From Potentials to Polyhedra: Inference in Structured Models

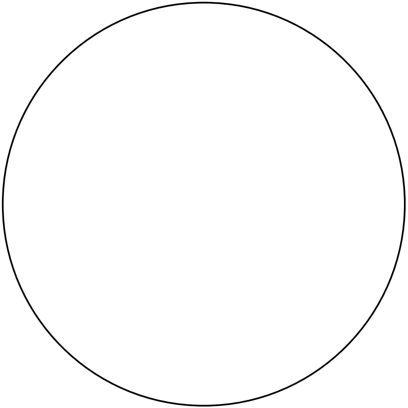
Sebastian Nowozin

Machine Learning and Perception Group
Microsoft Research Cambridge

Colorado Springs, 20th June 2011

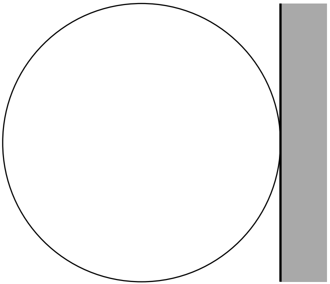
Microsoft Research

Approximating a Unit Disc



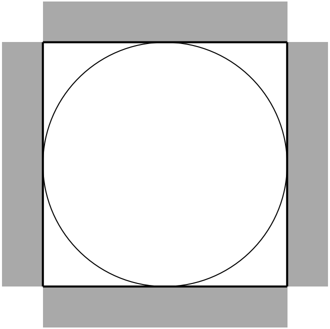
- Using linear inequalities, how can we approximate the unit disc?

Naive approach



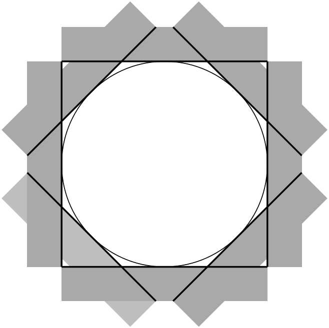
- Error $\epsilon = \frac{1}{\cos \frac{\pi}{k}} - 1 \approx \frac{\pi^2}{2k^2}$
- Inefficient, $\epsilon \leq 10^{-6}$ needs $k > 2200$
- Can we do better?

Naive approach



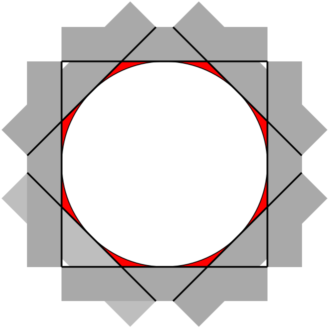
- Error $\epsilon = \frac{1}{\cos \frac{\pi}{k}} - 1 \approx \frac{\pi^2}{2k^2}$
- Inefficient, $\epsilon \leq 10^{-6}$ needs $k > 2200$
- Can we do better?

Naive approach



- Error $\epsilon = \frac{1}{\cos \frac{\pi}{k}} - 1 \approx \frac{\pi^2}{2k^2}$
- Inefficient, $\epsilon \leq 10^{-6}$ needs $k > 2200$
- Can we do better?

Naive approach



- Error $\epsilon = \frac{1}{\cos\frac{\pi}{k}} - 1 \approx \frac{\pi^2}{2k^2}$
- Inefficient, $\epsilon \leq 10^{-6}$ needs $k > 2200$
- Can we do better?

