Symbolic Methods for Probabilistic Inference, Optimization, and Decision-making

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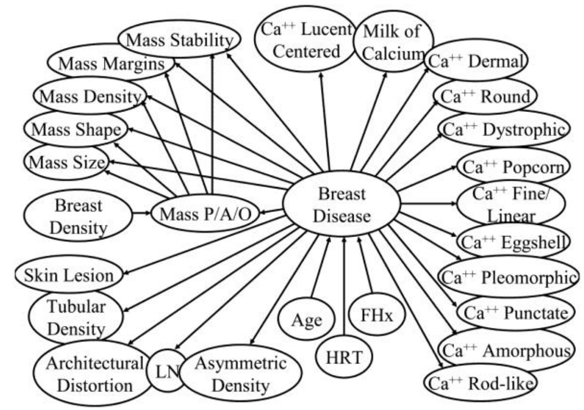
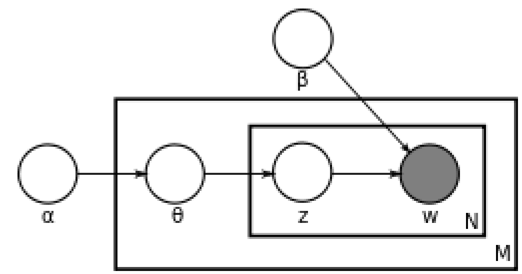
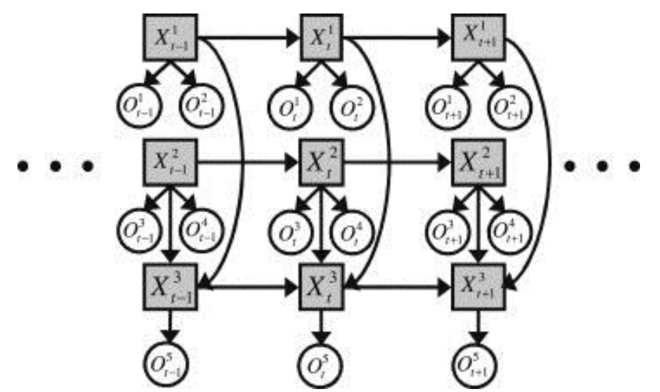
Graphical Models are Pervasive in AI

- Medical
  - Pathfinder: Expert System
  - BUGS: Epidemiology
- Text
  - LDA and 1,000 Extensions
- Vision
  - Ising Model!
- Robotics
  - Dynamics and sensor models







Graphical Models + Symbolic Methods

- Specify a graphical model for problem at hand
  - Text, vision, robotics, etc.

- Goal: efficient inference and optimization in this model
  - Be it discrete or continuous

Still partially a dream, but many recent advances

- Symbolic methods (e.g., decision diagrams) facilitate this!
  - Useful as building block in **any** inference algorithm
  - Exploit structure for compactness, efficient computation
    - Automagically!

Exploit more structure than graphical model alone

Tutorial Outline

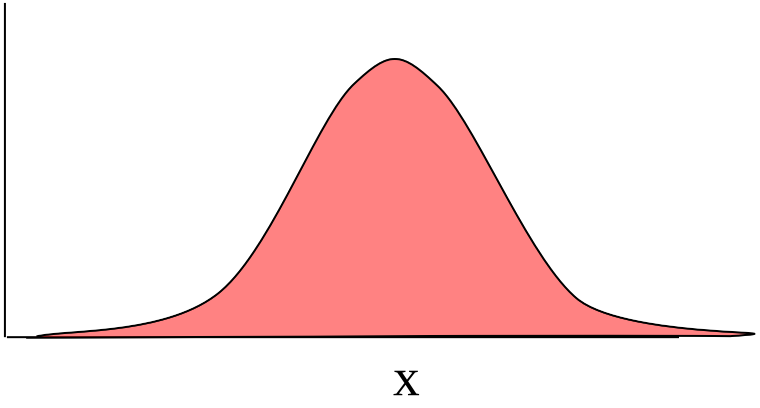
- Part I: Symbolic Methods for Discrete Inference
  - Graphical Models and Influence Diagrams
  - Symbolic Inference with Decision Diagrams
- Part II: Extensions to Continuous Inference
  - Case Calculus
  - Extended ADD (XADD)
- Part III: Applications
  - Graphical Model Inference
  - Sequential Decision-making
  - Constrained Optimization

Part II:

Extensions to Continuous Inference

General Form for Continuous Distributions?

- Probability density functions (pdfs), e.g.
  - $N(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{\sigma^2}}$



- Could be **piecewise** or **deterministic**
  - Mixture models (gates)
  - Stochastic programs (conditionals)
  - Utilities (step), decision-making (max), preferences (≥)
  - Dynamical controlled systems (switching control)
  - Deterministic (δ)

General 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)

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

- Continuous inference and optimization via the following piecewise calculus:
  - $f_1 \oplus f_2$, $f_1 \otimes f_2$
  - $\max(f_1, f_2)$, $\min(f_1, f_2)$
  - $\int_x f(x)$, $\int_x f(x)\delta(x - g(x))$
  - $\max_x f(x)$, $\min_x f(x)$

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?

$$\int_x \begin{cases} \phi_1 : & f_1 \\ \vdots & \vdots \\ \phi_k : & f_k \end{cases} dx$$

  - Just integrate case partitions, $\oplus$ results!

Partition Integral

-inf and +pos

1. Determine integration bounds

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

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

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

UB and LB are symbolic!

What constraints here?
- independent of x
- pairwise UB > LB

How to evaluate?

Definite Integral Evaluation

- How to evaluate integral bounds?

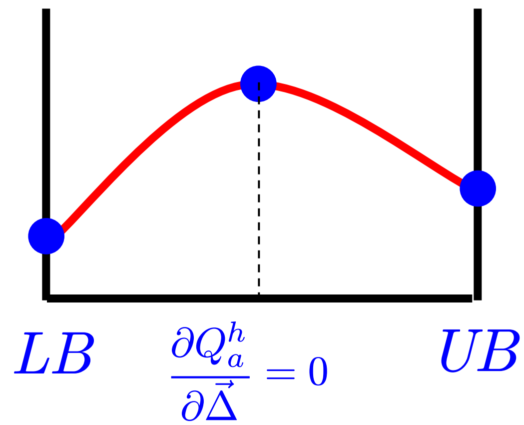
$$\int_{x=LB}^{UB} x^2 - xy \;=\; \frac{1}{3}x^3 - \frac{1}{2}x^2 y \Big|_{LB}^{UB}$$

- Can do polynomial operations on cases!

Symbolically, exactly evaluated!

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!

Integration with a δ: substitution

- Special case for integrals with δ-functions
  - $\int_x \delta[x - y] f(x) dx = f(y)$ triggers symbolic *substitution*
  - More generally: $\int_{x'_j} \delta[x'_j - g(\vec{x})] V' dx'_j = V'\{x'_j / g(\vec{x})\}$
  - E.g.,

$$\int_{x'_1} \delta[x'_1 - (x_1^2 + 1)] \left(\begin{cases} \underline{x'_1} < 2 : & \underline{x'_1} \\ \underline{x'_1} \geq 2 : & \underline{x'^2_1} \end{cases} \right) dx'_1 = \begin{cases} \underline{x_1^2 + 1} < 2 : & \underline{x_1^2 + 1} \\ \underline{x_1^2 + 1} \geq 2 : & \underline{(x_1^2 + 1)^2} \end{cases}$$

  - If *g* is *case*: need *conditional substitution*
    - see Sanner, Delgado, Barros (UAI 2011)

Recap

- Continuous inference and optimization problems represented by piecewise functions (cases)

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

- Continuous inference and optimization via the following piecewise calculus:
  - $f_1 \oplus f_2$, $f_1 \otimes f_2$
  - $\max(f_1, f_2)$, $\min(f_1, f_2)$
  - $\int_x f(x)\delta(x - g(x))$

  Closed-form for general case
  - $\int_x f(x)$ — Closed-form for linear piecewise polynomial, others
  - $\max_x f(x)$, $\min_x f(x)$ — Closed-form for linear piecewise quadratic

Cool… can we proceed to continuous inference?

Case partitions blow-up exponentially in number of operations.

Need to a compact form.

Case $\rightarrow$ XADD

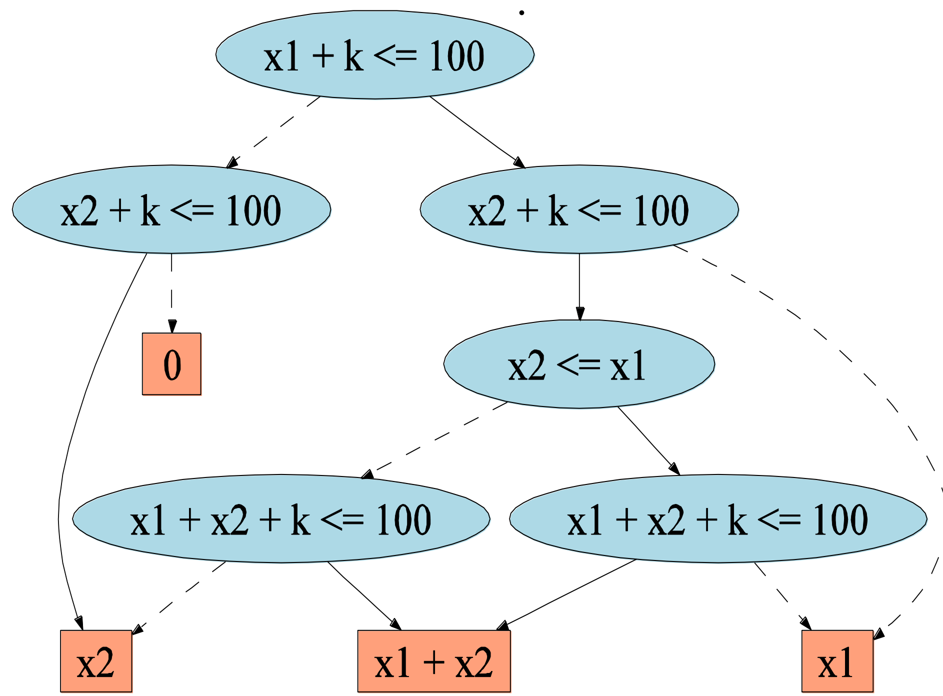
XADD = continuous variable e**x**tension
of **a**lgebraic **d**ecision **d**iagram

➔ compact, minimal case representation
➔ case operations can exploit structure

Case → XADD

Decisions can be inequalities of expressions, leaves are expressions

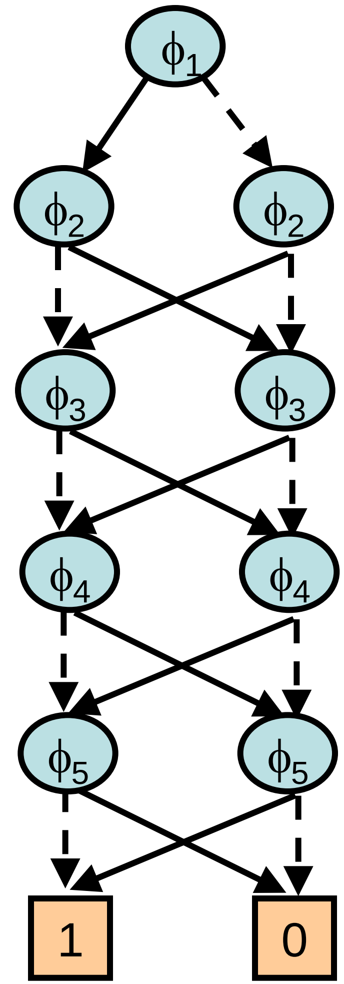
$$V = \begin{cases} x_1 + k > 100 \wedge x_2 + k > 100 : & 0 \\ x_1 + k > 100 \wedge x_2 + k \cdot\ 100 : & x_2 \\ x_1 + k \cdot\ 100 \wedge x_2 + k > 100 : & x_1 \\ x_1 + x_2 + k > 100 \wedge x_1 + k \cdot\ 100 \wedge x_2 + k \cdot\ 100 \wedge x_2 > x_1 : & x_2 \\ x_1 + x_2 + k > 100 \wedge x_1 + k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



