Fast approximation algorithms for partition functions of Gibbs distributions

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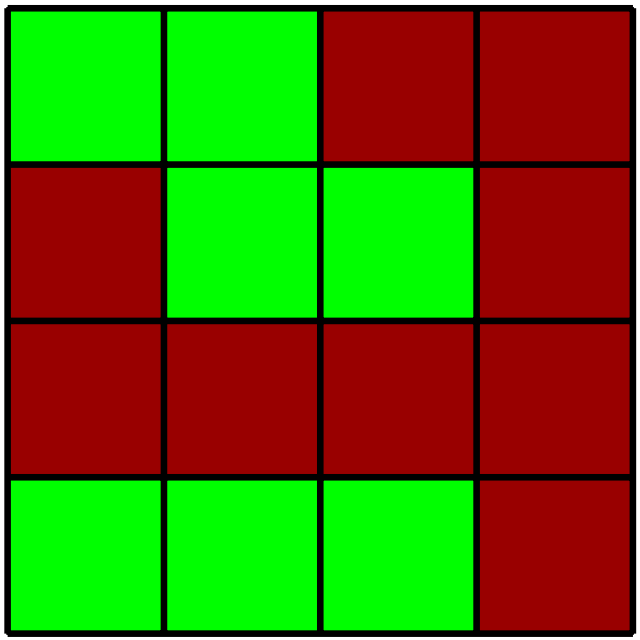
The Problem

Autonormal (Ising) model

Besag [1974] modeled soil plots as good (green) or bad (red)



$d(x) = 11$
(number of adj nodes that disagree)

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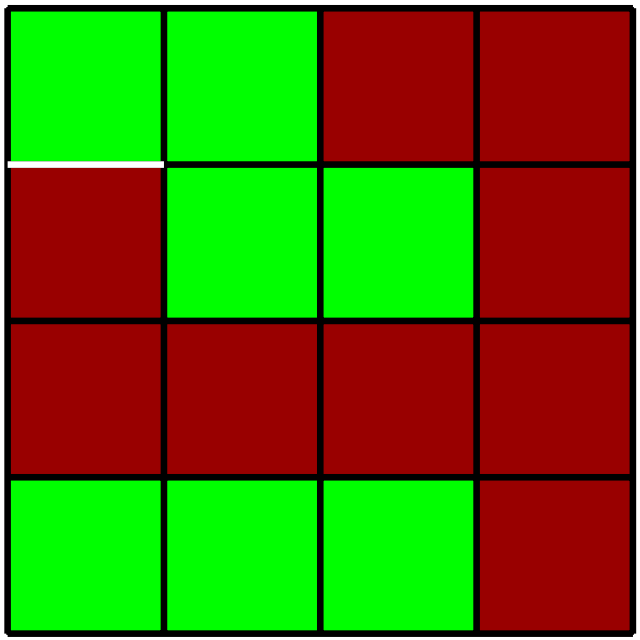

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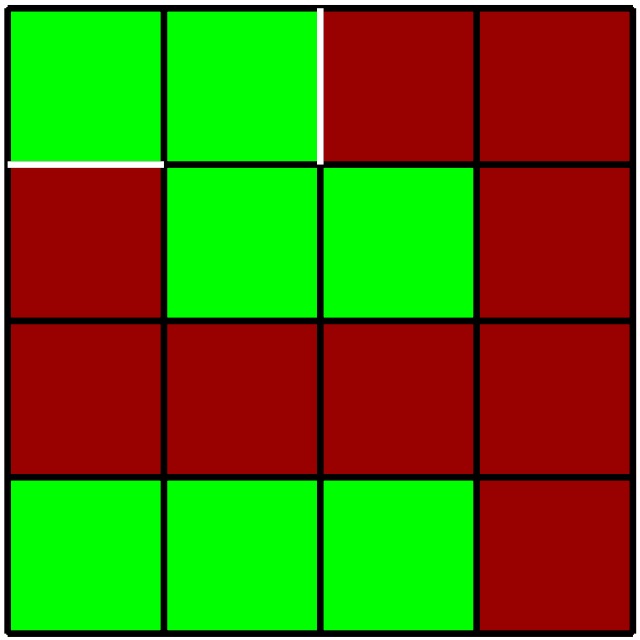

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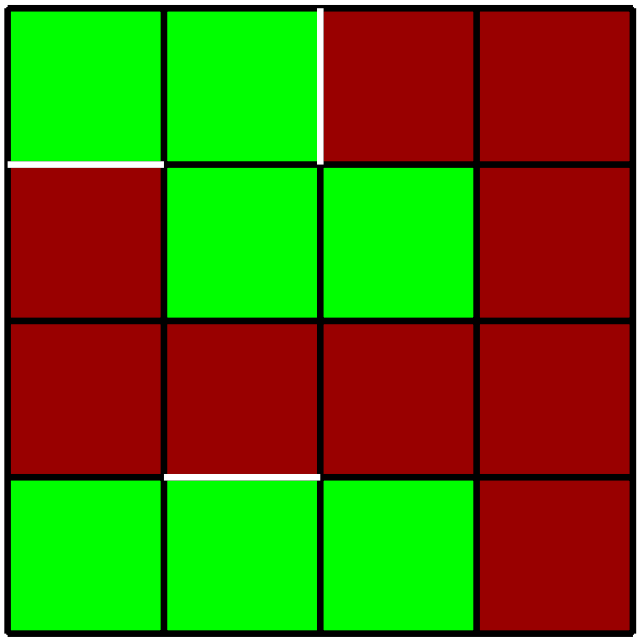

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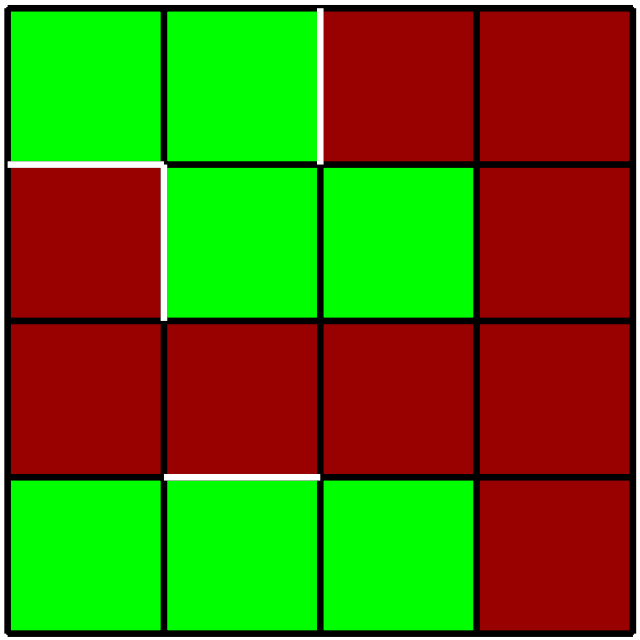