Extended Formulations

- Augment variable set (x_1, x_2) to $(x_1, x_2, \boldsymbol{\alpha})$
- Define set $\mathcal{S}$ on enlarged space
- Project

$$\mathcal{C} = \text{proj}_{x_1, x_2} \mathcal{S}$$

- Amazing fact in high dimensions:
  Simple $\mathcal{S}$ (small number of inequalities) can create complicated $\mathcal{C}$ (exponential number of inequalities)

Extended Formulations

- Augment variable set (x_1, x_2) to $(x_1, x_2, \boldsymbol{\alpha})$
- Define set $\mathcal{S}$ on enlarged space
- Project

$$\mathcal{C} = \mathrm{proj}_{x_1, x_2} \mathcal{S}$$

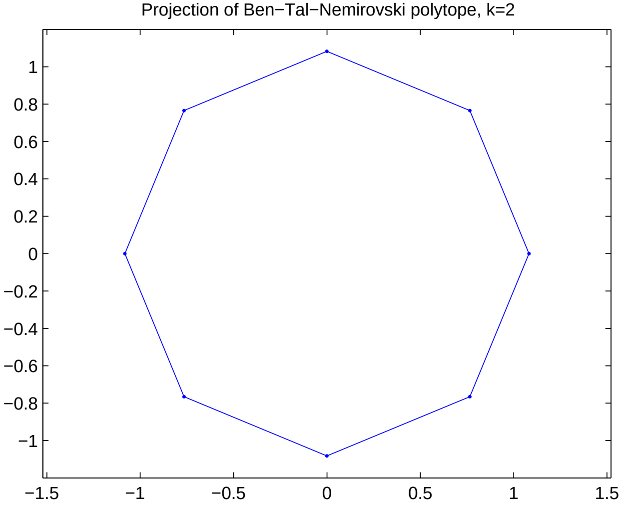
- Amazing fact in high dimensions:
  Simple $\mathcal{S}$ (small number of inequalities) can create complicated $\mathcal{C}$ (exponential number of inequalities)

Ben-Tal/Nemirovski Polyhedron

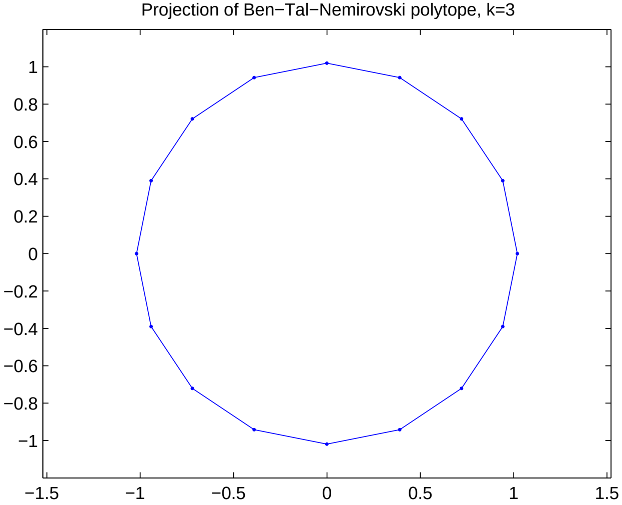
Variables x_1, x_2, and $\boldsymbol{\alpha} = (\xi^j, \eta^j)_{j=0,\dots,k}$, parameter k

$$
\begin{aligned}
&\xi^0 \geq x_1, \qquad \xi^0 \geq -x_1, \\
&\eta^0 \geq x_2, \qquad \eta^0 \geq -x_2, \\
&\xi^j = \cos\left(\frac{\pi}{2^{j+1}}\right)\xi^{j-1} + \sin\left(\frac{\pi}{2^{j+1}}\right)\eta^{j-1}, \qquad j = 1,\dots,k \\
&\eta^j \geq -\sin\left(\frac{\pi}{2^{j+1}}\right)\xi^{j-1} + \cos\left(\frac{\pi}{2^{j+1}}\right)\eta^{j-1}, \qquad j = 1,\dots,k \\
&\eta^j \geq \sin\left(\frac{\pi}{2^{j+1}}\right)\xi^{j-1} - \cos\left(\frac{\pi}{2^{j+1}}\right)\eta^{j-1}, \qquad j = 1,\dots,k \\
&\xi^k \leq 1, \\
&\eta^k \leq \tan\left(\frac{\pi}{2^{k+1}}\right)\xi^k.
\end{aligned}
$$