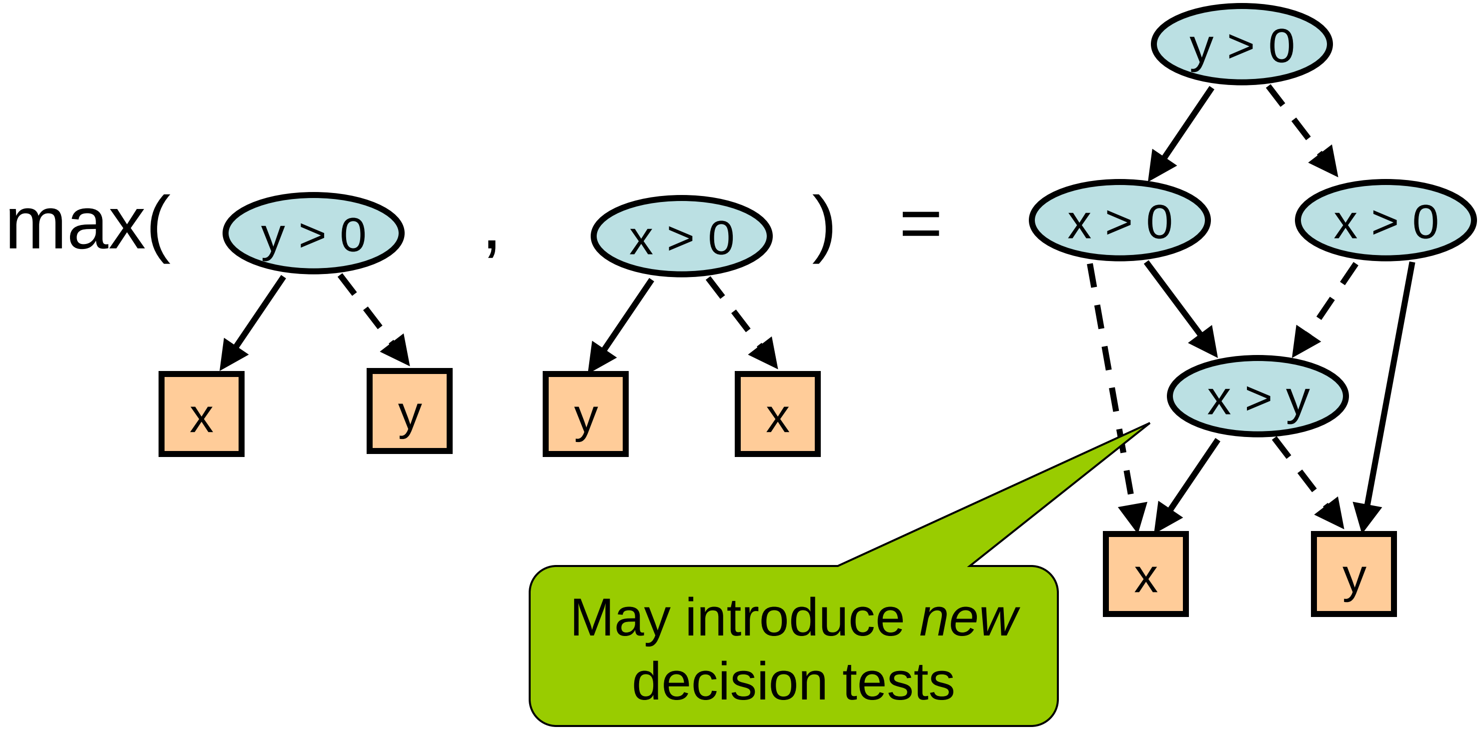
*Minimality and canonicity largely irrelevant because they are NP-Hard… but not required for correctness.

Compactness of (X)ADDs

- XADD linear in number of decisions ϕ_i
- **Case version** has exponential number of partitions!



XADD Maximization



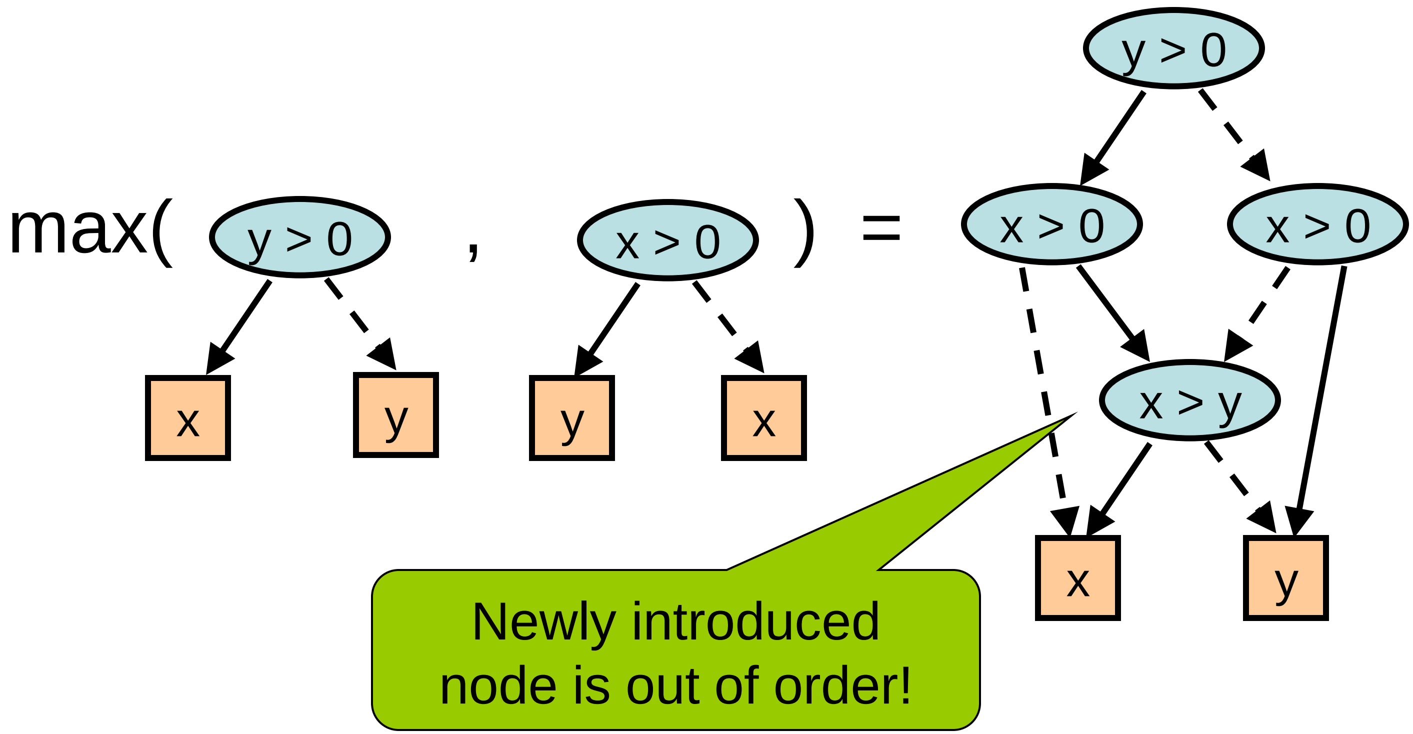
Operations exploit structure: O(|f||g|)

Maintaining XADD Orderings

- Max may get decisions out of order

Decision ordering (root→leaf)

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

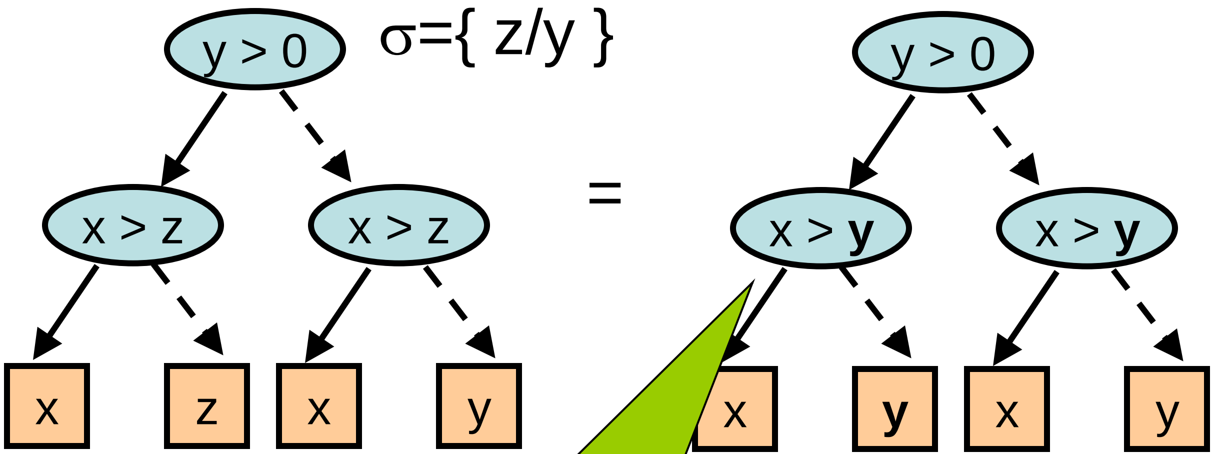


Maintaining XADD Orderings

- Substitution may get decisions out of order

Decision ordering (root→leaf):