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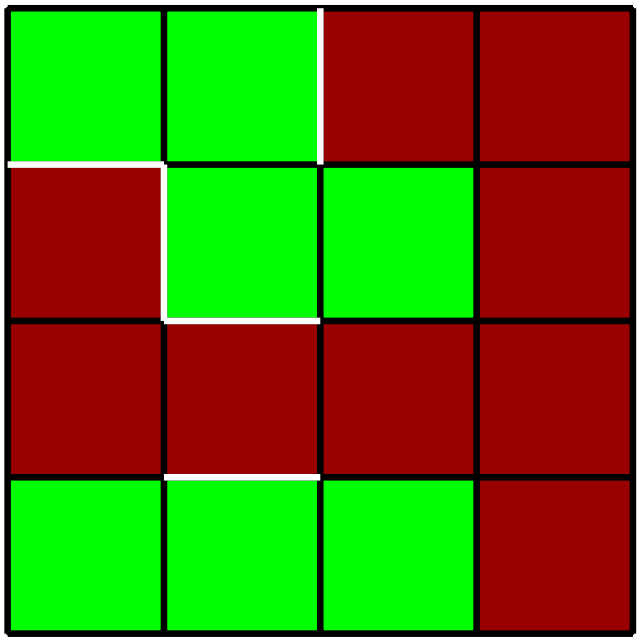

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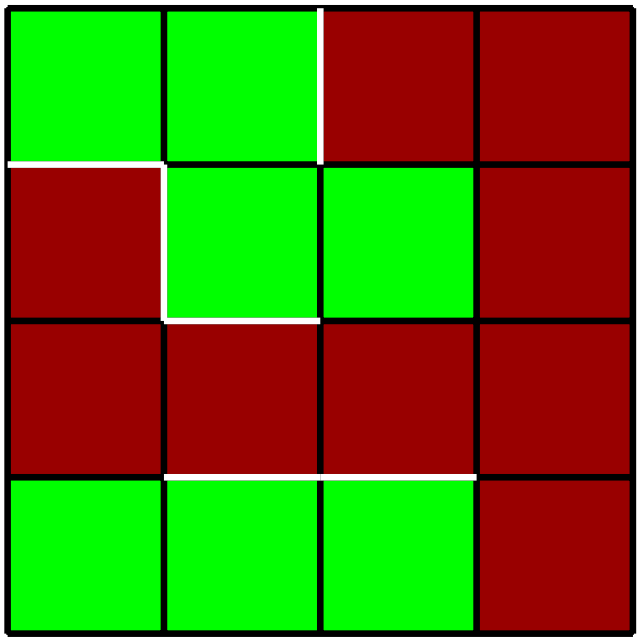

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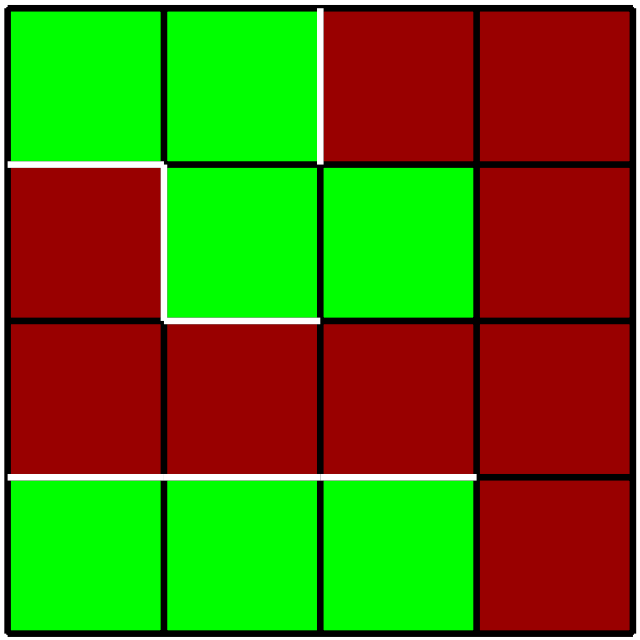

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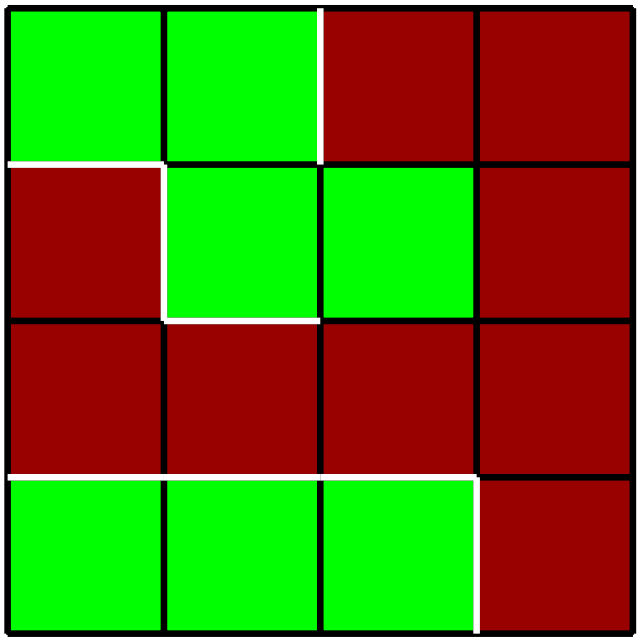

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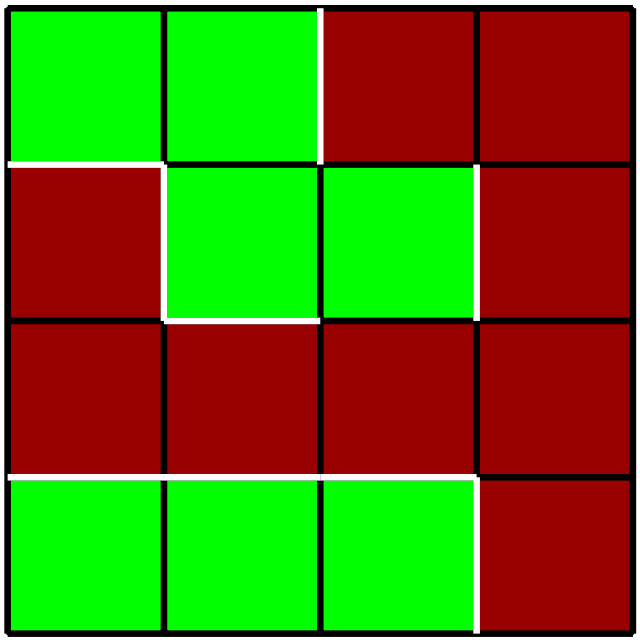

