ON THE DUALITY OF SAMPLING AND NEWTON'S METHOD IN CONSTRAINED OPT

FASTER CONVEX OPTIMIZATION

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THIS TALK — OUTLINE

- 1. The goal of Convex Optimization
- 2. Interior Point Methods and Path following
- 3. Hit-and-Run and Simulated Annealing
- 4. The Annealing-IPM Connection
- 5. Faster Optimization

GENERAL CONVEX OPTIMIZATION PROBLEM

Let K be a bounded convex set, we want to solve

$\min_{x \in K} \theta^{\top} x$

Can always convert non-linear objective into a linear one

$$\min_{x \in K} f(x) \longrightarrow \min_{\substack{(x,c) \in K \times \mathbb{R} \\ f(x) \le c}} c$$

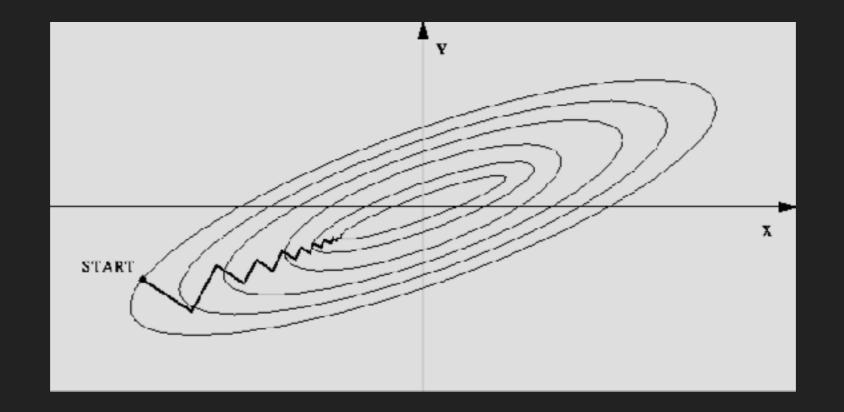
THE GRADIENT DESCENT ALGORITHM

The gradient descent algorithm:

For
$$t = 1, 2, \ldots$$
:
 $\tilde{x}_t = x_{t-1} - \eta \nabla f(x_{t-1})$
 $x_t = \operatorname{Proj}_K(\tilde{x}_t)$

Challenge: the Projection step can often be just as hard as the original optimization

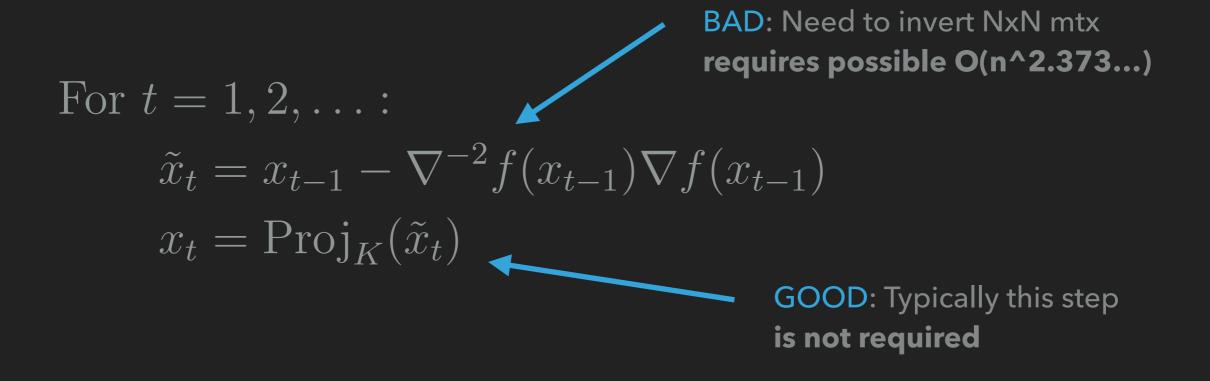
GD DOES POORLY WITH LOTS OF CURVATURE



The gradient descent algorithm doesn't use any knowledge of the curvature of objective function

BETTER: USE THE CURVATURE — NEWTON'S METHOD

Newton's Method is a "smarter" version of gradient descent, moves along the gradient after a transformation