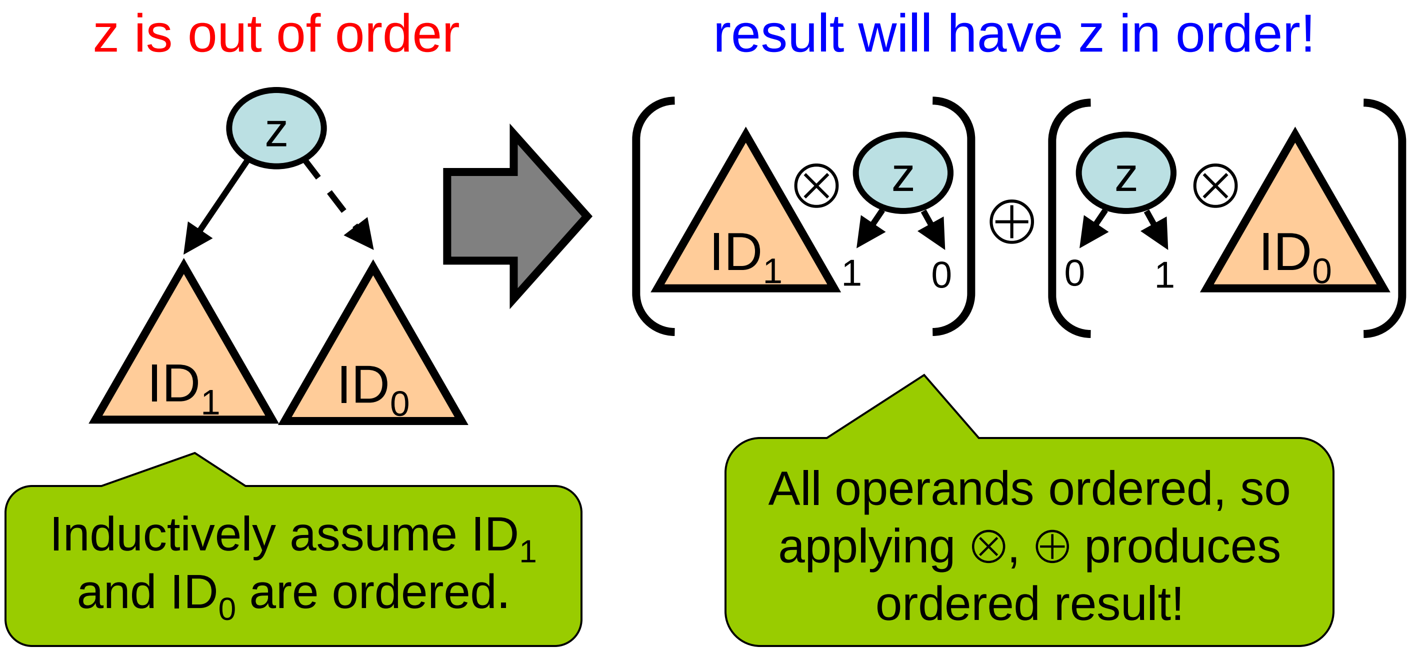
- x > y
- y > 0
- x > z



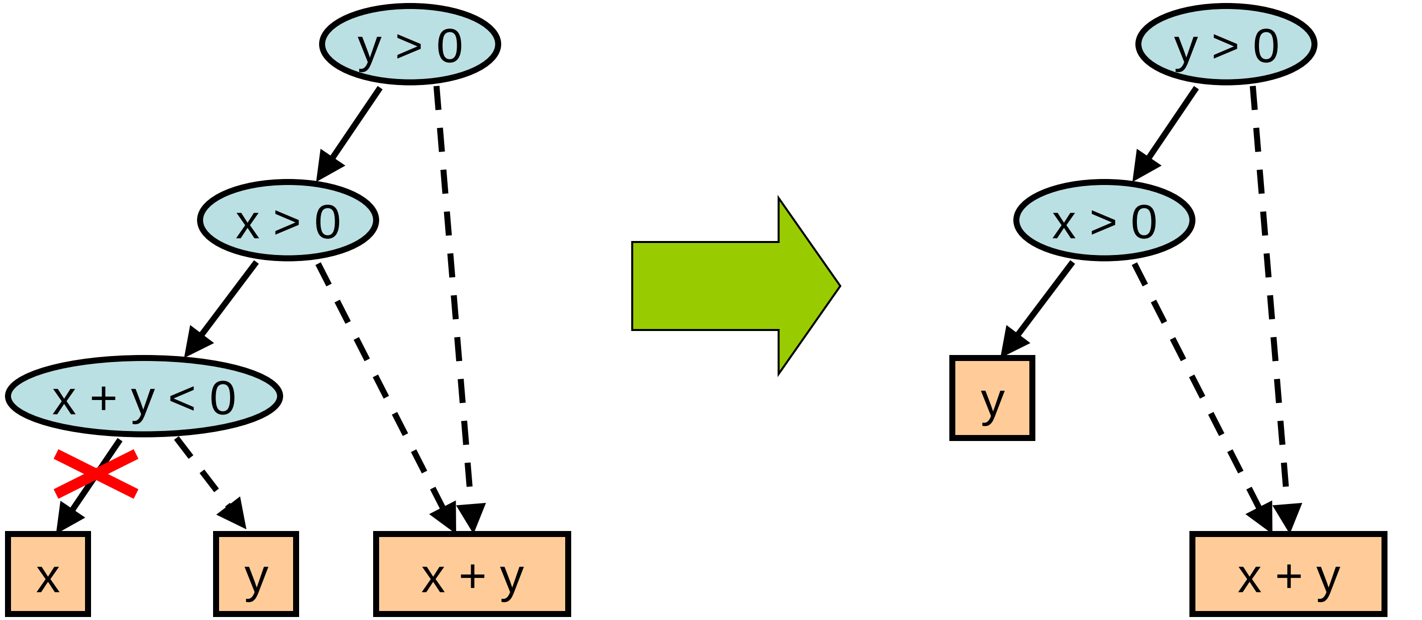
Substituted nodes are now out of order!

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

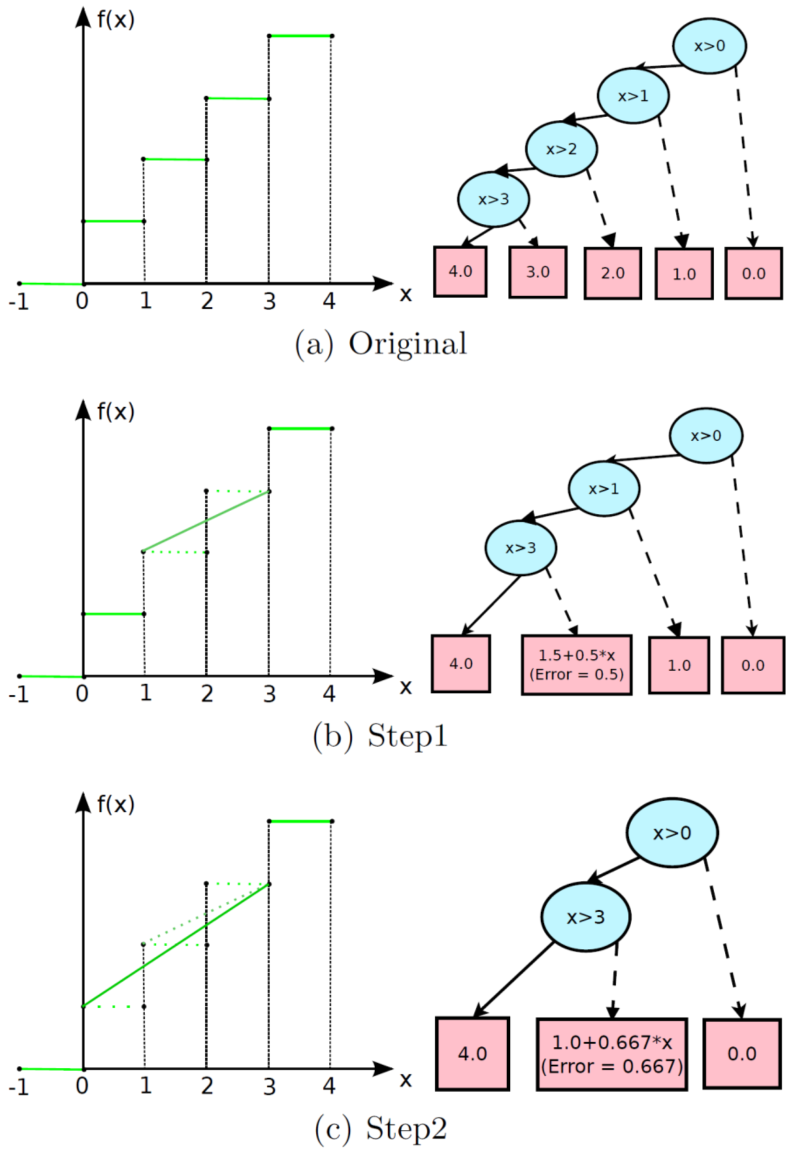
If **linear**, can detect with feasibility checker of LP solver & prune

More subtle prunings as well.

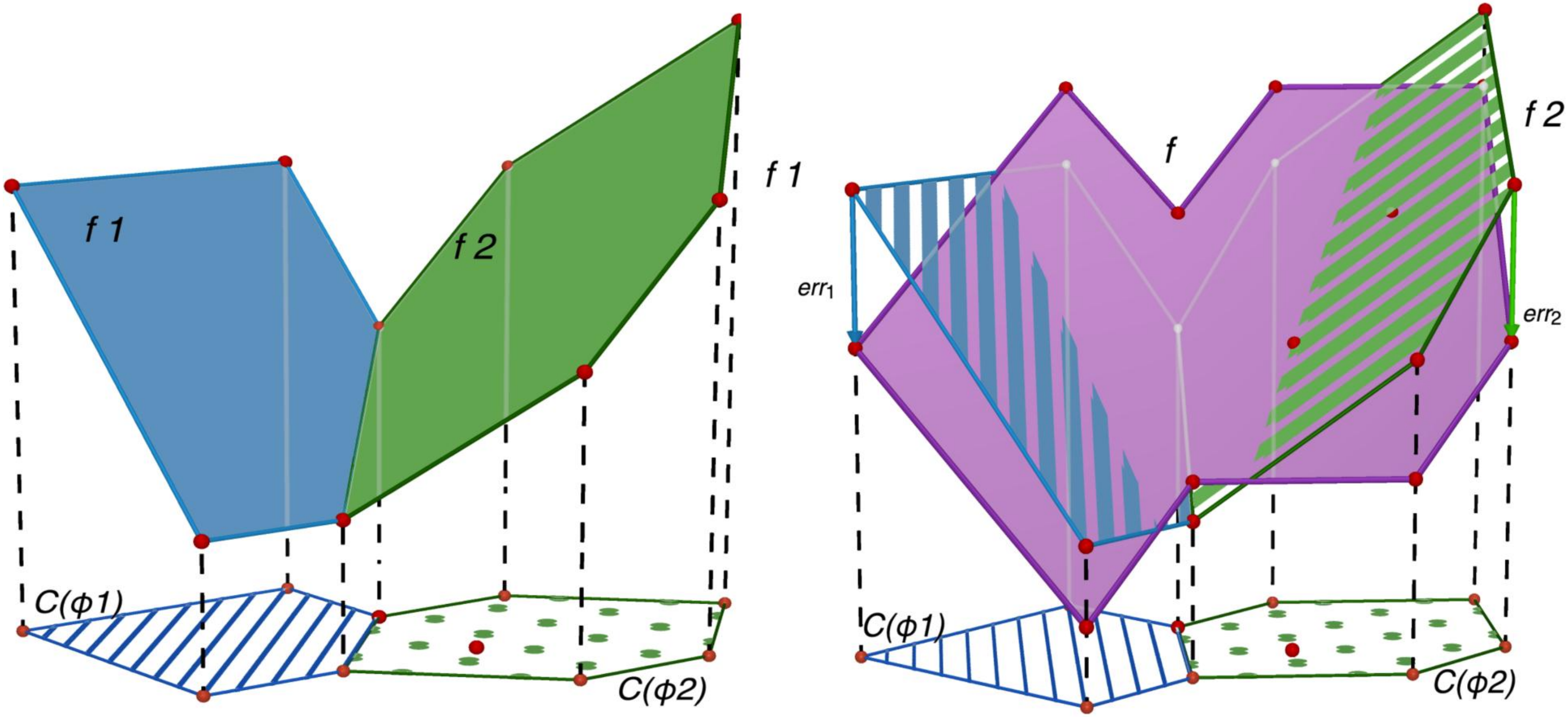
XADD Approximation

- Can we extend APRICODD-style approximations to XADDs?

