Adiabatic Optimization and the Fundamental Gap Theorem

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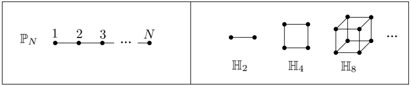
Our Problem

$$
\begin{aligned}
(1-s)\mathbf{L} + s\mathbf{W} &= (1-s)\left(\mathbf{L} + \frac{s}{1-s}\mathbf{W}\right) \\
H(\alpha) &\to \mathbf{L} + \mathbf{W}(\alpha)
\end{aligned}
$$

- **L** is a graph Laplacian
- **W** is a "convex" (quasiconvex) potential, diagonal in standard basis
- Use simple examples to study phenomena which may be relevant to real-world cases
  1. Path graphs
  2. Hypercube graphs (with Hamming-Symmetric **W**)
  3. Single-peaked ground states

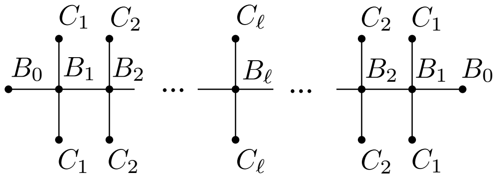


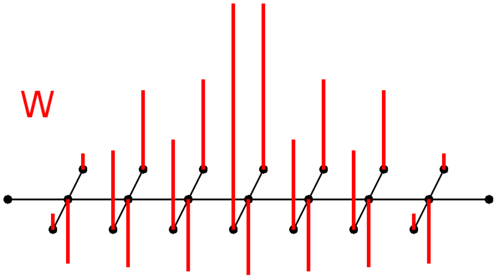
Example $\mathbf{H}$

Consider the simplest example, the path graph. Then,

$$\mathbf{H} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} + \begin{pmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 7 \end{pmatrix}$$

Caterpillar graph

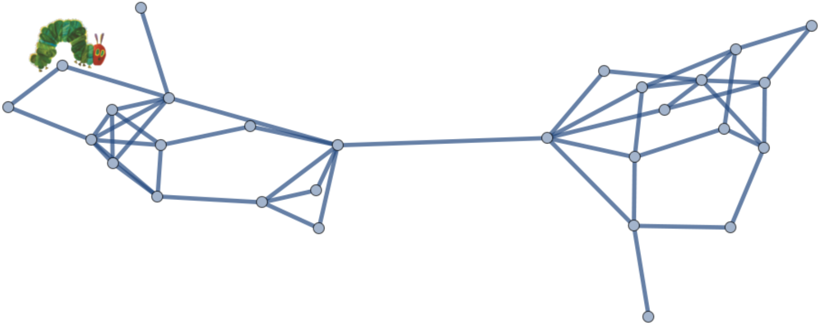




This has exponentially small gap! $\Gamma \sim O\left(2^{-\ell}\right)$.

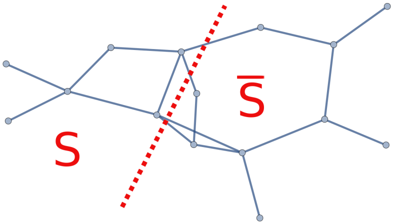
More general graphs

So, if the caterpillar graph has a small gap, what can we say about more general graphs with convex potentials?



Flow and Conductance – Random Walk [Sinclair 1993]

Let **P** be the transition matrix of a reversible ergodic random walk on graph G with vertices V_G and edges E_G. Let π be the corresponding limiting distribution. Let S be any non-empty subset of V_G and let $\bar{S} = V_G \setminus S$ be its complement. Let,



$$F_S = \sum_{\substack{(x,y)\in E_G \\ x\in S, y\in \bar{S}}} \pi_x P_{xy} \qquad \text{(Flow of } S\text{)}$$

$$C_S = \sum_{x\in S} \pi_x$$

$$\Phi_S(P) = \frac{F_S}{\min(C_S, C_{\bar{S}})}$$

$$\Phi(P) = \min_{S\subset V_G} \Phi_S(P) \qquad \text{(Conductance of } P\text{)}$$