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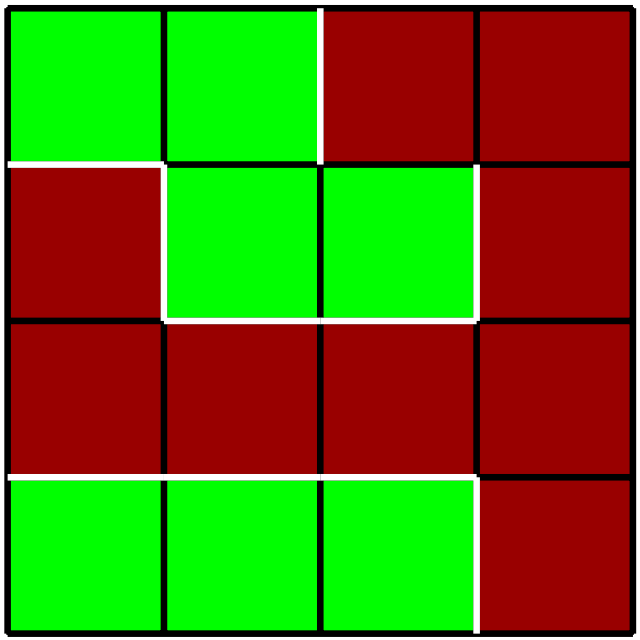

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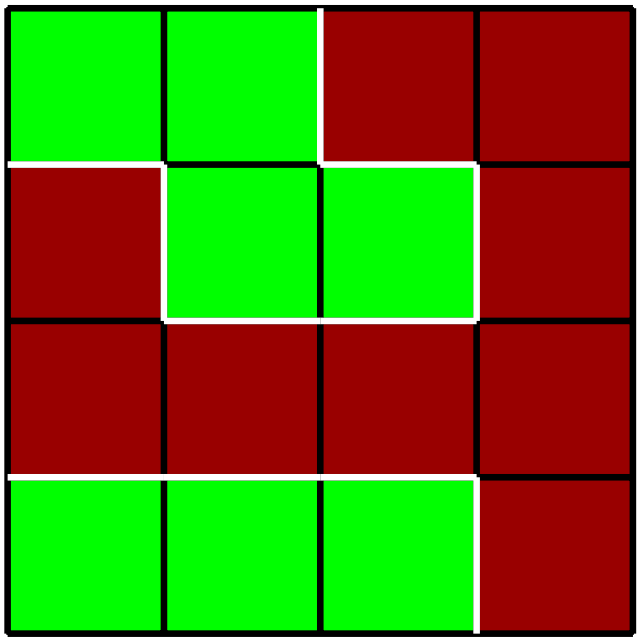

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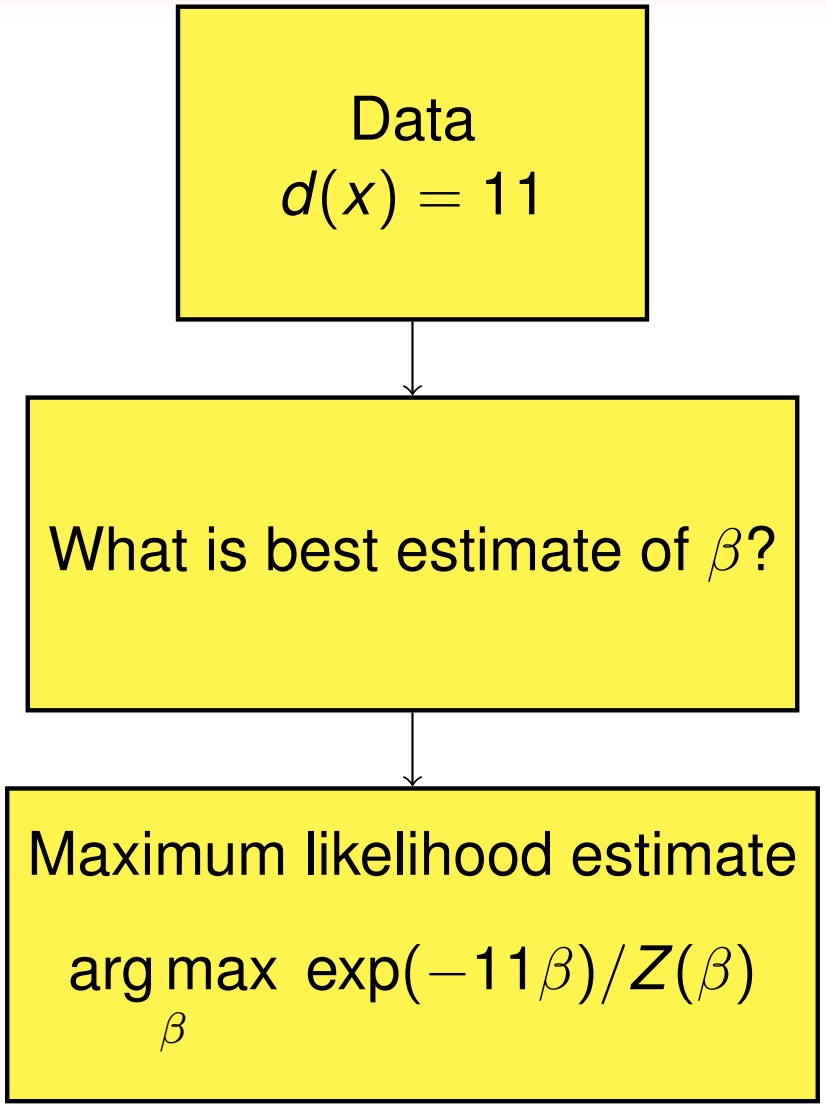
Basic inference



To use the MLE:

Need to know the function $Z(\beta)$ to find MLE
Typically hard to compute

Brute force computation $Z(\beta)$
Requires $2^{\#\text{ of vertices}}$ steps for autonormal model

Bayesian model selection also need $Z(\beta)$
$Z(\beta)$ appears in Bayes' Factor

$Z(\beta)$: The Partition Function

Partition function of Gibbs distribution

Ingredients:

State space $\Omega \subseteq \mathbb{R}^n$
Nonnegative function $H(x)$
Parameter β

Then the goal is to approximate:

$$Z(\beta) = \int_{x \in \Omega} \exp(-\beta H(x)) \, dx$$

Discrete version

Ingredients:

State space $\Omega \subseteq \{1, 2, \ldots, c\}^n$
Nonnegative function $H(x)$
Parameter β

Then the goal is to approximate:

$$Z(\beta) = \sum_{x \in \Omega} \exp(-\beta H(x))$$

Terminology

Definition (Gibbs distribution)

X has a (discrete) *Gibbs distribution* π_β if for all $x \in \Omega$,

$$\mathbb{P}(X = x) = \frac{1}{Z(\beta)} \exp(-\beta H(x)).$$

Definition (Partition function)

The *partition function* of a Gibbs distribution is

$$Z(\beta) = \sum_{x \in \Omega} \exp(-\beta H(x)).$$

Today's result

An approximation algorithm where

- Given $\epsilon > 0$, $\alpha > 0$
- Given the ability to sample from $\pi_{\beta'}$ for $\beta' \in [0, \beta]$
- Outputs $\hat{Z}(\beta)$ so that

$$\mathbb{P}\left(\frac{1}{1+\epsilon} \leq \frac{\hat{Z}(\beta)}{Z(\beta)} \leq 1+\epsilon\right) \geq 1-\alpha.$$

- Requires a number of samples

$$O(\ln(Z(0)/Z(\beta)))\ln(H_m)\epsilon^{-2}\ln(\alpha^{-1})],$$

$$H_m = \text{ median value of } H(X) \text{ where } X \sim \pi_0.$$

Is that good?