- Yes, but not as simple as averaging leaves…



Linear XADD Leaf Merging

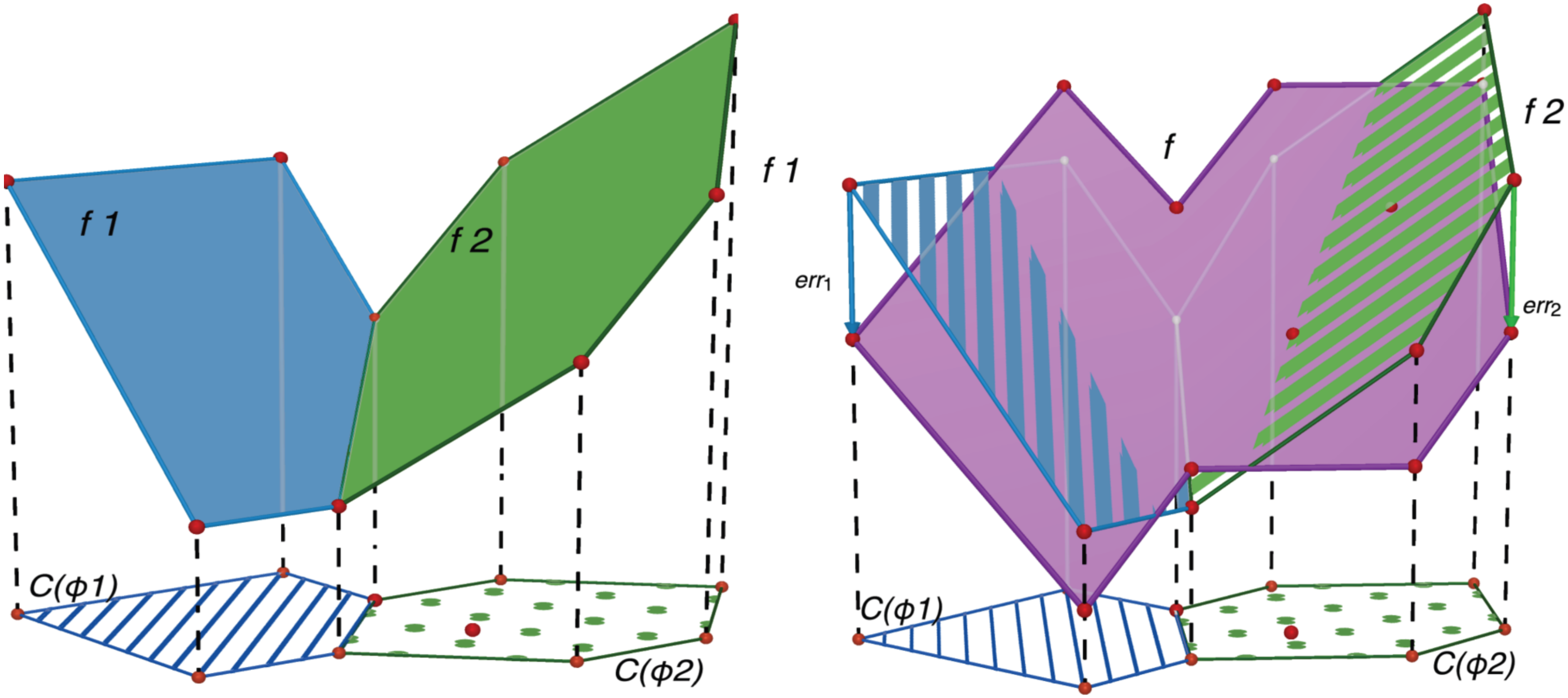


Best f*

Max error

$$\min_{\vec{c}^*} \max_{i\in\{1,2\}} \max_{\vec{x}\in S_{\phi_i}} \left| \underbrace{\vec{c}_i^{\,T}\begin{bmatrix}\vec{x}\\1\end{bmatrix}}_{f_i} - \underbrace{\vec{c}^{*T}\begin{bmatrix}\vec{x}\\1\end{bmatrix}}_{f^*} \right|$$

Linear XADD Leaf Merging

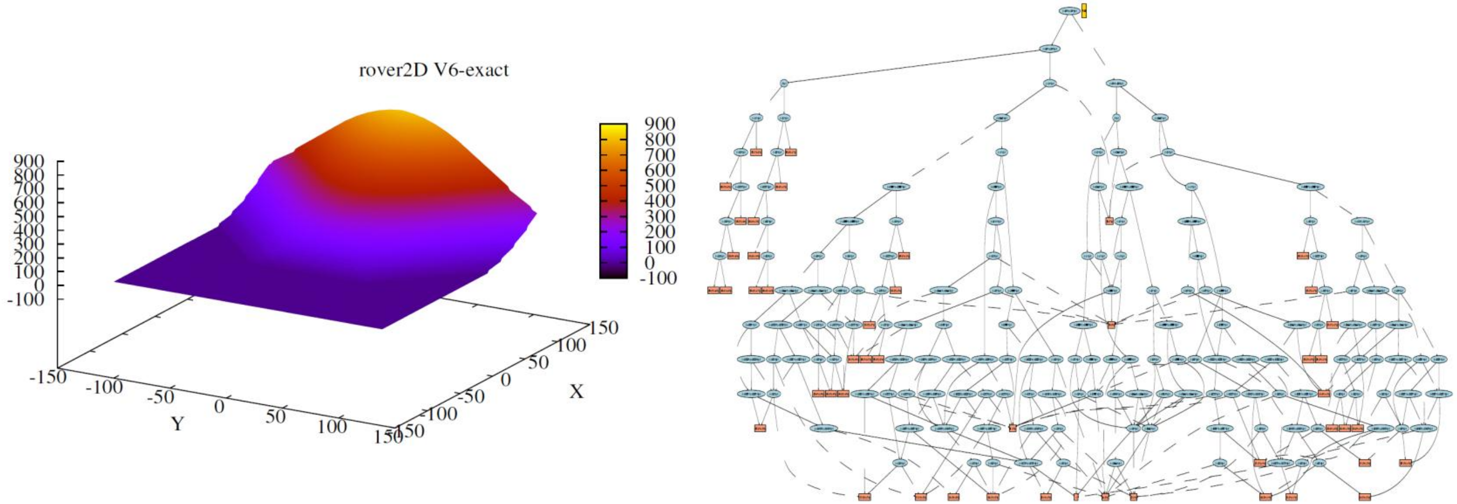


Constraint generation: for c*, use **LP** to generate max violated constraint

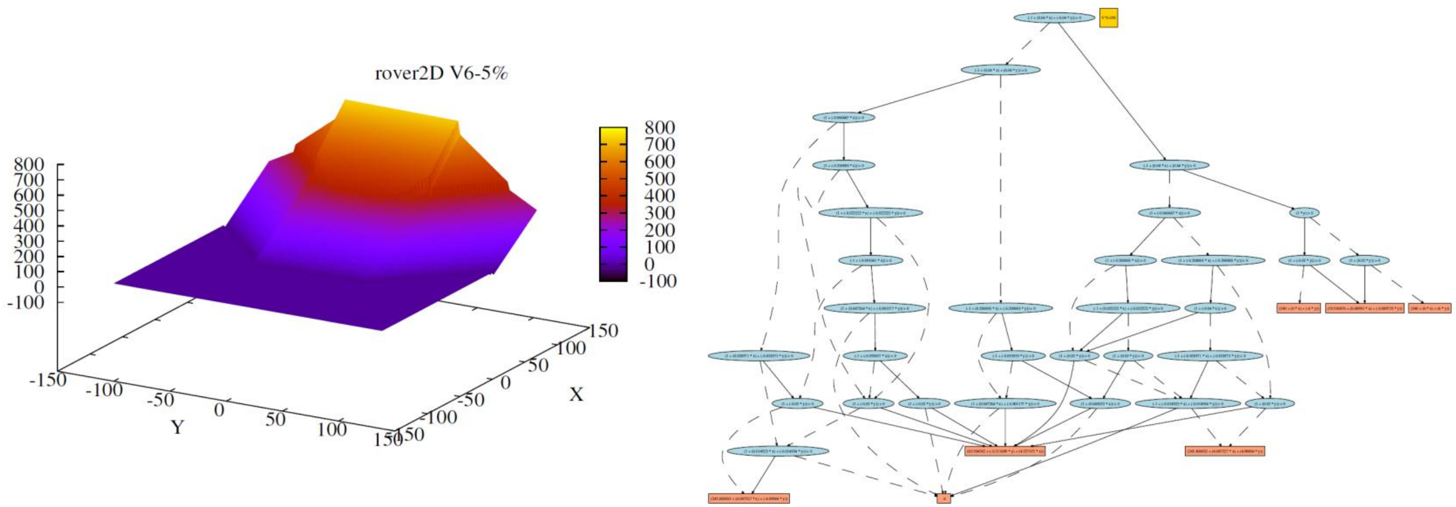
$$\min_{\vec{c}^*,\epsilon} \epsilon$$

$$s.t.\ \epsilon \geq \left| \vec{c}_i^{\,T} \begin{bmatrix} \vec{x}_{ij}^k \\ 1 \end{bmatrix} - \vec{c}^{*\,T} \begin{bmatrix} \vec{x}_{ij}^k \\ 1 \end{bmatrix} \right| ; \quad \forall i \in \{1,2\}, \forall \theta_{ij}, \forall k \in \{1 \ldots N_{ij}\}$$

Linear Approximation Example



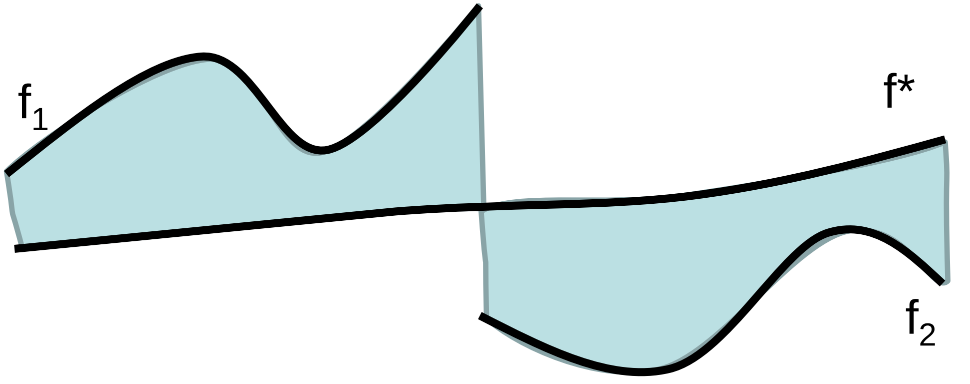
(a) Value at 6^{th} iteration for exact SDP.



(b) Value at 6^{th} iteration for 5% approximate SDP.

Nonlinear XADD Approximation?

- 1D Example



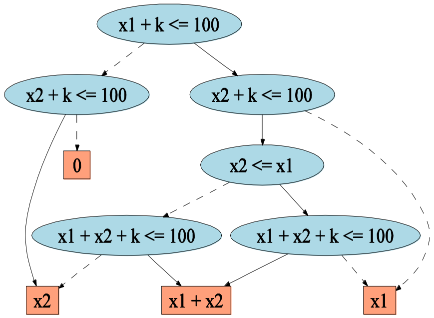
- Questions
  - What approximating class?
  - What error function?
    - Max not feasible
    - Volume of squared error? Integral is exact.

But many caveats vs. linear case

XADD Recap

- Represent case by XADD

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



XADD more **compact** than direct case representation

- Piecewise calculus operations exploit XADD structure:
  - $f_1 \oplus f_2$, $f_1 \otimes f_2$
  - $\max(f_1, f_2)$, $\min(f_1, f_2)$
  - $\int_x f(x)\delta(x - g(x))$
  - $\int_x f(x)$
  - $\max_x f(x)$, $\min_x f(x)$

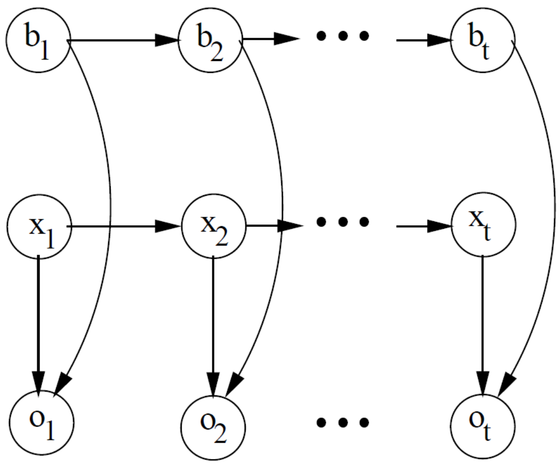
Bounded Linear XADD **approximation** possible.

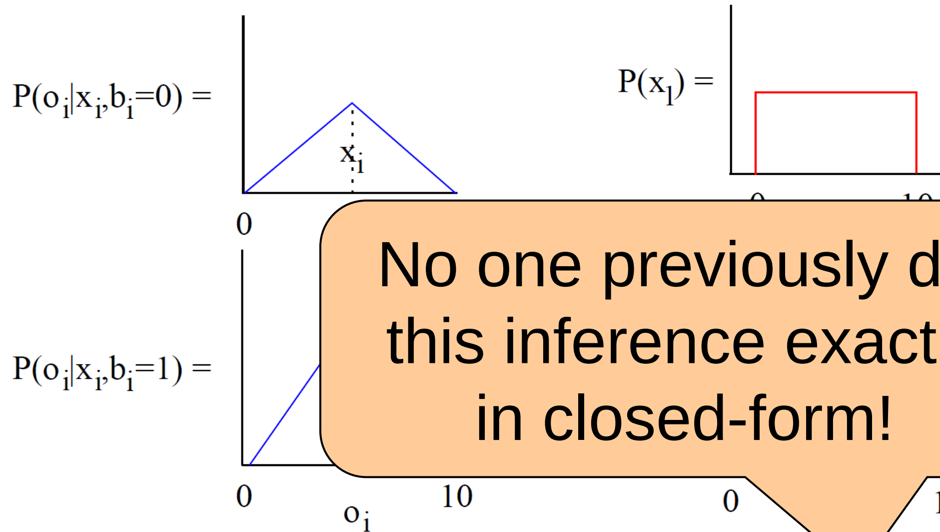
Working on nonlinear case.