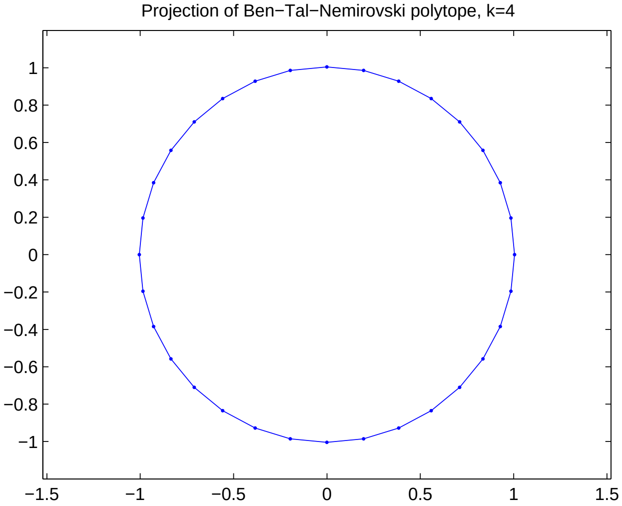
Ben-Tal/Nemirovski Polyhedron (cont)



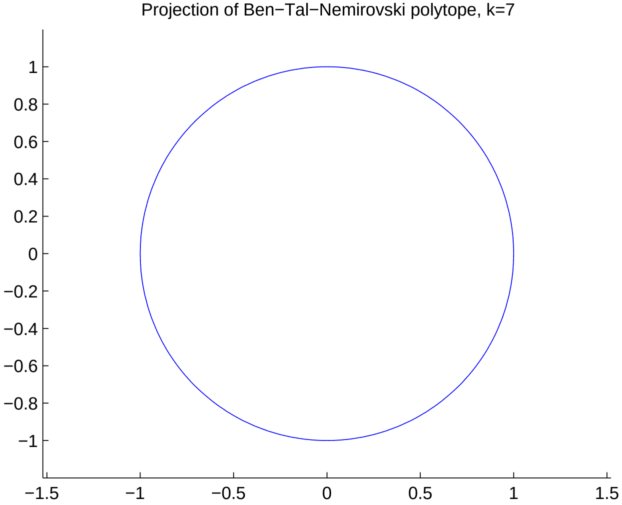
Ben-Tal/Nemirovski Polyhedron (cont)



Ben-Tal/Nemirovski Polyhedron (cont)



Ben-Tal/Nemirovski Polyhedron (cont)



Ben-Tal/Nemirovski Polyhedron (cont)

- BTN-k, for $k = 2, 3, 4, \ldots$
- Number of non-zero coefficients in system: $9k + 11$, linear in k
- Number of vertices in (x_1, x_2)-projection: 2^{k+1}

k	No. vert.	NNZ	ϵ
4	32	47	0.0048
5	64	56	0.0012
6	128	65	$3.0 \cdot 10^{-4}$
...	...	...	...
k	2^{k+1}	$9k + 11$	$O(\frac{1}{4^k})$

Ben-Tal/Nemirovski Polyhedron (cont)

- BTN-k, for $k = 2, 3, 4, \ldots$
- Number of non-zero coefficients in system: $9k + 11$, linear in k
- Number of vertices in (x_1, x_2)-projection: 2^{k+1}
- BTN: error $\epsilon = \frac{1}{\cos \frac{\pi}{2^{k+1}}} - 1 = O(\frac{1}{4^k})$ ($\epsilon \leq 3 \cdot 10^{-7}$ for $k = 12$)
- Naive: error $\epsilon = \frac{1}{\cos \frac{\pi}{k}} - 1 \approx \frac{\pi^2}{2k^2}$ ($\epsilon \leq 10^{-6}$ for $k = 2,200$)
- $\rightarrow$ A much better approximation

From Sets to Functions

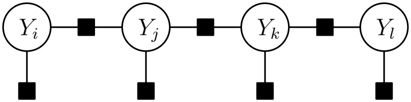
Connections to the Literature

- Extended formulations for polyhedral sets (Balas, 1975)
- Extended formulations for convex functions in integer programs (Miller and Wolsey, 2003)