Why is problem hard?

Typically $Z(\beta)$ is exponential in n, the input size of problem

Many methods for lowering variance

- Multistage Sampling [Valleau Card 1972]
- Bridge Sampling [Meng Wong 1996]
- Nested Sampling [Skilling 2006]

The above are not approximation algorithms

No *guarantee* on quality of estimate obtained
(But they could be faster in practice)

History of Approximation Algorithms

Let $q = \ln(Z(0)/Z(\beta))$ and ignore ϵ, α factors

Self-reducibility [Jerrum, Valiant, Vazirani 1986]
$O[q^2]$ time under best conditions, best constant ≈ 10

TPA [H., Schott 2010]
$O[q^2]$, and much simpler

SVV [Štefankovič, Vempala, Vigoda 2009]
$O[q \ln(M)^5]$
(where $H(x) \leq M$ for all x and with 10^{10} constant out in front)

Today [H. 2012]
$O[q + 1 + \beta \ln(H_m)] +$ preproccessing
(H_m median of $H(X)$ for $X \sim \pi_0$)

Applications

- Exact p values [Frequentist Statistics]
- Model selection [Bayesian Statistics]
- Phase Transitions [Statistical Physics]
- Approximation Algorithms for #P complete problems [Theoretical Computer Science]

The algorithm

New algorithm

Uses some old ideas

- Ratios of $Z(\beta)$ values at different values of β
- Importance sampling
- Product estimator/Self-reducibility

Also some new ideas

- Paired estimator
- Well balanced cooling schedule

Ratios of partition function values

$Z(\beta)$ **usually easy for some values of** β

- In discrete models $Z(0) = \#\Omega$
- For Ising model $Z(0) = 2^{\#\text{ of nodes in graph}}$
- To find $Z(\beta)$, instead estimate:

$$r = \frac{Z(\beta)}{Z(0)}$$

then multiply by $Z(0)$

Importance sampling

Suppose can sample X from π_0, let

$$W := \exp(-\beta H(X))$$

which makes

$$\mathbb{E}[W] = \frac{\sum_{x \in \Omega} \exp(-\beta H(X))}{Z(0)} = \frac{Z(\beta)}{Z(0)}$$

so it has the right mean!

Spread

Second moment

$$\begin{aligned}\mathbb{E}[W^2] &= \frac{\sum_{x\in\Omega}(\exp(-\beta H(X)))^2}{Z(0)} \\ &= \frac{\sum_{x\in\Omega}\exp(-2\beta H(X))}{Z(0)} \\ &= \frac{Z(2\beta)}{Z(0)}\end{aligned}$$

Relative variance (square of coefficient of variation)

$$\mathbb{V}_{\text{rel}}(W) = \frac{\mathbb{V}(W)}{\mathbb{E}[W]^2} = \frac{Z(2\beta)/Z(0)}{[Z(\beta)/Z(0)]^2} - 1 = \frac{Z(2\beta)Z(0)}{Z(\beta)^2} - 1$$

Standard Monte Carlo

Relative variance (square of coefficient of variation)

1. Let n be $\mathbb{V}_{\text{rel}}(\exp(-\beta H(X)))$, where $X \sim \pi_0$
2. Draw $X_1, \ldots, X_n$ iid from π_0
3. Let $\hat{r} = (1/n) \sum_{i=1}^{k} \exp(-\beta H(X_i))$

Properties

$$\mathbb{E}[\hat{r}] = Z(\beta)/Z(0), \quad \mathbb{V}(\hat{r}) = 1$$

So number of samples needed is on order of

$$\frac{Z(2\beta)Z(0)}{Z(\beta)^2} - 1$$

Understanding the relative variance

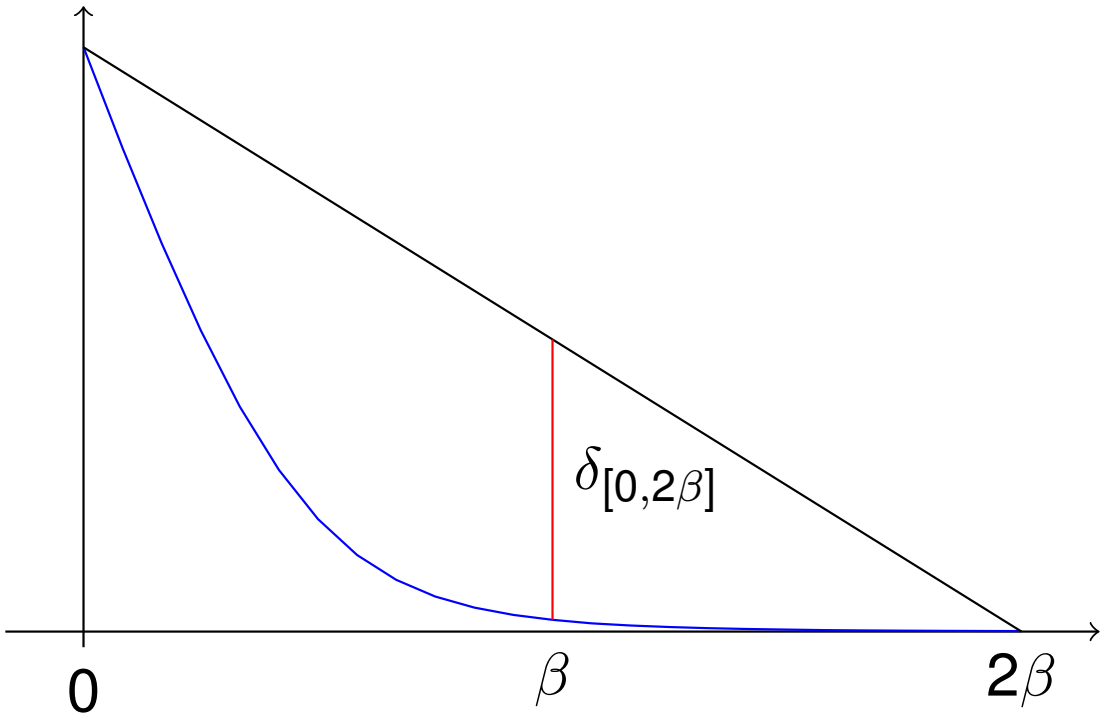
Easier to work in log space

$$z(\beta) := \ln(Z(\beta))$$

Then z is convex

$$\begin{aligned}
\ln\left(\frac{Z(2\beta)Z(0)}{Z(\beta)^2}\right) &= z(2\beta) + z(0) - 2z(\beta) \\
&= 2\left(\frac{z(2\beta) + z(0)}{2} - z(\beta)\right) \\
&= 2\delta_{[0,2\beta]}
\end{aligned}$$