Part III:
Applications

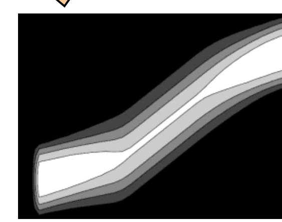
Graphical Models

Discrete & Continuous HMMs





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



Exact Inference in Cont. Graphical Models

- Fully Gaussian
  - Most inference
- 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?

Compact representations
and closed-form operations
on piecewise functions

Exact Graphical Model Inference!
(directed and undirected)

- Represent all factors as piecewise polynomials

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

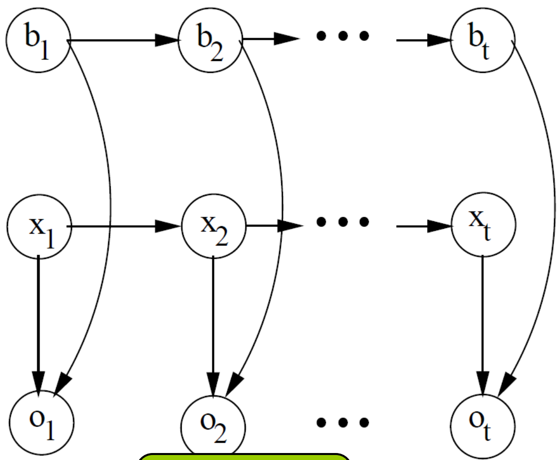
- Or an exact expectation of *any* polynomial

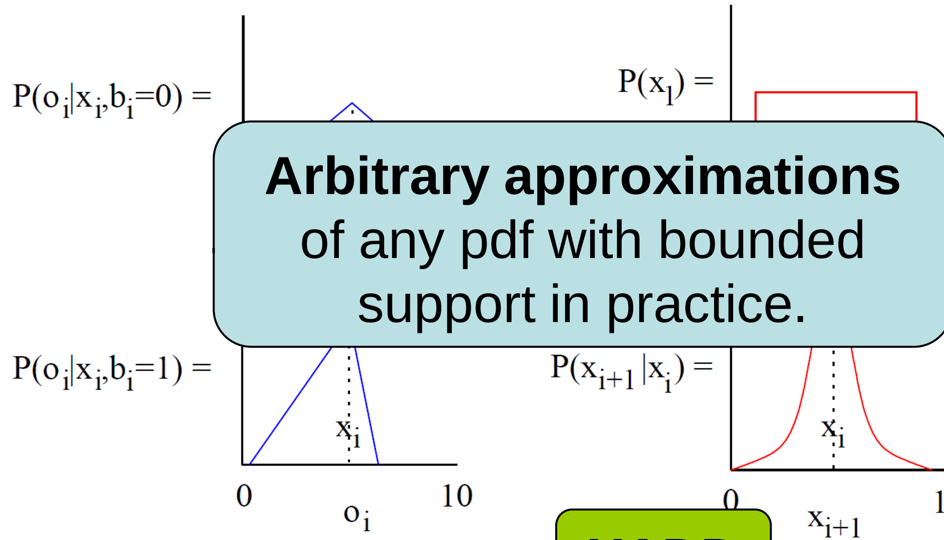
$$\mathbb{E}_{\mathbf{x} \sim p(\mathbf{x}|\mathbf{o})}[poly(\mathbf{x})|\mathbf{o}] = \int_{\mathbf{x}} p(\mathbf{x}|\mathbf{o}) poly(\mathbf{x}) d\mathbf{x}$$

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

All computed exactly in closed-form by **Symbolic Variable Elimination (SVE)**

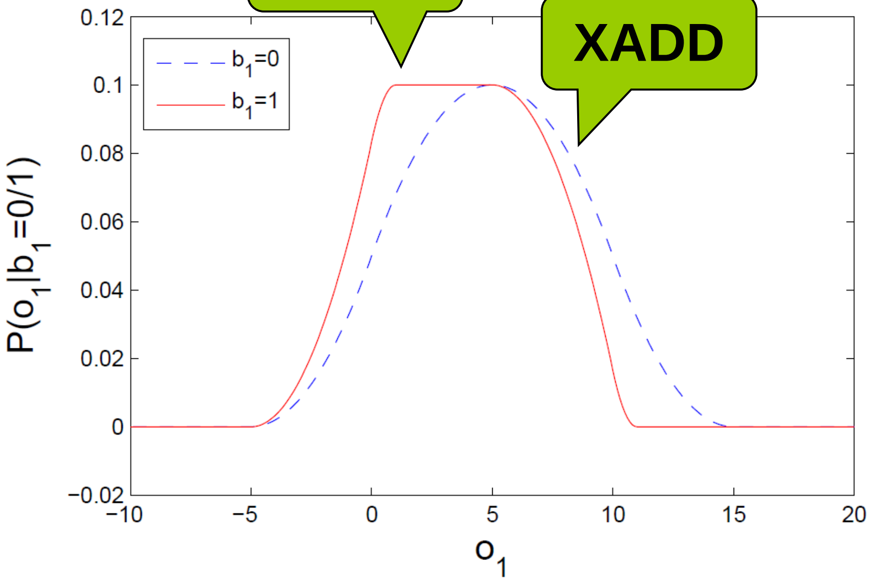
Voila: Closed-form Exact Inference via SVE!





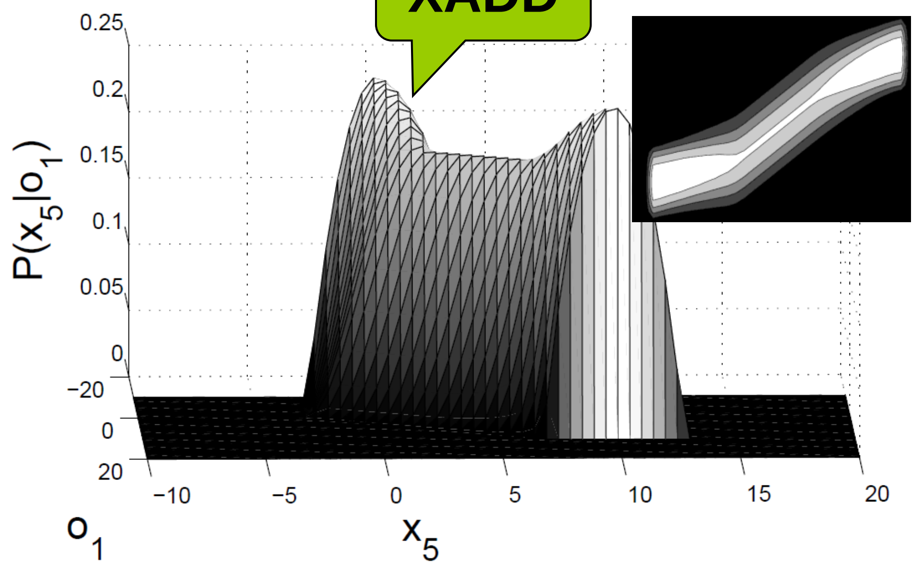
Arbitrary approximations of any pdf with bounded support in practice.

XADD



XADD

XADD



Computational Complexity?

- In theory for SVE on graphical models
  - Best-case complexity Ω(#operations)
  - Worst-case complexity is O(exp(#operations))
    - Not explicitly tree-width dependent!
    - **But worse:** integral may invoke 100's of operations!

Fortunately data structures mitigate worst-case complexity

An Expressive Conjugate Prior for Bayesian Inference

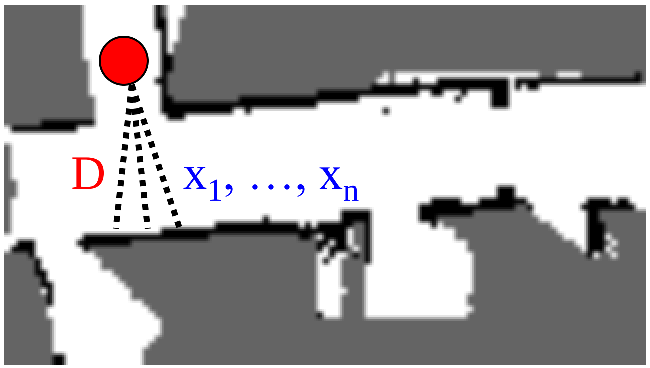
- General Bayesian Inference

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

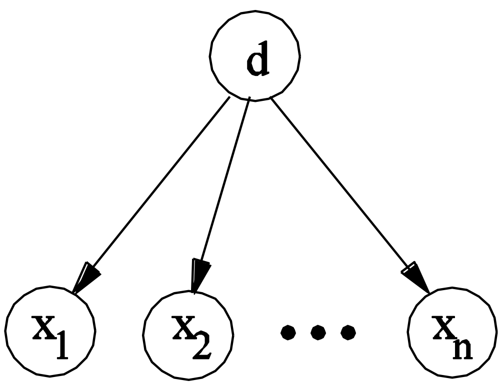
XADD XADD XADD

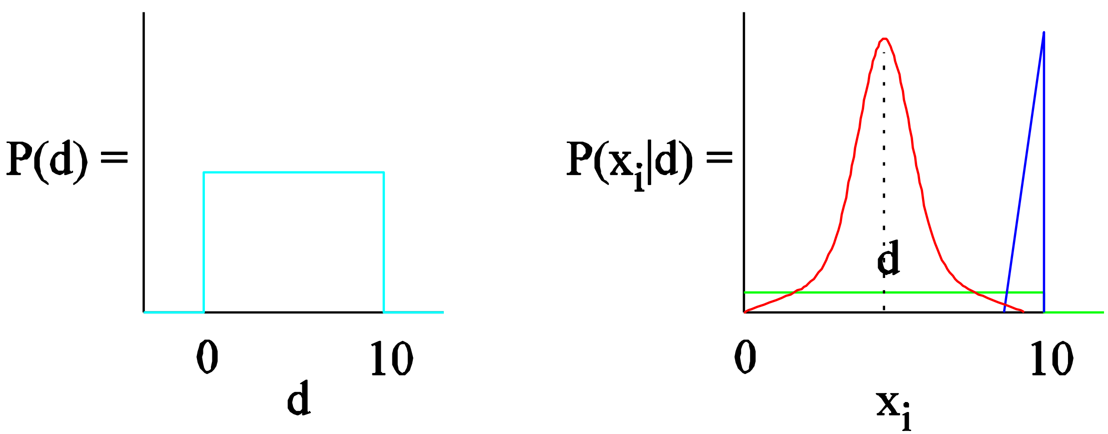
- Prior & likelihood for computational convenience?
  - No, choose as appropriate for your problem!

