Maximum Entropy Sampling

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Examples

- Coverage functions
  - Underlying finite universe U
  - Each $i \in N$ corresponds to a set $T_i \subset U$
  - $f(S) = |\cup_{i \in S} T_i|$, for $S \subset N$
  - Properties: monotone and nonnegagtive

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  - Properties: monotone and nonnegagtive
- Cut functions
  - (Di)Graph $G = (N, E)$ on vertex set N
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- Matroids / matroid intersection (e.g., trees / assignments)
  - $f(S) := r(S)$
  - $f(S) := r_1(S) + r_2(N \setminus S)$
    (min of f = maximum size of a set "independent" in M_1 and M_2)
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  - Properties: monotone and nonnegative
- (Differential/continuous) entropy of a finite set of Gaussian random variables
  - $f(S) :=$ log det $C[S]$, where $C[N]$ is positive semidefinite
  - Does not trivially have additional, nice properties

Information = Disorder

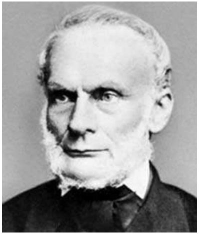
"Chance and chance alone has a message for us. Everything that occurs out of necessity, everything expected, repeated day in and day out, is mute. Only chance can speak to us. We read its message much as gypsies read the images made by coffee grounds at the bottom of a cup."

- Milan Kundera (The Unbearable Lightness of Being)

Entropy

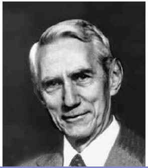
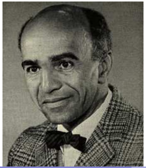
"I propose to name the magnitude $\mathcal{S}$ the entropy of the body from the Greek word $\eta\tau\rho o\pi\grave{\eta}$, a transformation. I have intentionally formed the word entropy so as to be as similar as possible to the word energy, since both these quantities, which are to be known by these names, as so nearly related to each other in their physical significance that a certain similarity in their names seemed to me advantageous ..."

— R. Clausius (1865)

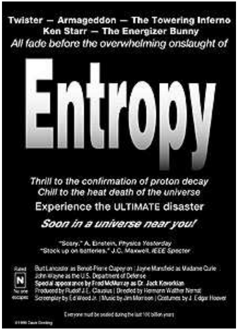


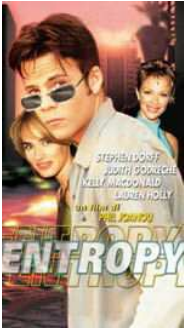
Historical Highlights

- R. Clausius (1865) — "entropy" (also Carnot and Kelvin in their versions of the 2nd law of thermodynamics), arrow of time *("What then is time? If no one asks me, I know what it is. If I wish to explain it to him who asks, I do not know." — St. Augustine)*
- L. Boltzmann (1877) — statistical mechanics
- C. Shannon (1948) — information theory
- D. Blackwell (1951) — statistics

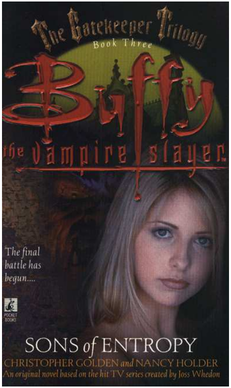



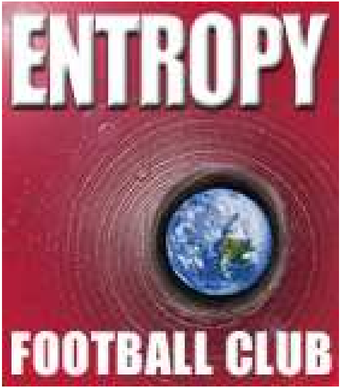
Entropy more recently...