Gap Bound – Random Walk

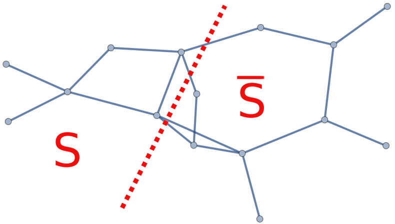
The conductance of $\mathbf{P}$ can be used to bound the gap γ between the two *largest* eigenvalues of $\mathbf{P}$:

$$\frac{\Phi(\mathbf{P})^2}{2} \leq \gamma \leq 2\Phi(\mathbf{P})$$

Our problem can be transformed into one about the eigenvalue gaps of Markov chains.

$$\mathbf{P} = \frac{1}{\lambda_0}\mathbf{D}^{-1}\mathbf{H}\mathbf{D}$$

$\mathbf{P}$ is row-stochastic. (Transition matrix.) Spectrum is inverted: the lowest eigenvalue of $\mathbf{P}$ corresponds to the highest eigenvalue of $\mathbf{H}$.

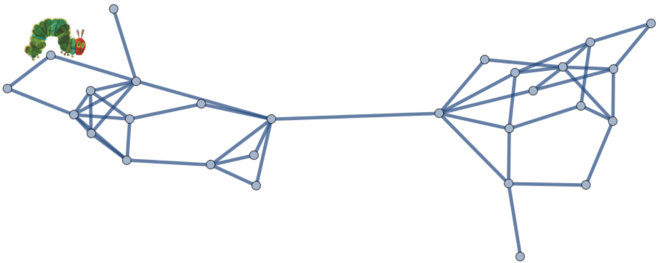


$$\Gamma \geq \frac{-1}{2\lambda_0}\left(\min_{S\subset V_G} \frac{F_S}{\min(C_S, C_{\bar{S}})}\right)^2$$

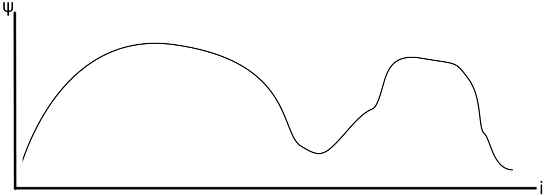
$$F_S = \sum_{\substack{(x,y)\in E_G \\ x\in S, y\in \bar{S}}} \psi(x)\psi(y)$$

$$C_S(\mathbf{P}) = \sum_{x\in S} \psi^2(x)$$

Bottlenecks and lobes



The above plot has a bottleneck. Corresponds to a "lobed" distribution.



Restriction to Single Peaks

Definition

We call a vector single-peaked if it has at most one connected region in its corresponding graph such that the vector is at a local maximum.

In certain graphs – such as the path graph – a single-basin potential is sufficient to demonstrate the single-peaked property for the ground state.

$$\Delta^2\psi(x) = (W_x - \lambda)\psi(x)$$

We expect (but do not yet have proof) that in many cases of interest the single peaked property is satisfied. (In fact, can be shown Dirichlet path is log-concave.)

Conductance Bound – Single Peaked

First consider shifted Hamiltonian with the same gap and eigenvectors, $\mathbf{H} \to \mathbf{H} - (W_{\max} + d)\mathbf{I}$

$$\Gamma \geq \frac{1}{2(|\mathbf{W}| + d)} \left(\min_{S \subset V_G} \frac{F_S}{\min(C_S, C_{\bar{S}})} \right)^2$$

Since ψ has a single peak, throw away extra flows

$$\boxed{\Gamma \geq \frac{1}{2(|\mathbf{W}| + d)|V_G|^2}}$$

For the path graph, $\Gamma \geq \frac{1}{2(|\mathbf{W}|+d)l^2}$.