In computer vision (under various names, often combined with an inference method)

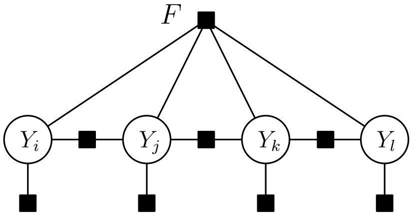
- (Rother and Kohli, 2011)
- (Ladicky et al., ECCV 2010)
- (Ishikawa, CVPR 2009)
- ...

Higher-order Interactions



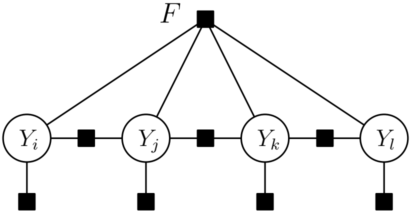
- Problem: graphical model formulation not expressive enough to capture structure of E_F,
- Decomposable higher-order interactions
  - Representable by a set of T new variables with state spaces S_t,
  - T, S_t bounded by a polynomial in the scope size and variable state spaces

Higher-order Interactions



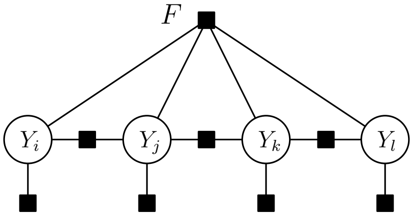
- Problem: graphical model formulation not expressive enough to capture structure of E_F,
- Decomposable higher-order interactions
  - Representable by a set of T new variables with state spaces S_t,
  - T, S_t bounded by a polynomial in the scope size and variable state spaces

Higher-order Interactions



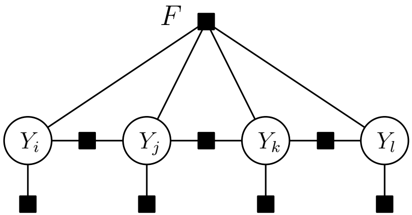
- Problem: graphical model formulation not expressive enough to capture structure of E_F,
- Decomposable higher-order interactions
  - Representable by a set of T new variables with state spaces S_t,
  - T, S_t bounded by a polynomial in the scope size and variable state spaces

Higher-order Interactions



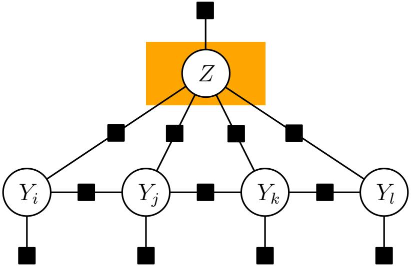
- Problem: graphical model formulation not expressive enough to capture structure of E_F,
- Decomposable higher-order interactions
  - Representable by a set of T new variables with state spaces S_t,
  - T, S_t bounded by a polynomial in the scope size and variable state spaces

Decomposable Higher-order Interactions



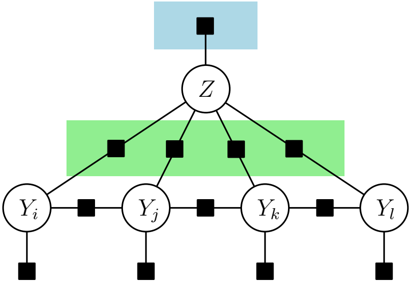
1. Partition $\mathcal{Y}_F$ into a small set $\mathcal{Z}$ of equivalence classes,
2. Introduce a new model variable $Z \in \mathcal{Z}$
3. Build simple energy model for each class (e.g. constant)
4. Integrate with original variables

Decomposable Higher-order Interactions



1. Partition $\mathcal{Y}_F$ into a small set $\mathcal{Z}$ of equivalence classes,
2. Introduce a new model variable $Z \in \mathcal{Z}$
3. Build simple energy model for each class (e.g. constant)
4. Integrate with original variables