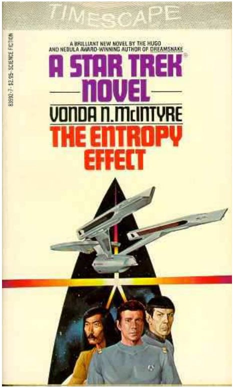

Twister — Armageddon — The Towering Inferno
Ken Starr — The Energizer Bunny
All fade before the overwhelming onslaught of
Entropy
Thrill to the confirmation of proton decay
Chill to the heat death of the universe
Experience the ULTIMATE disaster
Soon in a universe near you!
"Scary." A. Einstein, Physics Yesterday
"Stock up on batteries." J.C. Maxwell, IEEE Spectre
Rated
N
No one escapes
Burt Lancaster as Benoit-Pierre Clapeyron | Jayne Mansfield as Madame Curie
John Wayne as the U.S. Department of Defense
Special appearance by Fred McMurray as Dr. Jack Kevorkian
Produced by Rudolf J.E. Clausius | Directed by Hermann Walther Nernst
Screenplay by Ed Wood Jr. | Music by Jim Morrison | Costumes by J. Edgar Hoover
Everyone must be seated during the last 100 billion years
©1998 Dave Gosling



and more...


The Gatekeeper Trilogy
Book Three
Buffy the vampire slayer
The final battle has begun....
POCKET BOOKS
SONS of ENTROPY
CHRISTOPHER GOLDEN and NANCY HOLDER
An original novel based on the hit TV series created by Joss Whedon


ENTROPY
FOOTBALL CLUB


TIMESCAPE
83592-7 · $2.95 · SCIENCE FICTION
A BRILLIANT NEW NOVEL BY THE HUGO AND NEBULA AWARD-WINNING AUTHOR OF DREAMSNAKE
A STAR TREK NOVEL
VONDA N. McINTYRE
THE ENTROPY EFFECT

Maximum-Entropy Sampling

$N = \{1, 2, \ldots, n\}$

Random $Y_N = \{\, Y_j \;:\; j \in N\}$ with continuous density g_N

Goal: Choose $S \subset N$, with $|S| = s$, so that observing Y_S maximizes the "information" obtained about Y_N .

Entropy: $h(S) := -E[\ln g_S(Y_S)]$.

Motivation: Environmental Monitoring

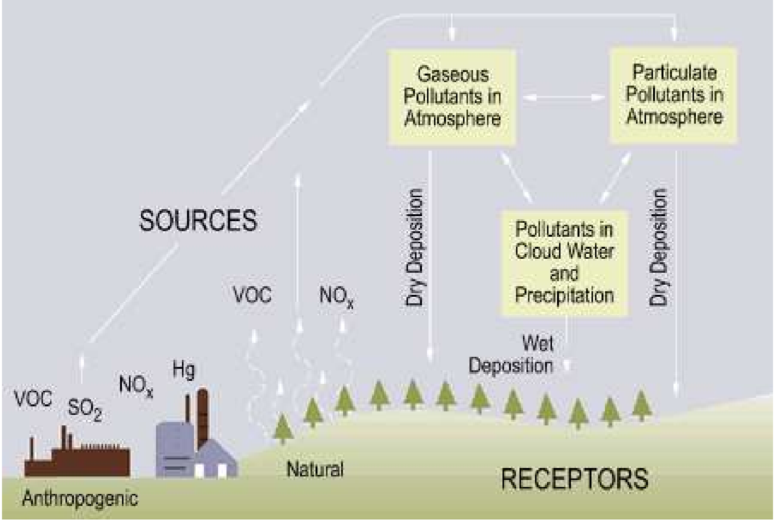
- Sites of emission $\Longrightarrow$ Causes
- Sites of deposition $\Longrightarrow$ Effects*

$*$ Clean Air Act of 1990 and its revisions mandate effects monitoring

National **A**cidic **D**eposition **P**rogram/
National **T**rends **N**etwork
`nadp.sws.uiuc.edu`