The relative variance picture



Why this is bad

Problems

- Only care about $[0, \beta]$ interval
- Variance involves Z function over $[0, 2\beta]$
- δ tends to grow linearly in problem size

$$\mathbb{V}_{\text{rel}}(W) = \exp(2\delta_{[0,2\beta]})$$

Paired Estimator

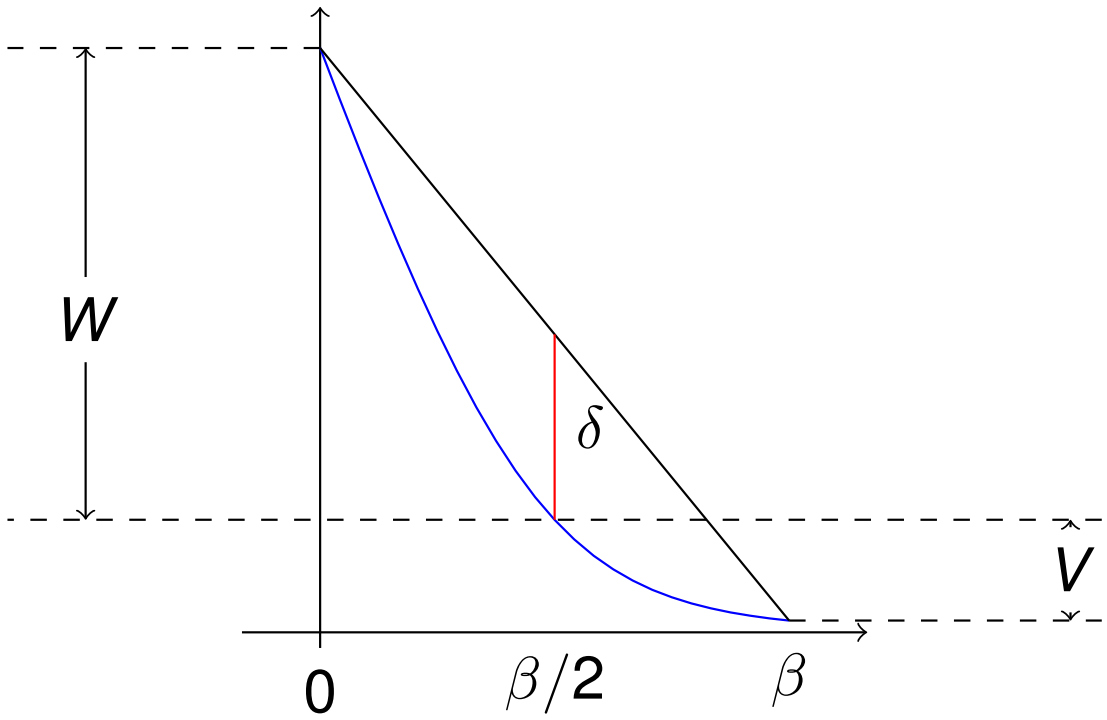
Use two estimators

$$X \sim \pi_0, \quad Y \sim \pi_\beta$$

$$W := \exp(-(\beta/2)H(X)), \quad V := \exp((\beta/2)H(Y))$$

$$W \text{ estimates } \frac{Z(\beta/2)}{Z(0)}, \quad V \text{ estimates } \frac{Z(\beta/2)}{Z(\beta)}$$

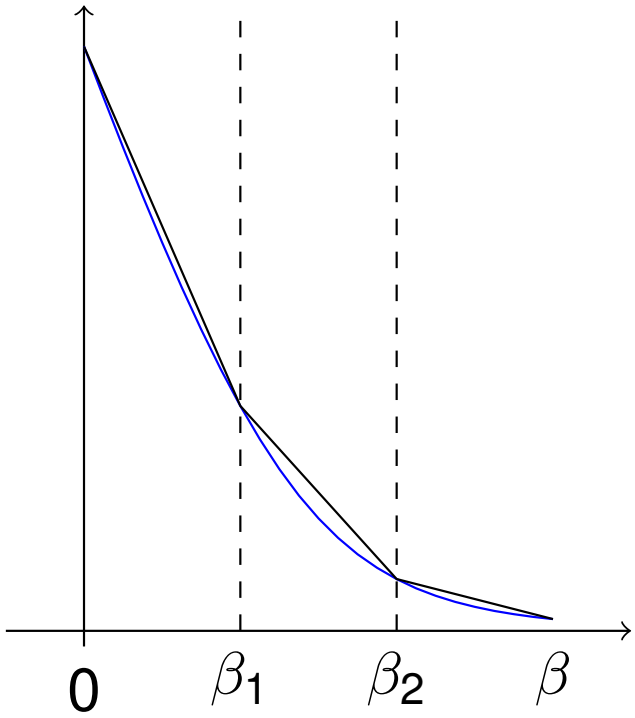
The relative variance for paired estimator



$$\mathbb{V}_{\mathrm{rel}}(W) = \mathbb{V}_{\mathrm{rel}}(V) = \exp(2\delta)$$

Breaking the interval

Multistage sampling [Valleau and Card 1972]



$$\frac{Z(\beta)}{Z(0)} = \frac{Z(\beta_1)}{Z(0)} \frac{Z(\beta_2)}{Z(\beta_1)} \frac{Z(\beta)}{Z(\beta_2)}$$

Paired Product Estimator

$$\frac{Z(\beta)}{Z(0)} = \frac{Z(\beta_1)}{Z(0)} \frac{Z(\beta_2)}{Z(\beta_1)} \frac{Z(\beta)}{Z(\beta_2)}$$

$$\frac{Z(\beta)}{Z(0)} \approx \frac{W_1}{V_1} \frac{W_2}{V_2} \frac{W_3}{V_3} = \frac{W}{V}$$

Analyzing Product Estimators

Variance of Product Estimator

Theorem

If $P = \prod P_i$ where the P_i are independent, then

$$\mathbb{E}(P) = \prod \mathbb{E}(P_i)$$

$$\mathbb{V}_{rel}(P) = -1 + \prod (1 + \mathbb{V}_{rel}(P_i))$$

For the products in our algorithm

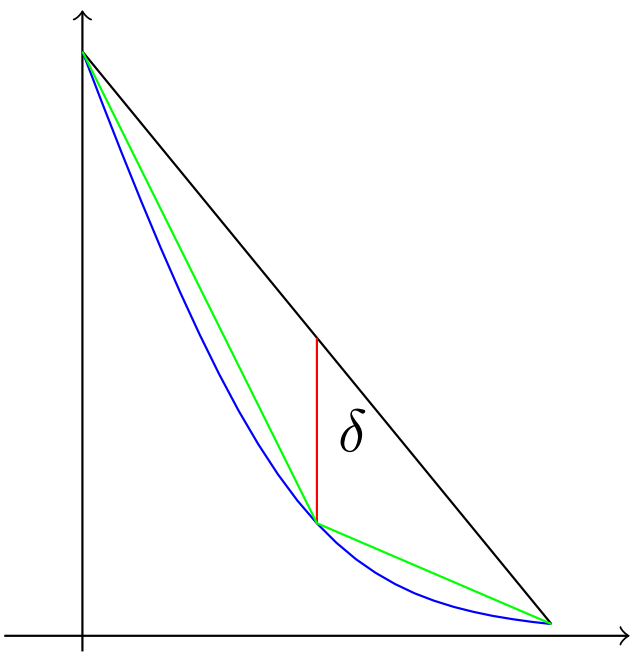
$$\mathbb{V}_{\text{rel}}(W_i) = \exp(2\delta_i) - 1 \Rightarrow \mathbb{V}_{\text{rel}}(W) = -1 + \exp\left(2\sum \delta_i\right)$$