Decomposable Higher-order Interactions



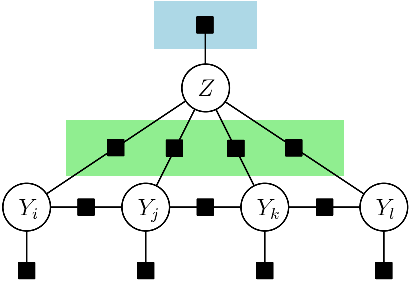
1. Partition $\mathcal{Y}_F$ into a small set $\mathcal{Z}$ of equivalence classes,
2. Introduce a new model variable $Z \in \mathcal{Z}$
3. Build simple energy model for each class (e.g. constant)
4. Integrate with original variables

Example 1: Pattern-based Potential

- (Rother et al., CVPR 2009), (Komodakis and Paragios, CVPR 2009)
- Match a small set of patterns with low energy or assign a default energy
- Pattern set $\mathcal{P}$,

$$E_F(y_F) = \begin{cases} C_{y_F} & \text{if } y_F \in \mathcal{P} \\ C_{\max} & \text{otherwise.} \end{cases}$$

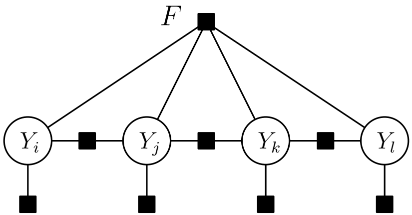
Example 1: Pattern-based Potential (cont)



$$E_F(y_F) = \begin{cases} C_{y_F} & \text{if } y_F \in \mathcal{P} \\ C_{\max} & \text{otherwise.} \end{cases}$$

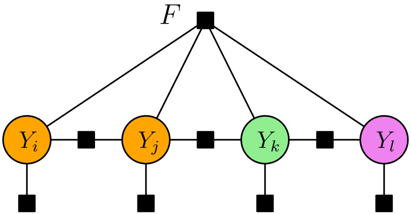
- Fix joint configuration y_F
- Pattern cost C_{y_F} or $C_{\max}$

Example 2: Co-occurence Potential



- (Ladicky et al., ECCV 2010), (Delong et al., CVPR 2010)
- Have a cost function based on what sets of labels appear (independent of their counts)

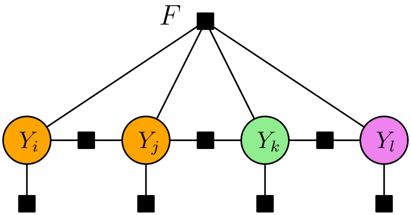
Example 2: Co-occurence Potential



$$E_F(y) = C(L(y)) = C(\{\bullet, \bullet, \bullet\})$$

- (Ladicky et al., ECCV 2010), (Delong et al., CVPR 2010)
- Have a cost function based on what sets of labels appear (independent of their counts)

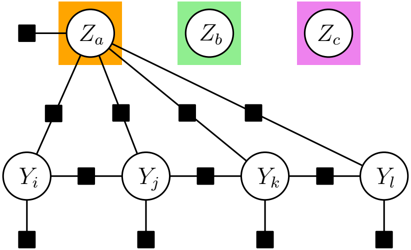
Example 2: Co-occurence Potential (cont)



$$E_F(y) = C(L(y)) = C(\{\bullet, \bullet, \bullet\})$$

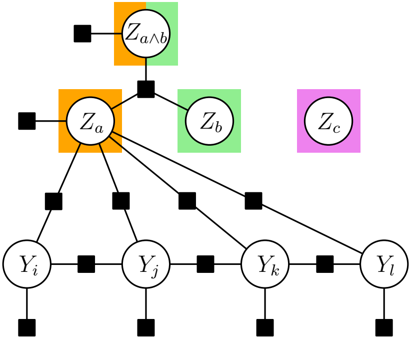
- Extended formulation with "has-color"-variable
- This extended formulation: further conditions required for E_F
- Extension possible for arbitrary E_F
- Size polynomial in the number of subsets