1978 - 22 stations. 2012 - $>$ 240 stations.
Precipitation collected weekly; analyzed for: Hydrogen (acidity as pH — 'acid rain'), Sulfate, Nitrate, Ammonia, Chloride, Calcium, Magnesium, Potassium, Sodium

Wet vs. Dry

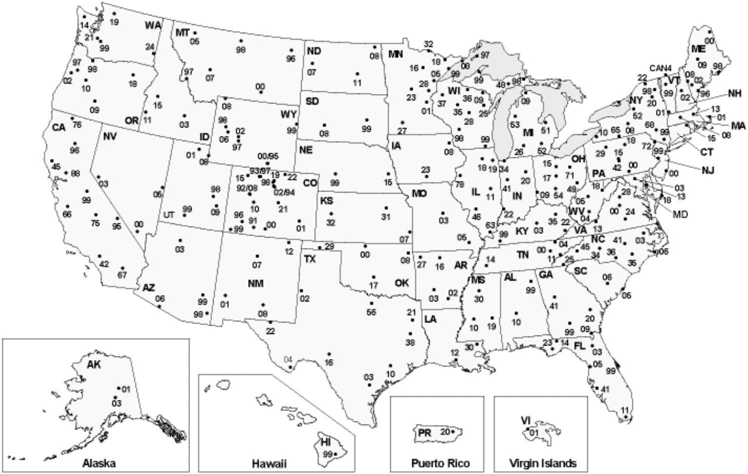

Gaseous Pollutants in Atmosphere
Particulate Pollutants in Atmosphere
SOURCES
Pollutants in Cloud Water and Precipitation
Dry Deposition
Dry Deposition
VOC
NO_x
Wet Deposition
Hg
NO_x
VOC
SO_2
Natural
RECEPTORS
Anthropogenic

TPC 3000 (Yankee Environ. Sys.)

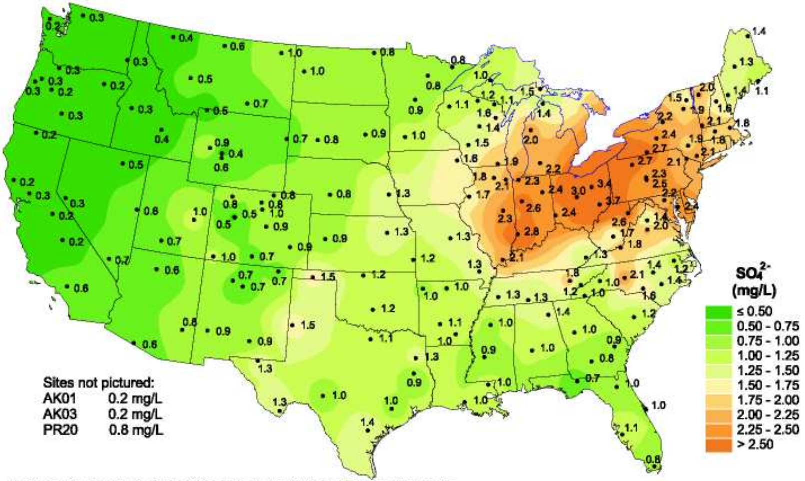
US Federal $

- YES has US federal funding of $300K to develop a new prototype over 2 years
- $3.5M federal funding for NTN ('99)
- $\sim$ $150M total US federal funding for environmental monitoring ('99)
    - much other monitoring focused on CO, NO_2, SO_2 and small particulate matter