Bayesian Robotics



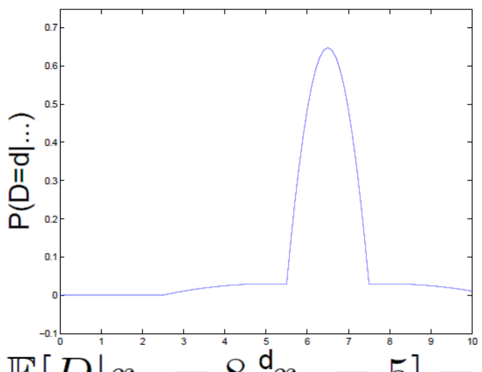
- D: true distance to wall
- $x_1, \ldots, x_n$: measurements
- want: $E[D \mid x_1,\ldots,x_n]$



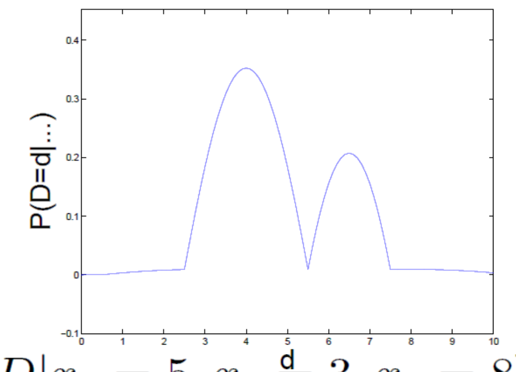


Bayesian Robotics: Results

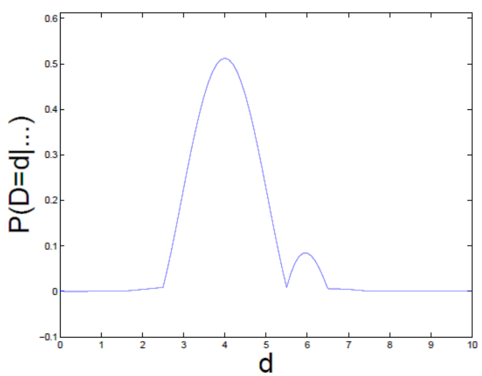
- Sample position posteriors and expectations…



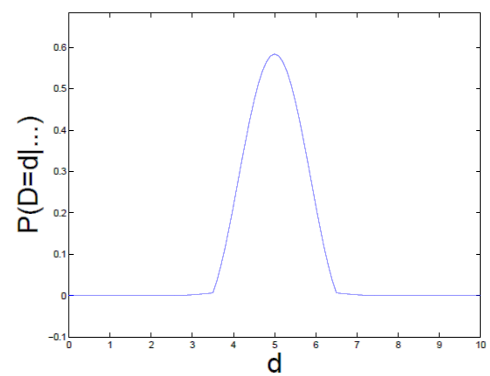
$$\mathbb{E}[D|x_1 = 8, x_2 = 5] = 6.0$$



$$\mathbb{E}[D|x_1 = 5, x_2 = 3, x_3 = 8] = 4.39$$



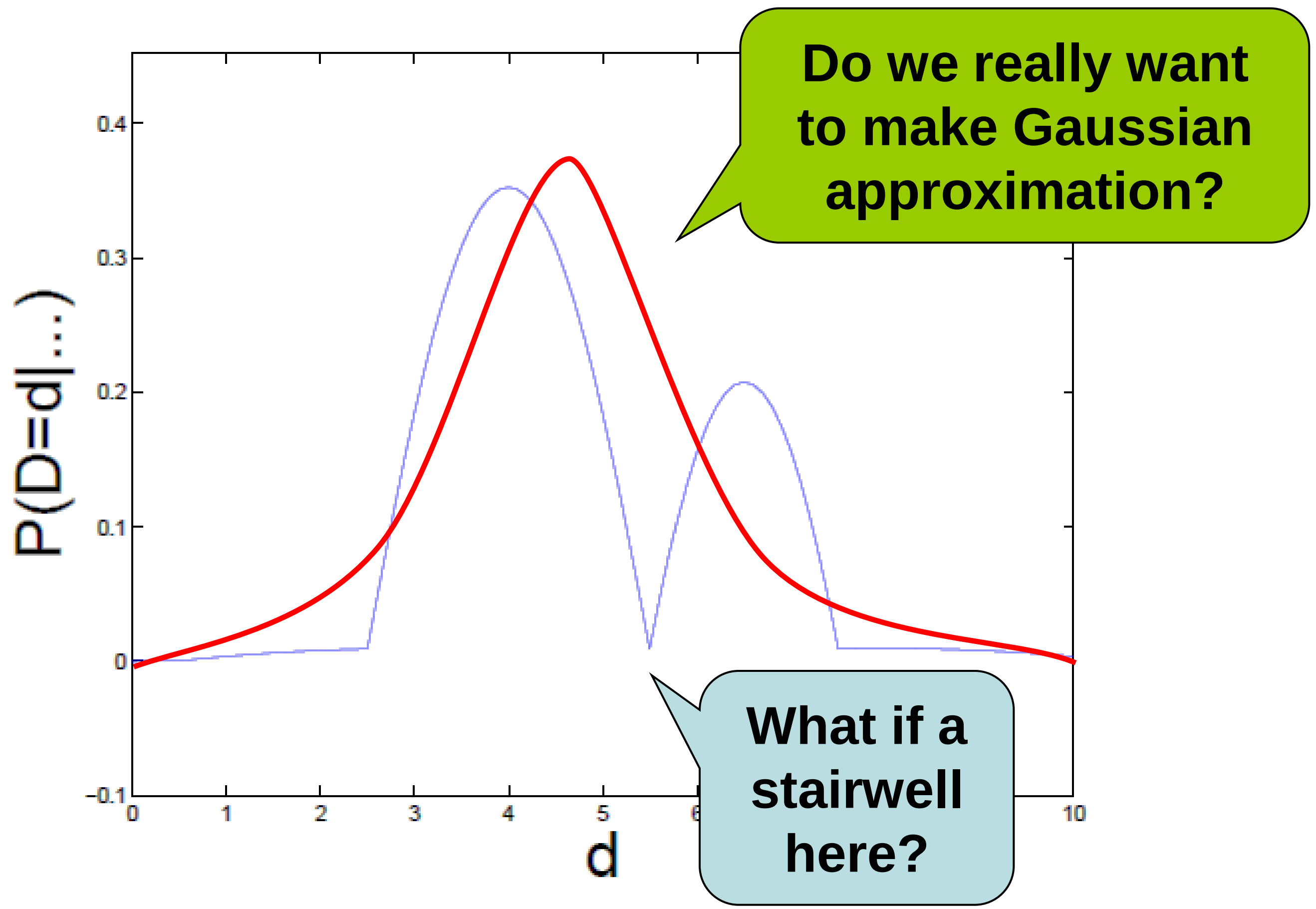
$$\mathbb{E}[D|x_2 = 1, x_2 = 3, x_3 = 4, x_4 = 8] = 5.45$$



$$\mathbb{E}[D|x_1 = 5, x_2 = 4, x_3 = 6, x_4 = 5] = 4.89$$

Bayesian Robotics: Results

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

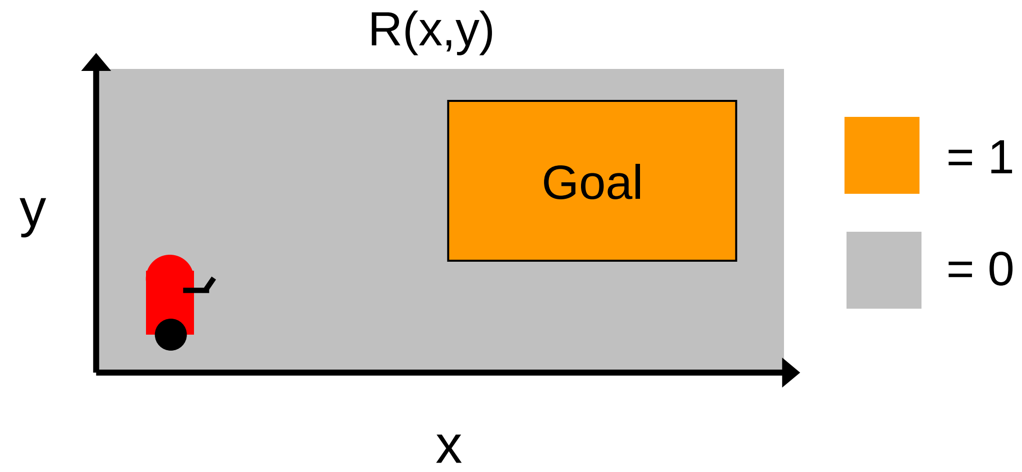


Part III:
Applications

Symbolic Dynamic Programming

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)]

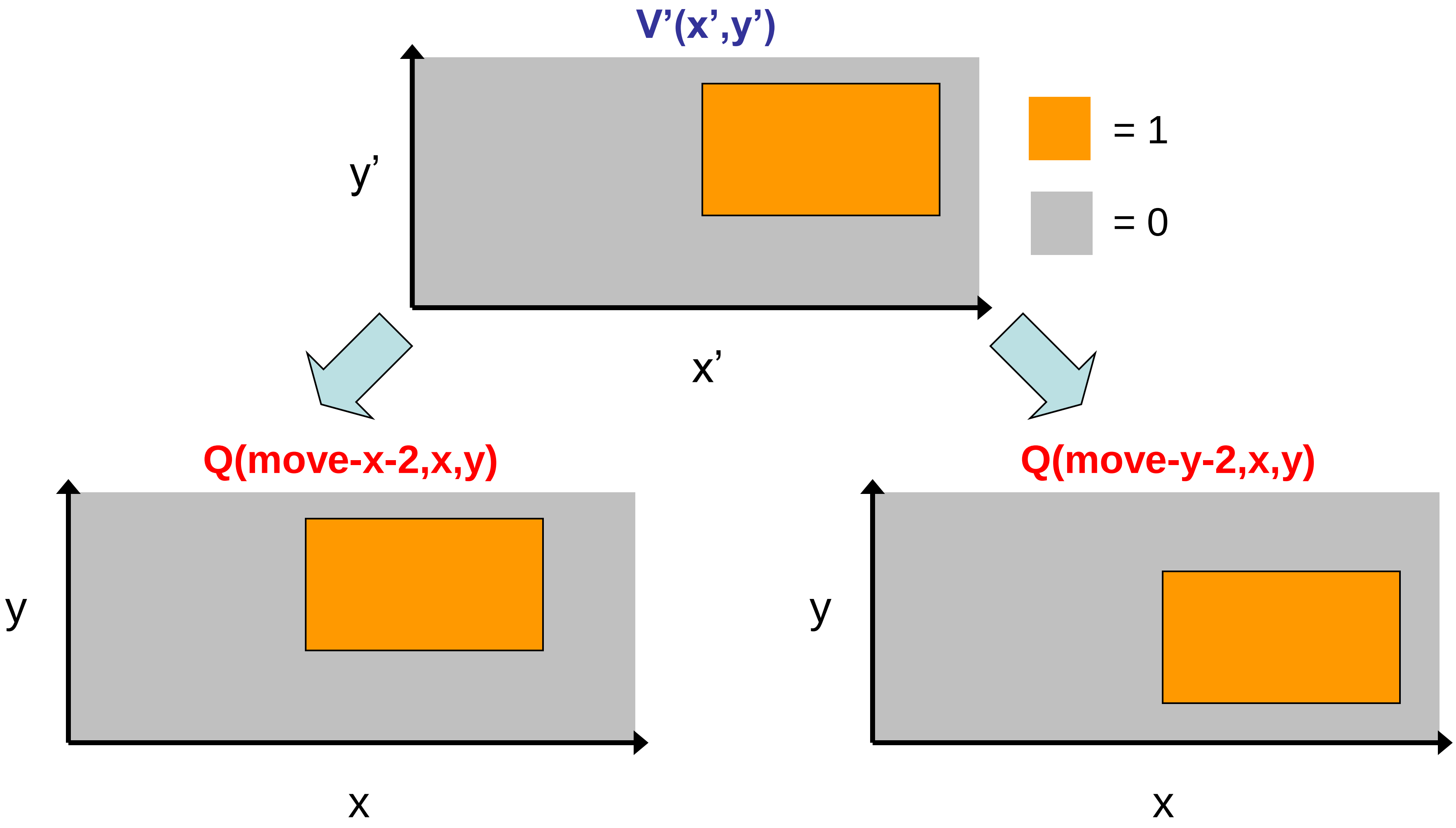


Feng *et al* (UAI-04) Assumptions:

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

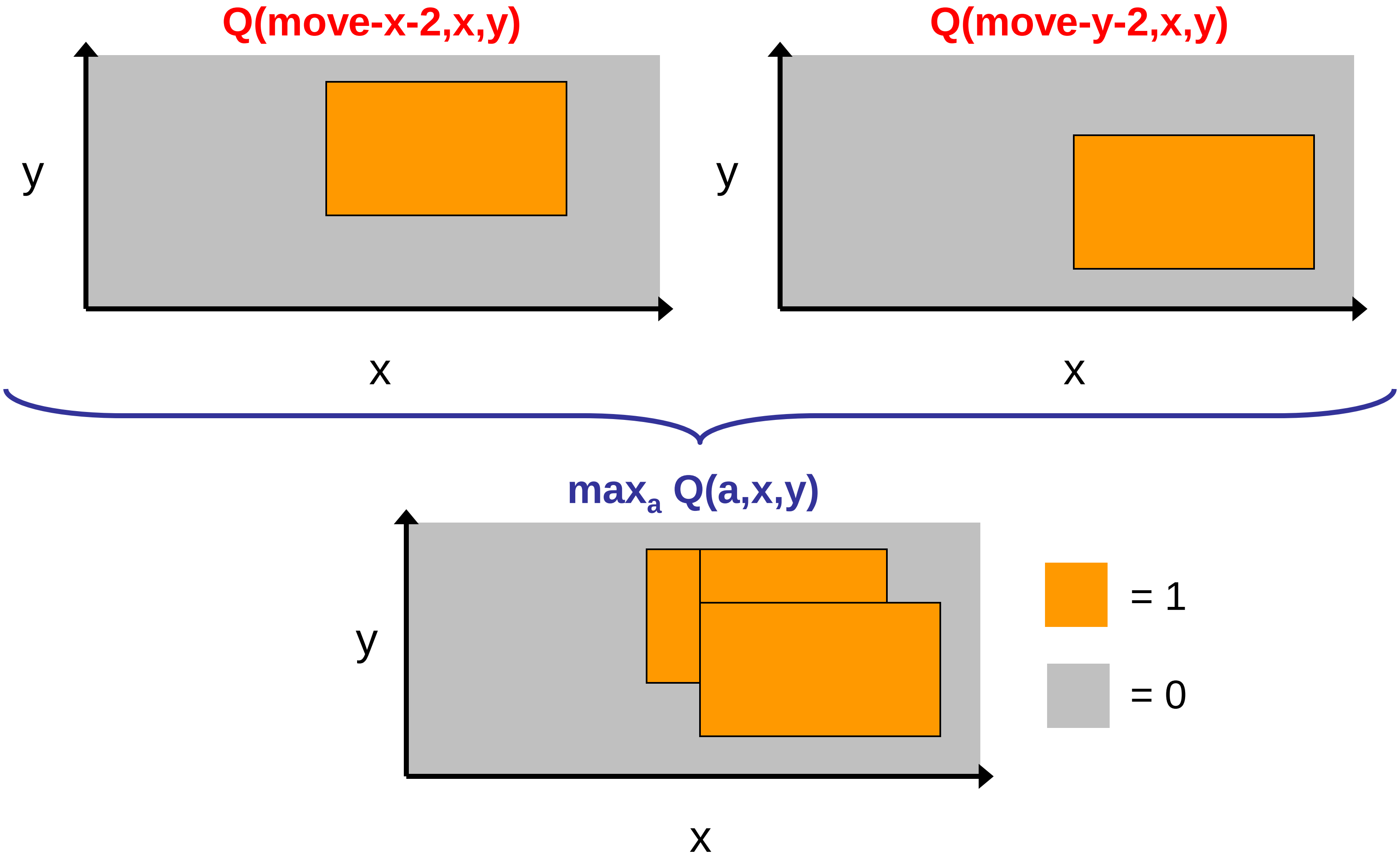
Exact Solutions to DC-MDPs: Regression

- Continuous regression is just translation of "pieces"



Exact Solutions to DC-MDPs: Maximization

- Q-value maximization yields piecewise rectilinear solution



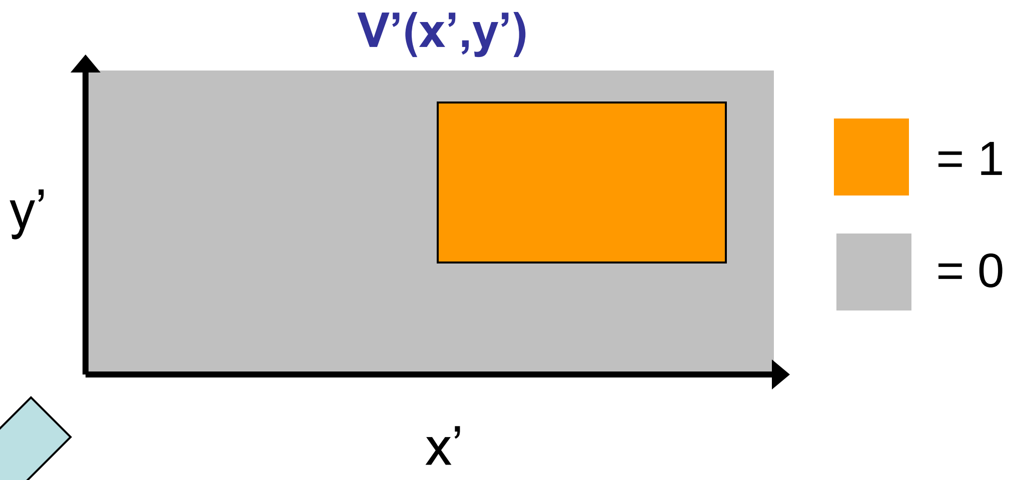
Previous Work Limitations I

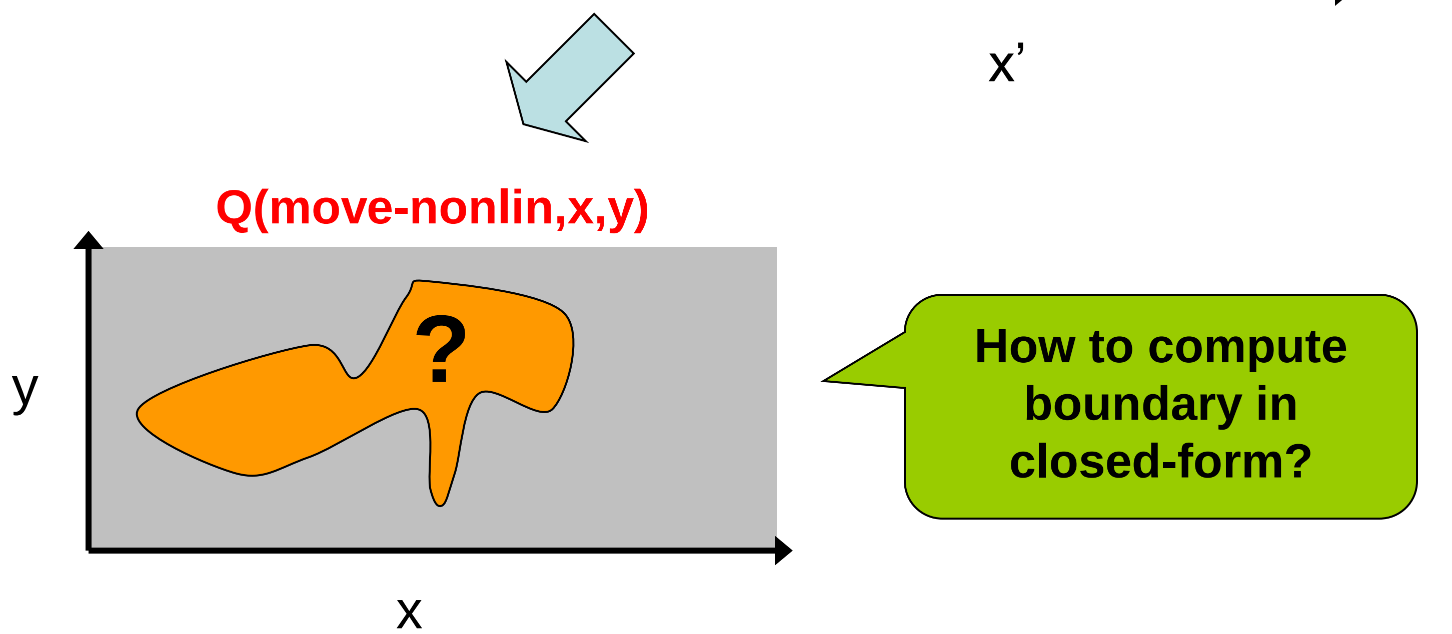
- Exact regression when transitions nonlinear?

Action move-nonlin:

– $x' = x^3 y + y^2$

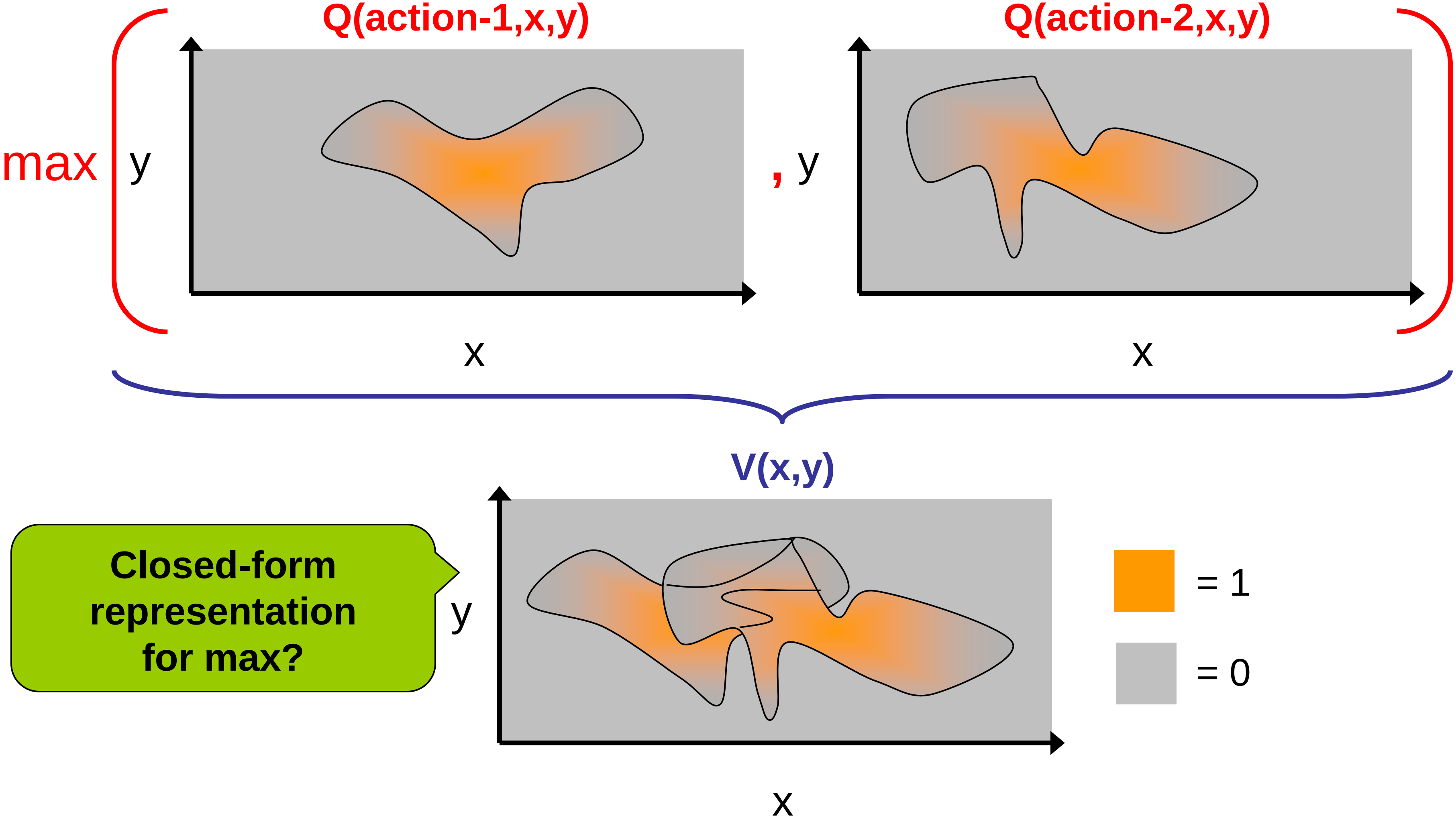
– $y' = y * \log(x^2 y)$





Previous Work Limitations II

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



Continuous State MDPs

Symbolic Dynamic Programming (SDP)… exact closed-form solution for **any** continuous state MDP!