Example 2: Co-occurence Potential (cont)



- Extended formulation with “has-color”-variable
- This extended formulation: further conditions required for E_F
- Extension possible for arbitrary E_F
- Size polynomial in the number of subsets

Example 2: Co-occurence Potential (cont)



- Extended formulation with "has-color"-variable
- This extended formulation: further conditions required for E_F
- Extension possible for arbitrary E_F
- Size polynomial in the number of subsets

Non-Decomposable Interactions

Non-decomposable,

- Not representable by a small set of new variables with small state spaces
- Requires analysis outside the graphical model framework

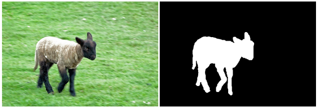
Examples of non-decomposable interactions

- Cooperative cuts (Jegelka and Bilmes, CVPR 2011)
- Topological constraints (Vicente et al., CVPR 2008), (Nowozin and Lampert, CVPR 2009), (Chen et al., CVPR 2011)

Connectivity: Connected Subgraph Polytope

Object segmentation

- "Connectedness": the resulting object segmentations should be connected
- (Nowozin and Lampert, CVPR 2009), (Nowozin and Lampert, SIAM IMS 2010)



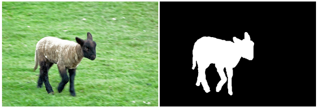
Steps

- Global potential ψ_V: connectivity
- Derive a polyhedral set which captures connected subgraphs
- This set is the *connected subgraph polytope*
- Use MAP-MRF linear programming relaxation, but *intersect* with this set

Connectivity: Connected Subgraph Polytope

Object segmentation

- "Connectedness": the resulting object segmentations should be connected
- (Nowozin and Lampert, CVPR 2009), (Nowozin and Lampert, SIAM IMS 2010)



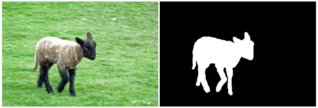
Steps

- Global potential ψ_V: connectivity
- Derive a polyhedral set which captures connected subgraphs
- This set is the *connected subgraph polytope*
- Use MAP-MRF linear programming relaxation, but *intersect* with this set

Connectivity: Connected Subgraph Polytope

Object segmentation

- "Connectedness": the resulting object segmentations should be connected
- (Nowozin and Lampert, CVPR 2009), (Nowozin and Lampert, SIAM IMS 2010)



Steps

- Global potential ψ_V: connectivity
- Derive a polyhedral set which captures connected subgraphs
- This set is the *connected subgraph polytope*
- Use MAP-MRF linear programming relaxation, but *intersect* with this set

Connected Subgraph Polytope (cont)

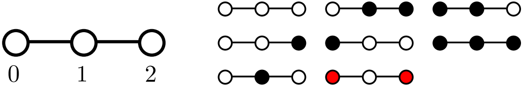
Definition (Connected Subgraph Polytope)

Given a simple, connected, undirected graph $G = (V, E)$, consider indicator variables $y_i \in \{0, 1\}$, $i \in V$. Let $C = \{\mathbf{y} : G' = (V', E') \text{ connected, with } V' = \{i : y_i = 1\}, E' = (V' \times V') \cap E\}$ denote the finite set of connected subgraphs of G. Then we call the convex hull $Z = \mathrm{conv}(C)$ the *connected subgraph polytope*.

Connected Subgraph Polytope (cont)

Definition (Connected Subgraph Polytope)

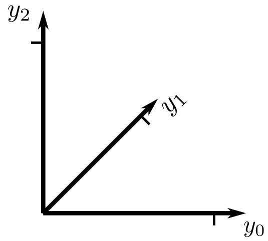
Given a simple, connected, undirected graph $G = (V, E)$, consider indicator variables $y_i \in \{0, 1\}$, $i \in V$. Let $C = \{\mathbf{y} : G' = (V', E') \text{ connected, with } V' = \{i : y_i = 1\}, E' = (V' \times V') \cap E\}$ denote the finite set of connected subgraphs of G. Then we call the convex hull $Z = \mathrm{conv}(C)$ the *connected subgraph polytope*.