National Atmospheric Deposition Program
National Trends Network



Sulfate ion concentration, 1994

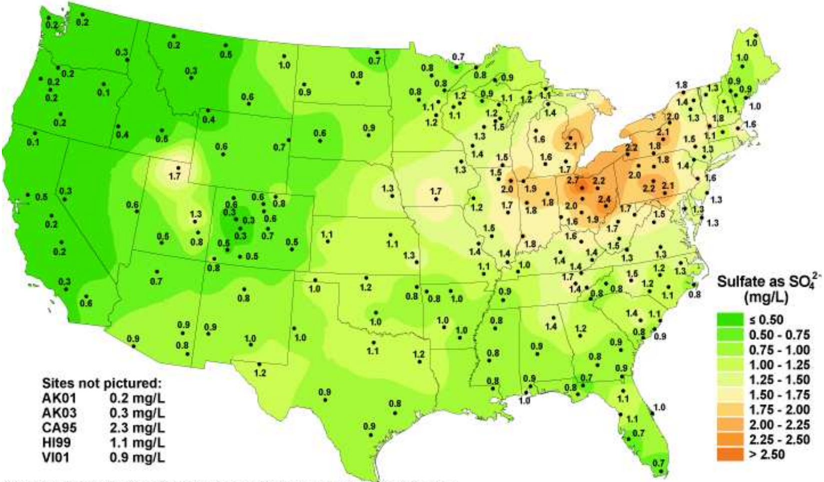


Sites not pictured:

AK01	0.2 mg/L
AK03	0.2 mg/L
PR20	0.8 mg/L

National Atmospheric Deposition Program/National Trends Network
http://nadp.sws.uiuc.edu

Sulfate ion concentration, 2002

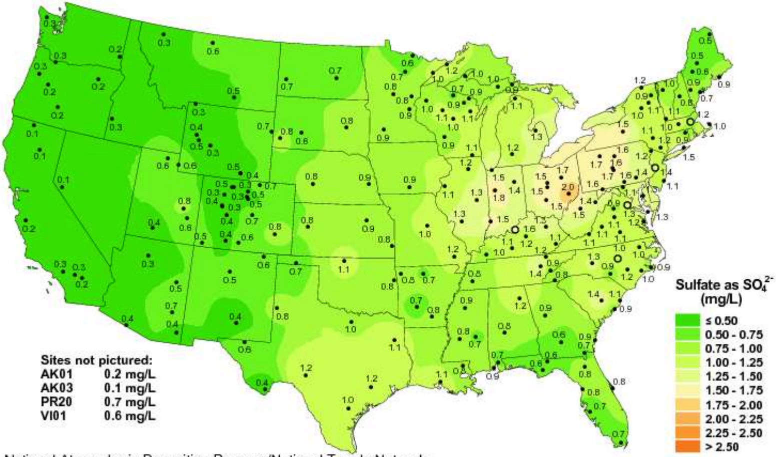


Sites not pictured:

AK01	0.2 mg/L
AK03	0.3 mg/L
CA95	2.3 mg/L
HI99	1.1 mg/L
VI01	0.9 mg/L

National Atmospheric Deposition Program/National Trends Network
http://nadp.sws.uiuc.edu

Sulfate ion concentration, 2008



Sulfate as SO_4^{2-} (mg/L)

- 🟩 ≤ 0.50
- 🟩 0.50 - 0.75
- 🟩 0.75 - 1.00
- 🟩 1.00 - 1.25
- 🟨 1.25 - 1.50
- 🟨 1.50 - 1.75
- 🟧 1.75 - 2.00
- 🟧 2.00 - 2.25
- 🟧 2.25 - 2.50
- 🟧 > 2.50

Sites not pictured:

AK01	**0.2 mg/L**
AK03	**0.1 mg/L**
PR20	**0.7 mg/L**
VI01	**0.6 mg/L**

National Atmospheric Deposition Program/National Trends Network
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Nice Properties of Entropy

- Submodularity ✓: $h(S \cup T) + h(S \cap T) \leq h(S) + h(T)$
- The Gaussian distribution maximizes the entropy for a given covariance matrix C
- Gaussian case: $h(S) = k_s + k \ln \det C[S, S]$
- Conditional Additivity:

$$h(N) = \overbrace{h(S)}^{\max} \overset{\Leftrightarrow}{+} \overbrace{h(N \setminus S|S)}^{\min}$$

  (justifies our objective function)