Curving the z function

Theorem

In interval $[\beta_i, \beta_{i+1}]$, either δ_i is small, or the derivative of z changes rapidly. To be precise, if $\epsilon_i = z(\beta_i) - z(\beta_{i+1})$, then

$$\frac{z'(\beta_{i+1})}{z'(\beta_i)} \leq \exp(-2\delta_i/\epsilon_i)$$



Given δ:

Green line has smallest change in ratio of derivative

Telescoping the derivative

Corollary

This implies that

$$\frac{z'(\beta)}{z'(0)} = \frac{z'(\beta_1)}{z'(0)} \cdot \frac{z'(\beta_2)}{z'(\beta_1)} \cdots \frac{z'(\beta)}{z'(\beta_{\ell-1})} \leq \exp\left(-2\sum \frac{\delta_i}{\epsilon_i}\right)$$

Invert the inequality in corollary

$$\frac{z'(0)}{z'(\beta)} \geq \exp(2\sum \delta_i/\epsilon_i)$$

If $\epsilon \geq \epsilon_i$ for all i:

$$\left[\frac{z'(0)}{z'(\beta)}\right]^{\epsilon} \geq \exp(2\sum \delta_i)$$

Result is the following theorem

Theorem

If $z(\beta_i) - z(\beta_{i+1}) \leq \epsilon$ *for all* i*, then*

$$\mathbb{V}_{rel}(W) \leq \left[\frac{z'(0)}{z'(\beta)}\right]^{\epsilon}$$

Corollary

If $z(\beta_i) - z(\beta_{i+1}) \leq 1/[\ln(-z'(0)) - \ln(-z'(\beta))]$ *for all* i *then*

$$\mathbb{V}_{rel}(W) \leq e$$

Sidebar: z' as probabilistic object

Fact

If $X \sim \pi_\beta$, then

$$-z'(\beta) = \mathbb{E}_{\pi_\beta}[H(X)]$$

Proof.

$$\begin{aligned}
-z'(\beta) &= -(d/d\beta) \ln \left(\sum \exp(-\beta H(x)) \right) \\
&= -\frac{\sum (d/d\beta) \exp(-\beta H(x))}{\sum \exp(-\beta H(x))} \\
&= -\frac{\sum -H(x) \exp(-\beta H(x))}{Z(\beta)} \\
&= \mathbb{E}[H(X)]
\end{aligned}$$

□

Our algorithm so far

Ingredients:

Cooling schedule with $z(\beta_i) - z(\beta_{i+1}) \leq \epsilon$
Ability to sample from π_{β_i} for all i

Output

Estimates W and V with $\mathbb{E}[W]/\mathbb{E}[V] = r$
$\mathbb{V}_{\text{rel}}(W) = \mathbb{V}_{\text{rel}}(V) \leq (z'(0)/z'(\beta))^{\epsilon}$

Natural questions

1. How long will the cooling schedule be?
2. How small should ϵ be?
3. What if $z'(0)$ is too large?
4. What if $z'(\beta)$ is too small?
5. How do we actually find the cooling schedule?

How long will the cooling schedule be?

For well balanced cooling schedule

- Suppose $z(\beta_i) - z(\beta_{i+1}) \approx \epsilon$ for all i
- Then length of cooling schedule about

$$\ell = [\ln(Z(0)) - \ln(Z(\beta))]/\epsilon$$

- Number of samples to get W and V is 2ℓ
- Make ϵ as large as possible: $1/\ln(z'(0)/z'(\beta))$ so

$$\mathbb{V}_{\text{rel}}(W) = \mathbb{V}_{\text{rel}}(V) \leq (z'(0)/z'(\beta))^{\epsilon} \leq e$$

What if $z'(0)$ is too big?

Making $z'(0)$ finite

- Technically, $z'(0)$ could be infinite!
- Trick: restrict state space using medians
- Let Ω_m be states with $H(x)$ value at most median of $H(X)$
- Only need two samples (on average) to get $X \in \Omega_m$
- For $X \in \Omega_m$, $\mathbb{E}[H(X)] \leq m$, always finite
- Estimating $Z(\Omega_m)/Z(\Omega)$ easy

Rarely needed in practice

- For Ising model, $z'(0)$ is half the edges in graph

What if $z'(\beta)$ is too small?

Easiest solution

- Form an adjusted H function:

$$H_{\text{adj}}(x) := 1 + H(x)$$

- Note π_β same with H_{adj} as with H
- $Z_{\text{adj}}(\beta) = \exp(-\beta)Z(\beta)$
- Which means

$$\ln(Z_{\text{adj}}(0)) - \ln(Z_{\text{adj}}(\beta)) = \beta + \ln(Z(0)) - \ln(Z(\beta))$$

- Always have $|z'_{\text{adj}}(\beta)| \geq 1$

How do we actually find the cooling schedule?

TPA algorithm [H.-Schott 2010]

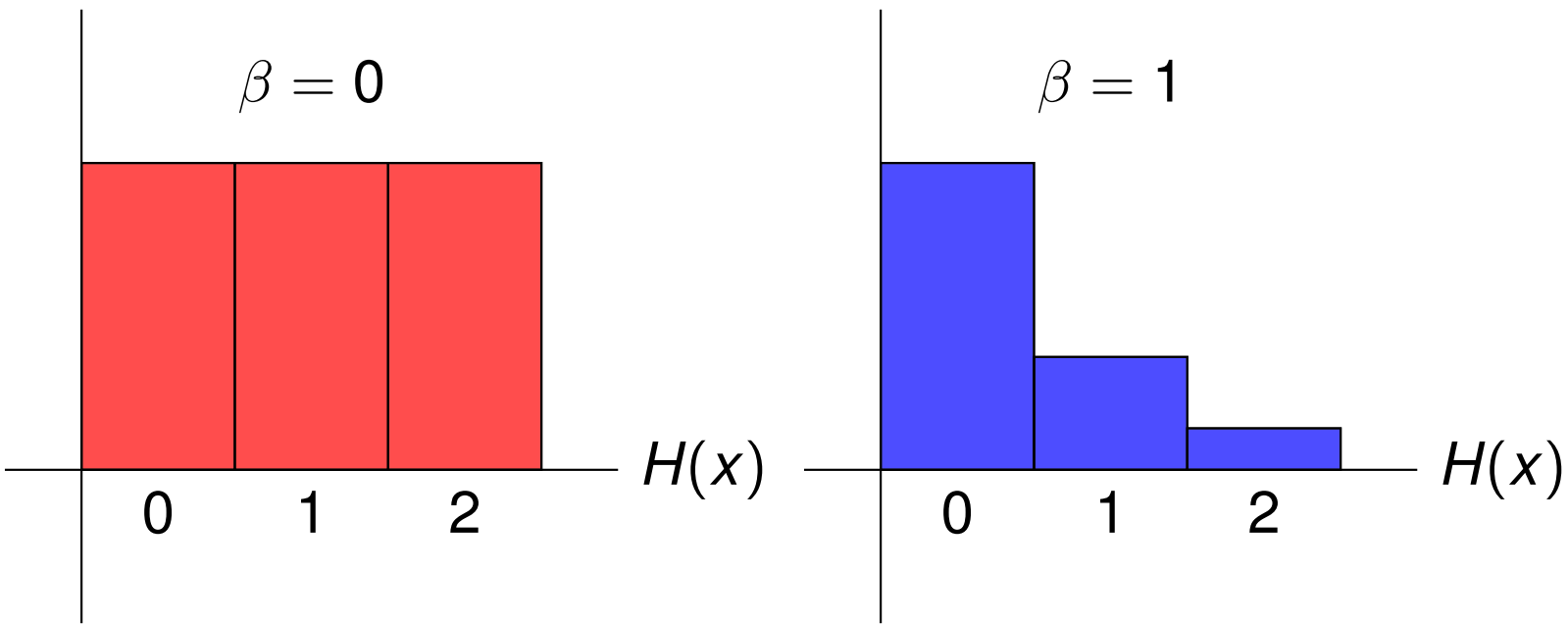
- Creates a well balanced schedule
- Number of samples used close to length of schedule