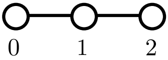


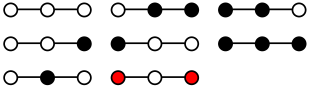
Connected Subgraph Polytope (cont)

Definition (Connected Subgraph Polytope)

Given a simple, connected, undirected graph $G = (V, E)$, consider indicator variables $y_i \in \{0, 1\}$, $i \in V$. Let $C = \{\mathbf{y} : G' = (V', E') \text{ connected, with } V' = \{i : y_i = 1\}, E' = (V' \times V') \cap E\}$ denote the finite set of connected subgraphs of G. Then we call the convex hull $Z = \mathrm{conv}(C)$ the *connected subgraph polytope*.



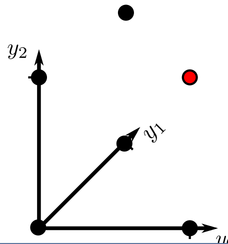


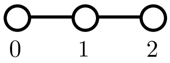


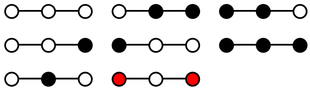
Connected Subgraph Polytope (cont)

Definition (Connected Subgraph Polytope)

Given a simple, connected, undirected graph $G = (V, E)$, consider indicator variables $y_i \in \{0, 1\}$, $i \in V$. Let $C = \{\mathbf{y} : G' = (V', E') \text{ connected, with } V' = \{i : y_i = 1\}, E' = (V' \times V') \cap E\}$ denote the finite set of connected subgraphs of G. Then we call the convex hull $Z = \mathrm{conv}(C)$ the *connected subgraph polytope*.



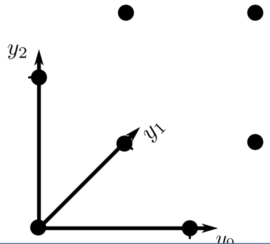


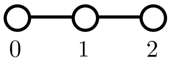


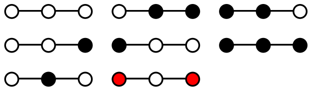
Connected Subgraph Polytope (cont)

Definition (Connected Subgraph Polytope)

Given a simple, connected, undirected graph $G = (V, E)$, consider indicator variables $y_i \in \{0, 1\}$, $i \in V$. Let $C = \{\mathbf{y} : G' = (V', E')\ \text{connected, with}\ V' = \{i : y_i = 1\}, E' = (V' \times V') \cap E\}$ denote the finite set of connected subgraphs of G. Then we call the convex hull $Z = \text{conv}(C)$ the *connected subgraph polytope*.



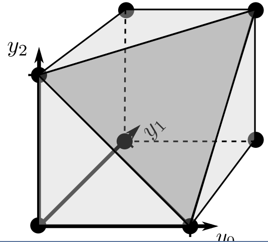


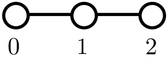


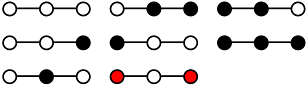
Connected Subgraph Polytope (cont)

Definition (Connected Subgraph Polytope)

Given a simple, connected, undirected graph $G = (V, E)$, consider indicator variables $y_i \in \{0, 1\}$, $i \in V$. Let $C = \{\mathbf{y} : G' = (V', E') \text{ connected, with } V' = \{i : y_i = 1\}, E' = (V' \times V') \cap E\}$ denote the finite set of connected subgraphs of G. Then we call the convex hull $Z = \mathrm{conv}(C)$ the *connected subgraph polytope*.