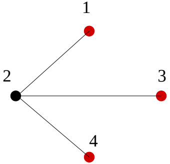
- Change coordinate systems: Entropy difference is logdet(Jacobian of transformation)
- Complementation:
  $\ln \det C[S, S] = \ln \det C + \ln \det C^{-1}[N \setminus S, N \setminus S]$

Not-So-Nice Property

Proposition [Ko, Lee, Queyranne]. The maximum-entropy sampling problem is NP-Hard (even for the Gaussian diagonally-dominant case)

Proof:

- **INDEPENDENT SET**: Does a simple undirected graph G on n vertices have an independent set of vertices of cardinality s ?
- Let $C := A(G) + 3nI$



$$\begin{pmatrix} 12 & 1 & 0 & 0 \\ 1 & 12 & 1 & 1 \\ 0 & 1 & 12 & 0 \\ 0 & 1 & 0 & 12 \end{pmatrix}$$

(KLQ) Branch . . .

- **Fixing j out of S:**
  ⇒ Strike out row and column j : $C[N,N] \rightarrow$

$$C[N-j, N-j]$$

- **Fixing j in S:**
  ⇒ Schur complement of $C[j,j]$: $C[N,N] \rightarrow$

$$C[N-j, N-j] - C[N-j, j]\, C^{-1}[j,j]\, C[j, N-j]$$

(and solution/bounds are shifted by $\ln C[j,j]$).

. . . and Bound

- Lower bounds: Greedy, local-search, rounding heuristics
- Upper bounds:
  - Spectral based bounds
    - ⋆ Ko, Lee, Queyranne '95 (original B&B and spectral bound)
    - ⋆ Lee '98 (extension to side constraints)
    - ⋆ Hoffman, Lee & Williams '01 (spectral partition bounds)
    - ⋆ Lee, Williams '03 (tightening HLW via ILP and matching)
    - ⋆ Anstreicher, Lee '04 (generalization of HLW)
    - ⋆ Burer, Lee '07 (another approach to computing the AL bound)
  - NLP relaxation
    - ⋆ Anstreicher, Fampa, Lee & Williams '96 (continuous NLP relaxation and parallel B&B)

Complementary Bounds (Anstreicher, Fampa, Lee, Williams)

$$\ln \det C[S,S] = \ln \det C + \ln \det C^{-1}[N \setminus S, N \setminus S]$$

- So a maximum entropy s-subset of N with respect to C is the complement of a maximum entropy $(n-s)$-subset of N with respect to C^{-1}
- So a bound on the complementary problem plus the entropy of the entire system is a bound on the original problem
- These complementary bounds can be quite effective

NLP Bound (AFLW)

$$\max f(x) := \ln\det\left(\mathrm{Diag}(x_j^{p_j})\ C\ \mathrm{Diag}(x_j^{p_j}) + \mathrm{Diag}(d_j^{x_j} - d_j x_j^{p_j})\right)$$

$$\text{subject to } \sum_{j\in N} a_{ij}x_j \le b_i, \forall i; \quad \Longleftarrow \text{CONSTRAINTS}$$

$$\sum_{j\in N} x_j = s;$$

$$0 \le x_j \le 1, \forall j,$$

where the constants $d_j > 0$ and $p_j \geq 1$ satisfy $d_j \leq \exp(p_j - \sqrt{p_j})$, and $\mathrm{Diag}(d_j) - C[N,N] \succeq 0$.

