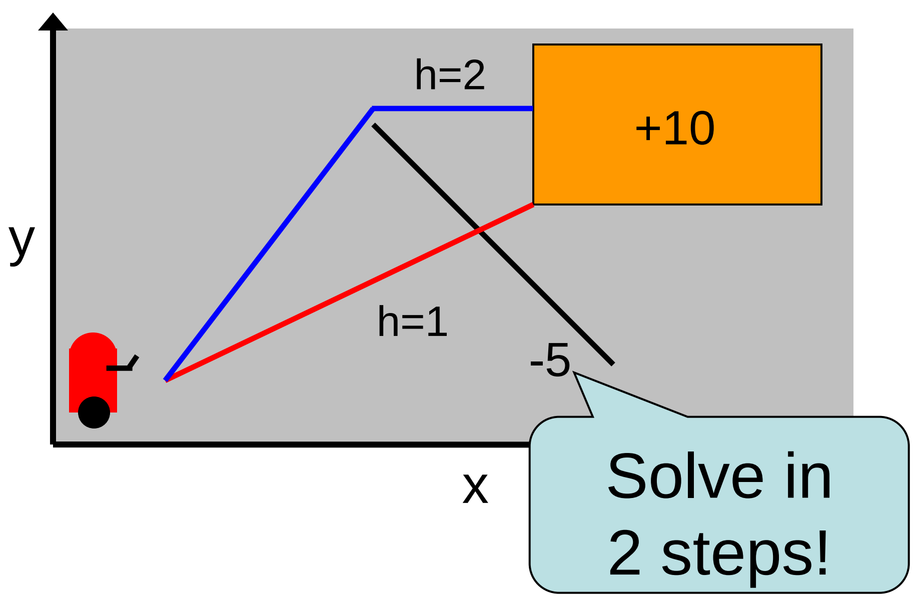
Could not even do a single integral or maximization without it!

Open Problems

Continuous Actions, Nonlinear

- **Robotics**
  - Continuous position, joint angles
  - Represent exactly with polynomials
    - Radius constraints

- **Obstacle Navigation**
  - 2D, 3D, 4D (time)
  - Don't discretize!
    - ~~Grid worlds~~
  - But nonlinear ☹

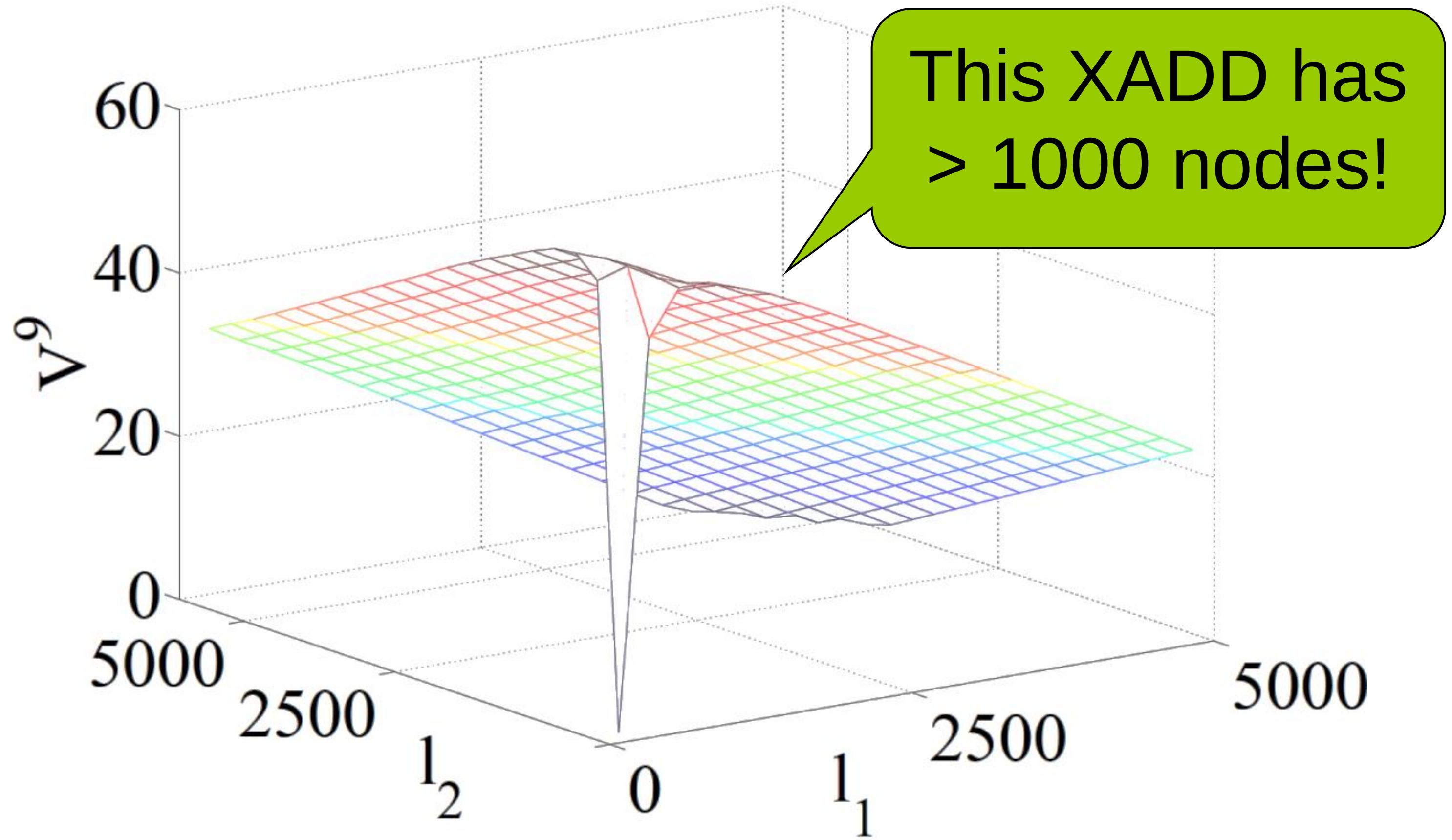


Multilinear, quadratic extensions.

In general: algebraic geometry.

Open Problems

- Bounded (interval) approximation



Recap

- Defined a calculus for piecewise functions
    - $f_1 \oplus f_2$, $f_1 \otimes f_2$
    - $\max(f_1, f_2)$, $\min(f_1, f_2)$
    - $\int_x f(x)$
    - $\max_x f(x)$, $\min_x f(x)$
- **Defined XADD to efficiently compute with cases**
- **Makes possible**
    - **Exact inference in continuous graphical models**
    - **New paradigms for optimization and sequential control**
    - **New formalizations of machine learning problems**

Symbolic Piecewise Calculus + XADD

= Expressive Continuous Inference, Optimization, & Control

Thank you!

Questions?