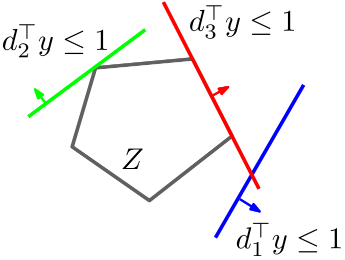
Facets and Valid Inequalities

Convex polytopes have two equivalent representations

- As a convex combination of extreme points
- As a set of facet-defining linear inequalities

A linear inequality with respect to a polytope can be

- *valid*, does not cut off the polytope,
- *representing a face*, valid and touching,
- *facet-defining*, representing a face of dimension one less than the polytope.



Warmup

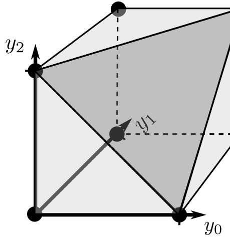
Some basic properties about the connected subgraph polytope Z. Note that Z depends on the graph structure.

Lemma

If G is connected, $dim(Z) = |V|$, that is, Z has full dimension.

Lemma

For all $i \in V$, the inequalities $y_i \geq 0$ and $y_i \leq 1$ are facet-defining for Z.

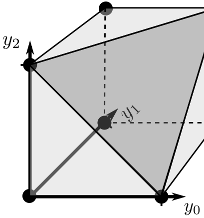


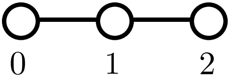
An Exponential-sized Class of Facet-defining Inequalities

Theorem

The following linear inequalities are facet-defining for $Z = conv(C)$.

$$y_i + y_j - \sum_{k \in S} y_k \leq 1, \quad \forall (i,j) \notin E : \forall S \in \bar{\mathcal{S}}(i,j). \qquad (1)$$





$$y_0 + y_2 - y_1 \leq 1.$$

Intuition

$$y_i + y_j - \sum_{k \in S} y_k \leq 1, \quad \forall (i,j) \notin E : \forall S \in \bar{\mathcal{S}}(i,j)$$

If two vertices i and j are selected ($y_i = y_j = 1$, shown in black), then any set of vertices which separate them (set S) must contain at least one selected vertex.

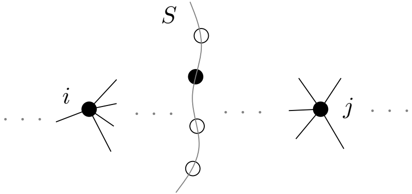


Figure: Vertex i and j and one vertex separator set $S \in \bar{\mathcal{S}}(i,j)$.

Formulation

Theorem

C, the set of all connected subgraphs, can be described exactly by the following constraint set.

$$y_i + y_j - \sum_{k \in S} y_k \leq 1, \forall (i,j) \notin E : \forall S \in \mathcal{S}(i,j), \qquad (2)$$

$$y_i \in \{0, 1\}, \qquad i \in V. \qquad (3)$$

This means

- inequalities together with integrality are a *formulation* of the set of connected subgraphs,
- we can attempt to relax (3) to

$$y_i \in [0; 1], \qquad i \in V.$$

- (Problem): number of inequalities (2) is exponential in $|V|$.

Conclusions

- Discrete graphical models are just one way to capture structure
- There are other tractable/approximable structures
  - Extended formulations (latent variables with specific tying)
  - Polyhedral combinatorics

Open questions

- How to perform probabilistic inference in higher-order models?
- How to parametrize and learn higher-order models?
- (Is there a more suitable formalism than either graphical models or polytopes?)

Conclusions

- Discrete graphical models are just one way to capture structure
- There are other tractable/approximable structures
  - Extended formulations (latent variables with specific tying)
  - Polyhedral combinatorics

Open questions

- How to perform probabilistic inference in higher-order models?
- How to parametrize and learn higher-order models?
- (Is there a more suitable formalism than either graphical models or polytopes?)

Thank you!

feedback most welcome

`nowozin@gmail.com`