NLP Bound, cont'd

$$\max f(x) := \ln \det \left(\mathrm{Diag}(x_j^{p_j})\ C\ \mathrm{Diag}(x_j^{p_j}) + \mathrm{Diag}(d_j^{x_j} - d_j x_j^{p_j}) \right)$$

For $(\overbrace{1, 1, \ldots, 1}^{S}, \overbrace{0, 0, \ldots, 0}^{N \setminus S})$

- $\mathrm{Diag}(d_j^{x_j} - d_j x_j^{p_j}) = \mathrm{Diag}(\overbrace{0, 0, \ldots, 0}^{S}, \overbrace{1, 1, \ldots, 1}^{N \setminus S})$.
- $\mathrm{Diag}(x_j^{p_j})\, C\, \mathrm{Diag}(x_j^{p_j}) = \left(\begin{array}{c|c} C[S,S] & 0 \\ \hline 0 & 0 \end{array} \right)$

NLP Bound: Properties

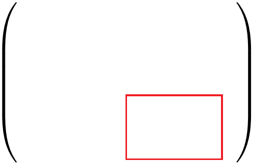
- Concavity: Assume $D \succeq C$, $p_j \geq 1$, $0 < d_j \leq \exp(p_j - \sqrt{p_j})$. Then f is concave for $0 < x \leq e$
- Dominance: Assume that p and d satisfy the above, and $p' \geq p$. Let f' be defined as above, but using p' for p. Then $f'(x) \geq f(x)$ $\forall$ $0 < x \leq e$
- Scaling C by γ adds $s \ln(\gamma)$ to the obj. Let $f_\gamma(x) := \ln\det\left(\gamma X^{p/2}(C-D)X^{p/2} + (\gamma D)^x\right) - s\ln(\gamma)$
  - Scaling: Assume $I \succeq D \succeq C$, $p = e$. Then $f_\gamma(x) \geq f(x)$ $\forall$ $0 \leq x \leq e$, $e^T x = s$ and $0 < \gamma \leq 1$
  - Assume $D \succeq C$, $D \succeq I$. Then $f_\gamma(x) \geq f(x)$ $\forall$ $0 < x \leq e$, $e^T x = s$ and $\gamma \geq 1$, where p is chosen as above

These results give us some guidance for choosing the p_j, d_j and γ

Spectral Bound (KLQ)

$$z \leq \sum_{l=1}^{s} \ln \lambda_l(C)$$

- Determinant = product of eigenvalues.
- Eigenvalue interlacing.



$$\begin{array}{ccc} \lambda_1 & \geq & \lambda_1' \\ \lambda_2 & \geq & \lambda_2' \\ \lambda_3 & \geq & \lambda_3' \\ & \vdots & \\ \lambda_s & \geq & \lambda_s' \end{array}$$

Lagrangian Spectral Bound (Lee)

For handling linear side constraints

$$\min_{\pi \in \mathbb{R}^m_+} v(\pi)$$

where

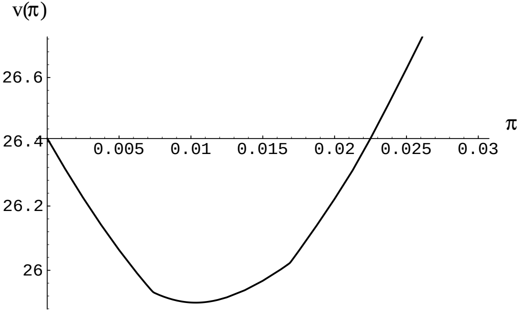
$$v(\pi) := \left\{ \sum_{l=1}^{s} \ln \lambda_l \left(D^\pi \;\; C \;\; D^\pi \right) + \sum_{i \in M} \pi_i b_i \right\},$$

and D^π is the diagonal matrix having

$$D^\pi_{jj} := \exp \left\{ -\frac{1}{2} \sum_{i \in M} \pi_i a_{ij} \right\}$$

Optimizing the Lagrangian Spectral Bound

- v_π is convex (in π)
- v_π is analytic when $\lambda_s\left(D^\pi \; C \; D^\pi\right) > \lambda_{s+1}\left(D^\pi \; C \; D^\pi\right)$



Optimizing the Bound, cont'd

- Let x^l be the eigenvector (of unit Euclidean norm) associated with λ_l.
- Define the <u>continuous solution</u> $\tilde{x} \in \mathbb{R}^N$ by $\tilde{x}_j := \sum_{l=1}^{s} \left(x_j^l\right)^2$, for $j \in N$.
- Define $\gamma \in \mathbb{R}^M$ by $\gamma_i := b_i - \sum_{j \in N} a_{ij}\tilde{x}_j$.