Definition (Canonical Paths)

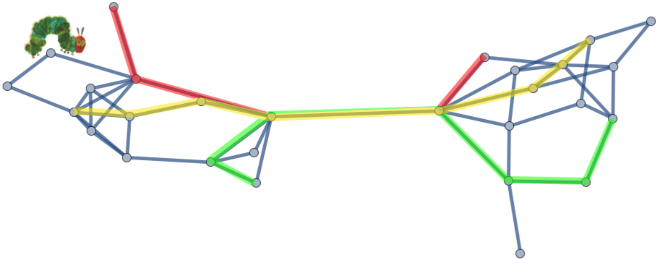
Let G be an undirected graph with edge set E and vertex set V. For each $(x, y) \in V \times V$ with $x \neq y$, choose a unique oriented path t_{xy} from x to y. We call the set of all such paths $T = \{t_{xy} | (x, y) \in V \times V, x \neq y\}$ the canonical paths.

Then, for the random walk on this graph, the Poincaré inequality states that $\gamma \geq \frac{1}{\kappa(S)}$ where

$$\kappa(T) = \max_{e} \sum_{t_{xy} \ni e} |t_{xy}| \pi_x \pi_y$$

where

$$|t_{xy}| = \sum_{(x',y') \in t_{xy}} \left(\pi_{x'} P_{x'y'}\right)^{-1}$$



If too many paths cross the same edge, there is again a bottleneck and a "lobed" distribution. Imposing single-peakededness, we can recover the asymptotically tight bound (to within π^2) for the path graph

$$\Gamma \geq \frac{1}{l(l+1)}$$

Take Home Lessons

- Open possibility for huge loss to your favorite method (eg. gradient descent)
- but, we don't *prove* it is slower
- Single local minima of W insufficient for fast runtime
- Single local maximum of ψ sufficient
- Hard(?) to demonstrate single-peakededness
- Some cases are easy, other cases can sometimes be transformed or approximated as these

Fundamental Gap Conjecture

- But, can we get this tight?
- The graph Laplacian is similar to the continuum Laplacian

$$-\nabla^2 + V(x) \to \mathbf{\Delta}^2 + \mathbf{W}$$

- Fundamental gap conjecture was a longstanding conjecture about continuum Laplacians, recently proven by Andrews and Clutterbuck
- Tight lower bound to a Schrödinger operator with convex potential $(\nabla^2 + V)$ on convex domain $\Omega \subset \mathbb{R}^n$ with Dirichlet boundary conditions
- $\Gamma \geq \frac{3\pi^2}{d^2}$ where d is the diameter of Ω

Fundamental Gap Conjecture

- Expect that for large N grid graphs (and convex subgraphs) should behave like the continuum
- Lots of work done on this problem over the past 30 years
- Behavior of the discrete case should be similar to that of the continuum case, so we can borrow the same intuition
- Although getting correct asymptotic bound, difficult to tightly bound class
- First attack: Lavine's approach. This gives us the discrete analogue to his result in the continuum. [Lavine 1994]
- Extending these techniques to additional problems looks promising.

Our problem:

$$\mathbf{H} = \mathbf{L} + \mathbf{W}(\alpha)$$

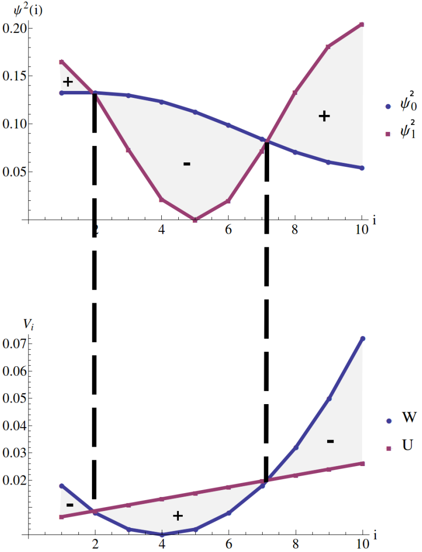
Hellman-Feynman Theorem:

$$\frac{d\lambda_i}{d\alpha} = \left\langle \frac{d\mathbf{W}}{d\alpha} \right\rangle_{\psi_i}$$