- Value Iteration for h∈0..H
  - Regression step:

$$Q_a^{h+1}(\vec{b},\vec{x}) = R_a(\vec{b},\vec{x}) + \gamma \cdot \sum_{\vec{b}'} \int_{\vec{x}'} \left(\prod_{i=1}^{n} P(b_i'|\vec{b},\vec{x},a) \prod_{j=1}^{m} P(x_j'|\vec{b},\vec{b}',\vec{x},a) \right) V^h(\vec{b}',\vec{x}')d\vec{x}'$$

  - Maximization step:

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

XADD

XADD

XADD

XADD

XADD

XADD

Continuous Actions?

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

Continuous Actions

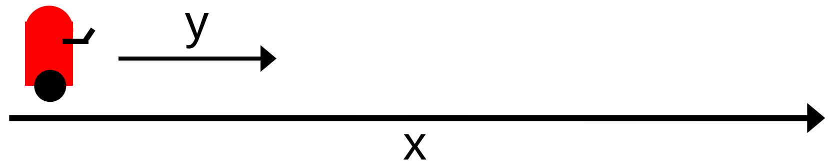
- Inventory control
  - Reorder based on stock, future demand
  - Action: $a(\vec{\Delta});\ \vec{\Delta} \in \mathbb{R}^{|a|}$

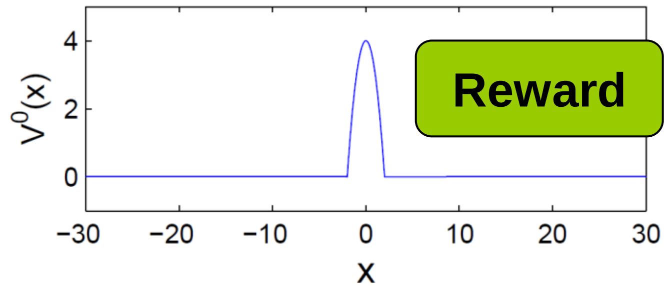
- Need $\max_{\Delta}$ in Bellman backup

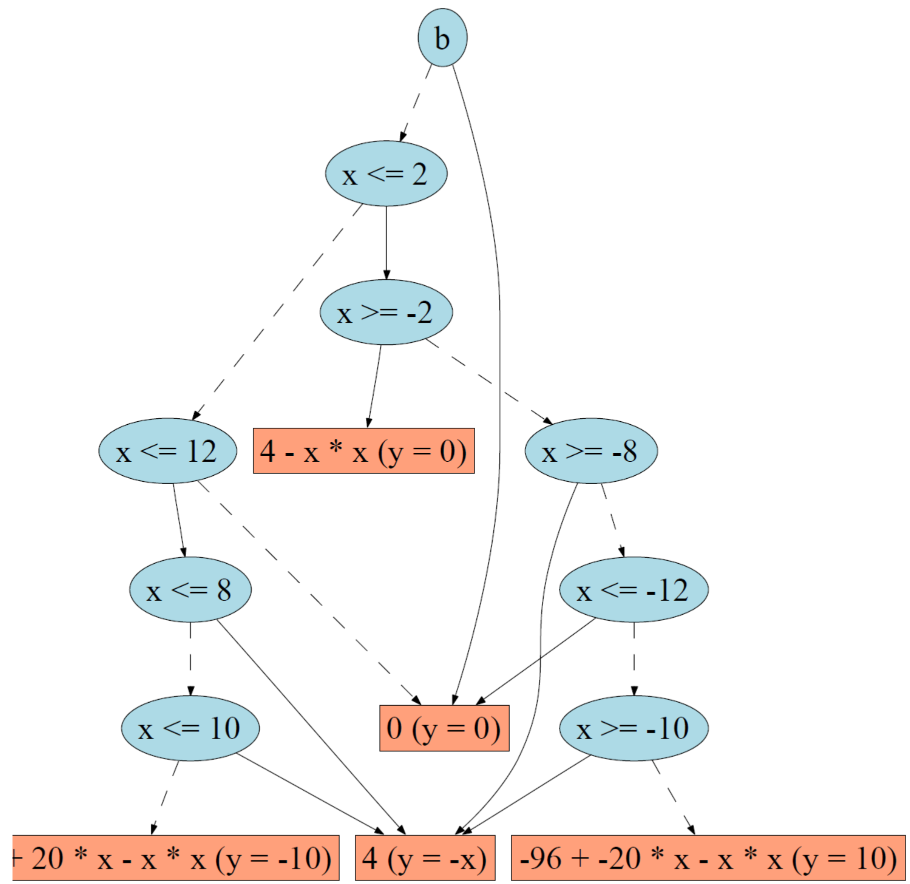
$$V_{h+1} = \max_{a \in A} \max_{\vec{\Delta}} Q_a^{h+1}(\vec{\Delta})$$

- $\max_x$ case(x) previously defined case(x)
  - Can track maximizing Δ substitutions to recover π

Illustrative Value and Policy







Value (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**
  - Robust solutions with continuous noise **IJCAI-13**

All papers co-authored with Sanner

Part III:
Applications

Optimization

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

- Conditional constraints
  - E.g., if (x > y) then (y < z)
  - Not 0-1 MILP, MIQP equivalent

Can encode with "big-M trick", but requires careful tuning of M to avoid numerical precision issues.

- 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!

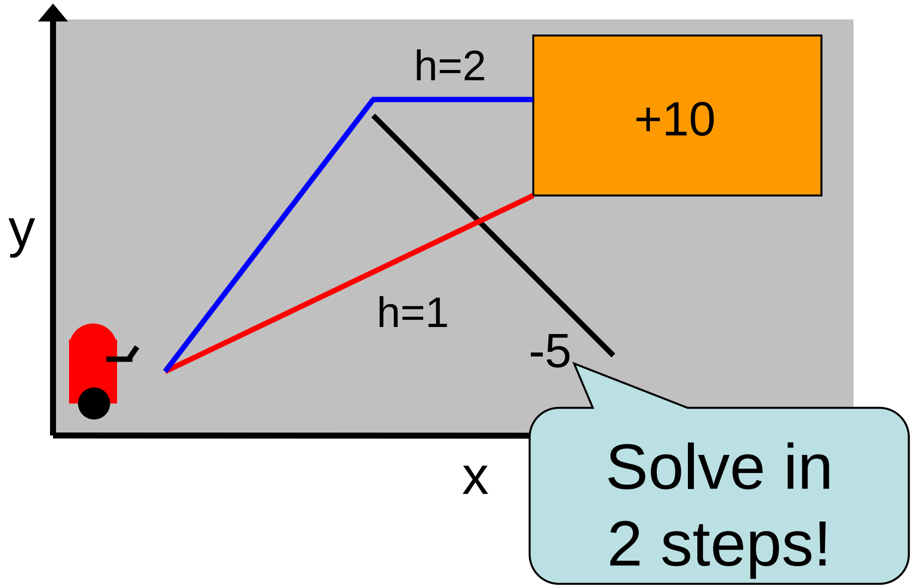
- Parameterized optimization
  - $f(y) = \max_x f(x,y)$
  - Maximum value, substitution as a **function of y**

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 ☹

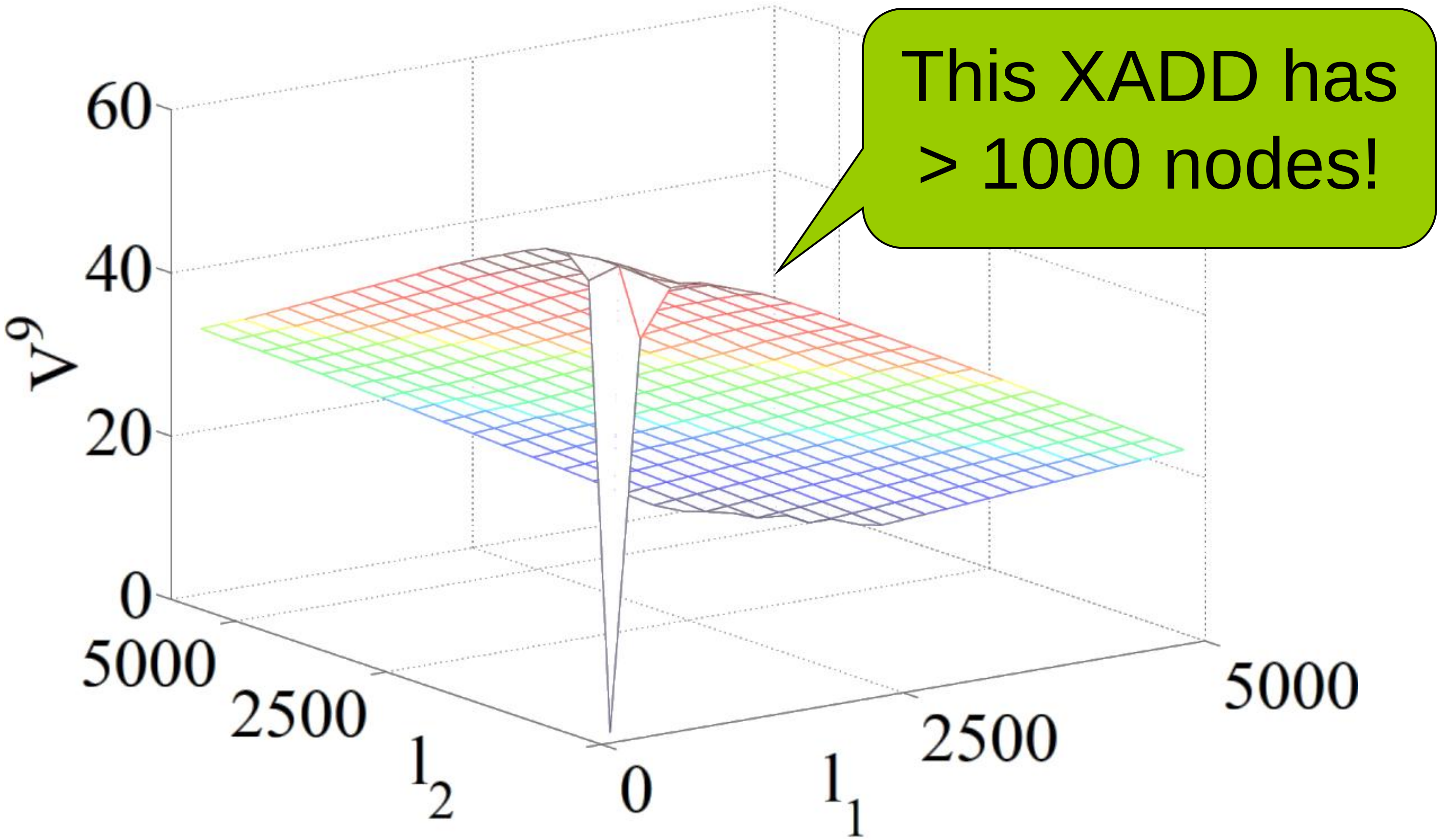


Multilinear, quadratic extensions.

In general: algebraic geometry.

Open Problems

- Bounded approximation for nonlinear XADDs



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**
    - **Unprecedented expressive sequential optimization and control**
    - **New approaches for optimization**

Symbolic Piecewise Calculus + XADD

= Expressive Continuous Inference & Optimization

Thank you!

Questions?