- If $\lambda_s > \lambda_{s+1}$, then γ is the gradient of f at π.
- Can incorporate this in a Quasi-Newton (or, with an expression for the Hessian, a Newton) method for finding the minimum. (Implemented using LBFGS-B (Zhu, Byrd, Nocedal) and a coarse line search)

Spectral Partition Bound (Hoffman, Lee, Willaims)

Let $\mathcal{N} = \{N_1, N_2, ..., N_n\}$ denote a partition of N. Let $C' = 0$ except for $C'[N_k, N_k] = C[N_k, N_k]$.

$$z \leq \sum_{l=1}^{s} \ln \lambda_l(C')$$

- Based on “Fischer’s Inequality”
- For $\mathcal{N} = \{\{1\}, \{2\}, \ldots, \{n\}\}$ we have “the diagonal bound”
- For $\mathcal{N} = \{N, \emptyset, \emptyset, \ldots, \emptyset\}$ we have the ordinary spectral bound
- As we partition N, the optimal value with respect to C' cannot decrease, <u>but the bound can decrease</u>

ILP Bound (Lee, Williams)

Observation: Why calculate eigenvalue based bounds for small blocks of a partition? Just solve the small blocks exactly.
$x_k(i) = 1 \iff$ pick k elements from block N_i

$$
\begin{aligned}
g_s(\mathcal{N}) := \quad & \max \sum_{i=1}^{p} \sum_{k=1}^{|N_i|} f_k(N_i) x_k(i) \\
& \text{s.t. } \sum_{k=1}^{|N_i|} x_k(i) \le 1, \ \text{for } i = 1, 2, \ldots, p; \\
& \sum_{i=1}^{p} \sum_{k=1}^{|N_i|} k x_k(i) = s \\
& x_k(i) \in \{0, 1\}, \ \text{for } i = 1, 2, \ldots, p, \\
& \qquad\qquad\qquad\qquad k = 1, 2, \ldots, |N_i|.
\end{aligned}
$$

ILP Bound, cont'd

- Refines the spectral partition bound.
- Calculate via dynamic programming
  (assuming $|N_i|$ is bounded):

  Boundary conditions:

  $v_t(j) := -\infty$ when $\sum_{i=1}^{j} |N_i| < t \leq s$;

  $v_0(0) := 0$.

  $$v_t(j) = \max_{0 \leq k \leq \min\{|N_j|, t\}} \left\{ f_k(N_j) + v_{t-k}(j-1) \right\}.$$

  Then $v_s(p) = g_s(\mathcal{N})$
- Can even calculate via Edmonds' min-weight matching algorithm when $|N_i| \leq 2$.

Masked Spectral Bound (Anstreicher, Lee)

A mask is a (symmetric) $X \succeq 0$ having $\mathrm{diag}(X) = e$. The associated masked spectral bound is

$$\xi_{C,s}(X) := \textstyle\sum_{l=1}^{s} \ln\left(\lambda_l\left(C \circ X\right)\right)$$

Special combinatorial cases:

- Spectral bound $X := E$
- Diagonal bound $X := I$
- Spectral partition bound $X := \mathrm{Diag}_i(E_i)$

Validity

Based on

- $\det A = \prod_l \lambda_l(A)$
- “Oppenheim’s Inequality”

$$\det\ A \le \det\ A \circ B / \textstyle\prod_{j=1}^{n} B_{jj}\ ,$$

where $A \succeq 0$ and $B \succeq 0$

- the eigenvalue inequalities $\lambda_l(A) \ge \lambda_l(A')$, where $A \succeq 0$, and A' is a principal submatrix of A

Some References

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