So that for the gap,

$$\begin{aligned} \frac{d\Gamma}{d\alpha} &= \frac{d\lambda_1}{d\alpha} - \frac{d\lambda_0}{d\alpha} \\ &= \left\langle \frac{d\mathbf{W}}{d\alpha} \right\rangle_{\psi_1} - \left\langle \frac{d\mathbf{W}}{d\alpha} \right\rangle_{\psi_0} \end{aligned}$$

Convex Potentials Lower Bounded by Linear Potentials [Lavine 1994]



$$\frac{d\mathbf{W}}{d\alpha} := \mathbf{U} - \mathbf{W}$$

$$\frac{d\Gamma}{d\alpha} = \langle \mathbf{U} - \mathbf{W} \rangle_{\psi_1} - \langle \mathbf{U} - \mathbf{W} \rangle_{\psi_0} \leq 0$$

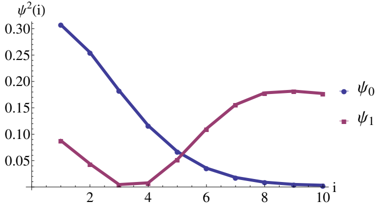
This converges arbitrarily close to some linear potential!

Linear Potentials Lower Bounded by Flat Potentials

$$\mathbf{H} = \mathbf{L} + \alpha \mathbf{U}$$

Hellman-Feynman becomes,

$$\frac{d\mathbf{\Gamma}}{d\alpha} = \langle \mathbf{U} \rangle_{\psi_1} - \langle \mathbf{U} \rangle_{\psi_0}$$



$$\Gamma \geq 2\left(1 - \cos\left(\frac{\pi}{N}\right)\right) \sim \frac{\pi^2}{N^2} + O\left(\left(\frac{\pi}{N}\right)^4\right)$$

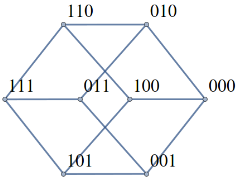
Analogous to Payne and Weinberger (1960)

Hypercube

$$\mathbf{H} = -\sum_i \sigma_x^{(i)} + \alpha \mathbf{W}$$

- Start with Hypercube graph with vertices indexed by bit-strings
- Now, **W** convex function of Hamming weight
- $|010111000\rangle$ has Hamming weight 4
- Connecting vertices with Hamming distance 1 equivalent to σ_x terms
- $|010111000\rangle \sim |110111000\rangle$

$$\left(N + \alpha W_{|b_i|} - \lambda\right)\psi_i = \sum_{(V_i,V_j)\in E} \psi_j$$



Hypercube

- Represent Hypercube in Symmetric subspace

$$\phi_m = \sqrt{\binom{N}{m}} \sum_{|b_i|=m} \psi_i$$

- Result has similar structure to path graph (Jacobi matrix)

$$(N + \alpha W_m - \lambda)\phi_m = \sqrt{m(N-m+1)}\phi_{m-1} + \sqrt{(m+1)(N-m)}\phi_{m+1}$$

- Apply previous results (with some massage) to get that Convex, Hamming-symmetric potentials are lower bounded by Linear, Hamming-symmetric potentials
- Linear, Hamming-symmetric potentials have an exactly solvable spectrum
- $\Gamma \geq 2$

Lessons Learned

Findings:

1. Convex potentials insufficient to prevent exponentially small gap
2. Separated localization results in a small gap
3. Localization without local minima is okay

Mathematical Tools Introduced:

1. Poincaré's Inequality
2. Variational Methods adapted from Fundamental Gap Literature
3. Both yielded tighter bounds than conductance methods
4. Adaptable to harder and useful optimization problems?
5. Other Fundamental Gap literature?