Rough idea

- Start with $b = \beta$
- Draw $X \sim \pi_b$, $Y \sim \text{Unif}([0, \exp(-\beta H(X))]$
- Let b be smallest value such that $Y \in [0, \exp(-bH(X))]$
- Repeat until $b = 0$.
- Set of β values is approximately 1-balanced schedule

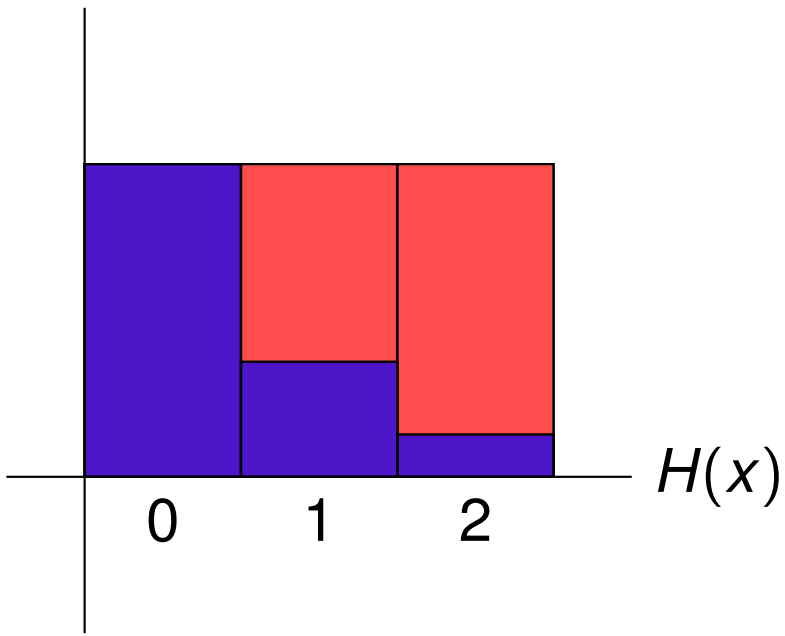
Geometric view

$$Z(\beta) = 1 + \exp(-\beta) + \exp(-2\beta)$$



Combining...

$$Z(\beta) = 1 + \exp(-\beta) + \exp(-2\beta)$$



TPA

- Draw (X, Y) uniformly from red region
- Find b so that point just touches blue region

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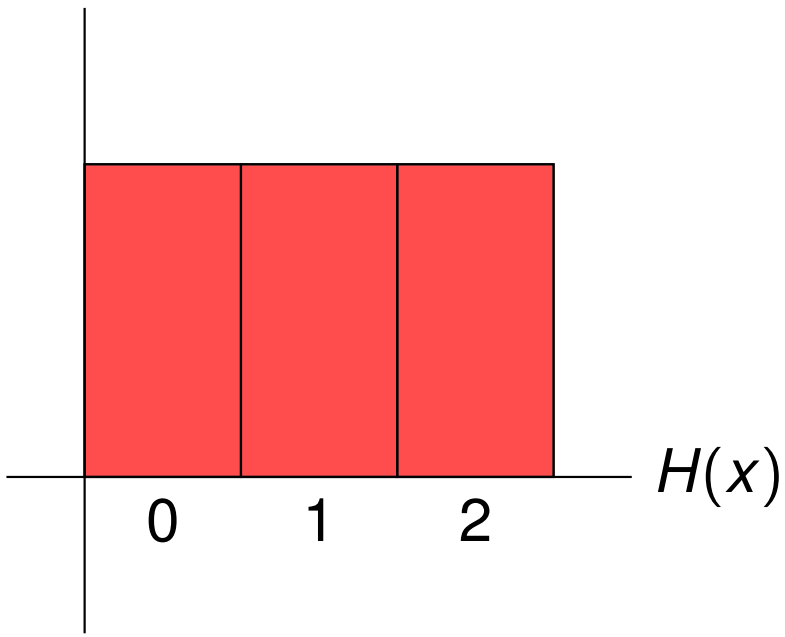

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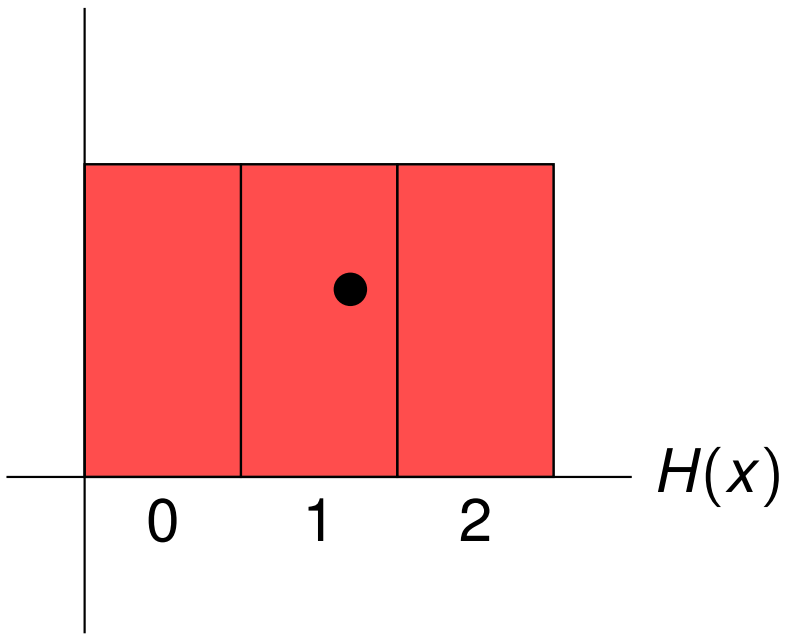

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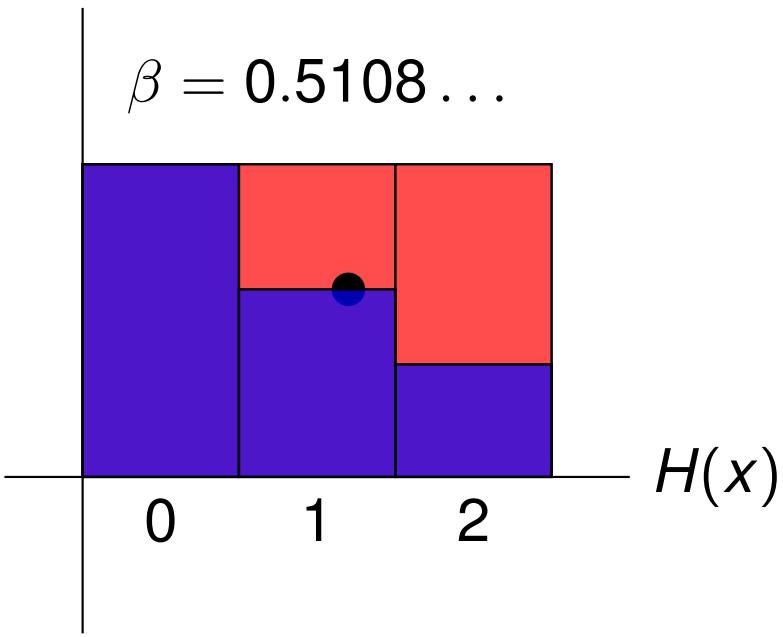


The result

Example run:

$$(1, .5108, 0.1342, 0)$$

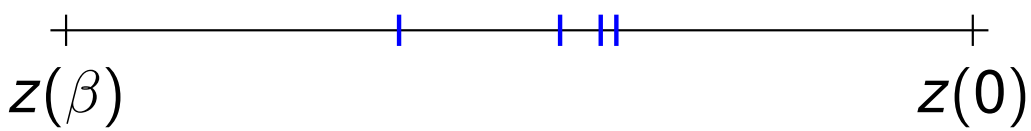
Fact (H.-Schott 2010)

If the values found in a run of TPA are $\beta = b_0, b_1, \ldots, b_k = 0$*, then* $z(b_1), z(b_2), \ldots, z(b_k)$ *form a Poisson point process on the interval* $[z(\beta), z(0)]$*.*

Why Poisson point process (PPP)?

Works as follows

- At each step, ratio of blue area to red area is random
- Random variable is uniform over $[0, 1]$
- Take $-\ln(U)$, get exponential distribution
- When differences exponential, get PPP



Poisson process

Fact (H.-Schott 2010)

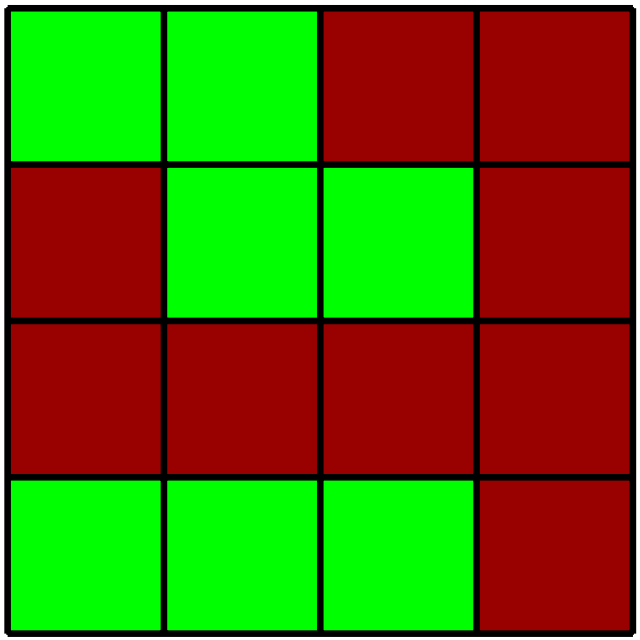
If the values found in a run of TPA are $\beta = b_0, b_1, \ldots, b_k = 0$*, then* $z(b_1), z(b_2), \ldots, z(b_k)$ *form a Poisson point process on the interval* $[z(\beta), z(0)]$*.*

- Run TPA several times to build large set of β values
- Points roughly evenly spaced (uniformly distributed)

Back to the Autonormal model

Autonormal (Ising) model

Besag [1974] modeled soil plots as good (green) or bad (red)



$d(x) = 11$
(number of adj nodes that disagree)

Model:

$$\mathbb{P}(X = x) = \frac{\exp(-\beta d(x))}{Z(\beta)}$$

Initial changes

What we want

- Cooling schedule for $Z(\beta)$ for all $\beta \in [0, \infty)$
- Let $h(x) = d(x) + 1$
- Since $d(x) \in [0, m]$, this means $h(x) \in [1, m + 1]$ (where $m =$ the number of edges)
- So $\ln(z'(0)/z'(\infty)) \leq \ln(m + 1)$
- Also $Z(0) = 2^n$ ($n =$ number of nodes)
- So length of schedule about $\ln(m + 1) \cdot n \cdot \ln(2)$

Procedure

1. Use TPA [H.-Schott 2010] to find a good cooling schedule
2. Generate W and V, use W/V as estimate

For better accuracy

- Generate several copies of W and V
- Find the sample average $\bar{W}$ and $\bar{V}$
- The estimate is then $\bar{W}/\bar{V}$

Initial changes

Improvement for 2D lattices

- Here $m \leq 4n$, β constant (below phase transition)
- Cooling schedule for $Z(\beta)$ for all $\beta \in [0, \infty)$
- Let $h(x) = d(x) + m$
- Since $d(x) \in [0, m]$, this means $h(x) \in [m, 2m]$ (where $m =$ the number of edges)
- So $\ln(z'(0)/z'(\infty)) \leq \ln(2)$
- Also $Z(0) = 2^n$ ($n =$ number of nodes)
- So length of schedule about $\ln(2) \cdot n \cdot \ln(2) + \beta m$
- Result: method linear in m

Future work

Running method in practice

Obtaining samples

- Simulated tempering runs all β values simultaneously
- Omnithermal sampling
- Lose analysis based on independence
- Gain from many more samples

Preprocessing TPA output

- Some temperatures will be too close together
- Use some fast samples to eliminate bunched β values

Ideas:

1. Is the $\ln(H_m)$ part really necessary? (Computer experiments indicate no)
2. Take advantage of the form:

$$Z(\beta) = \sum_{i=1}^{n} a_i \exp(-i\beta)$$

3. Flattening $Z(\beta)$ function by substracting median $H(x)$

Summary

Most imporant thing

First practical approx alg (nearly) linear in dimension

Uses some old ideas

Importance Sampling, Multistage Sampling, Product Estimator

Add some new ideas

Paired Product Estimator, Well-balanced schedule

The resulting approximation algorithm

Relatively simple to implement, guaranteed quality of estimate

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