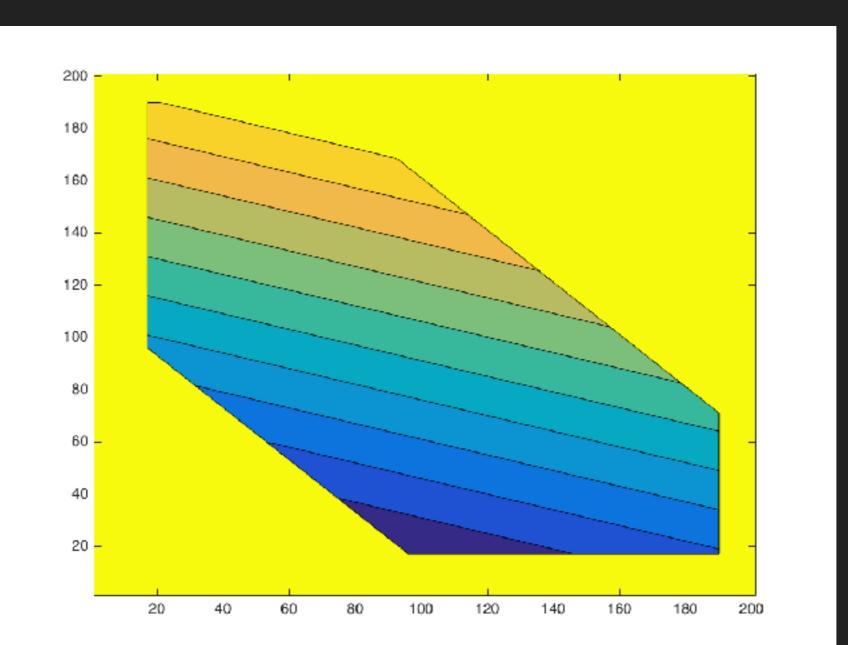
WAIT! OUR ORIGINAL OBJECTIVE ISN'T CURVED...

How does this help us with linear optimization?

$$\min_{x \in K} \theta^\top x + \phi(x)$$

- Add a curved function ϕ () to the objective!
- $\blacktriangleright \phi$ () should be "super-smooth" (more on this later)
- ▶ ϕ () should be a "barrier", i.e. goes to ∞ on the boundary, but not too quickly! In a sense, ϕ () encodes constraints K.

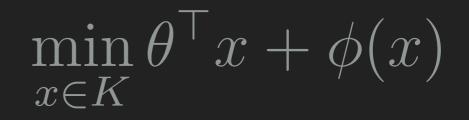
OPTIMIZATION WITHOUT A BARRIER

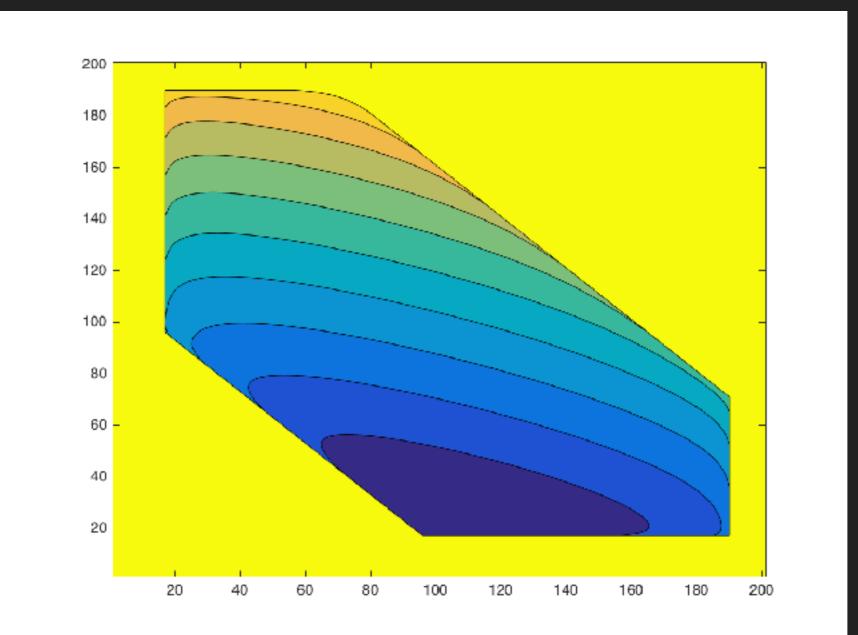


 $\min \theta^\top x$

 $x \in K$

OPTIMIZATION WITH A BARRIER





WHAT IS A GOOD BARRIER?

- > What is needed for this "barrier func." ϕ ()?
- Canonical example: if set is a polytope K = {x : Ax ≤ b} then the logarithmic barrier suffices: φ(x) = -∑_i log(b_i - A_ix)
- In general, Nesterov and Nemirovski proved that the following two conditions are sufficient. Any function satisfying these conditions is a *self-concordant barrier*:

$$abla^3 \phi[h,h,h] \leq 2(
abla^2 \phi[h,h])^{3/2}, \text{ and}$$

 $abla \phi[h] \leq \sqrt{\nu \nabla^2 \phi[h,h]},$

v is the barrier parameter which will be important later

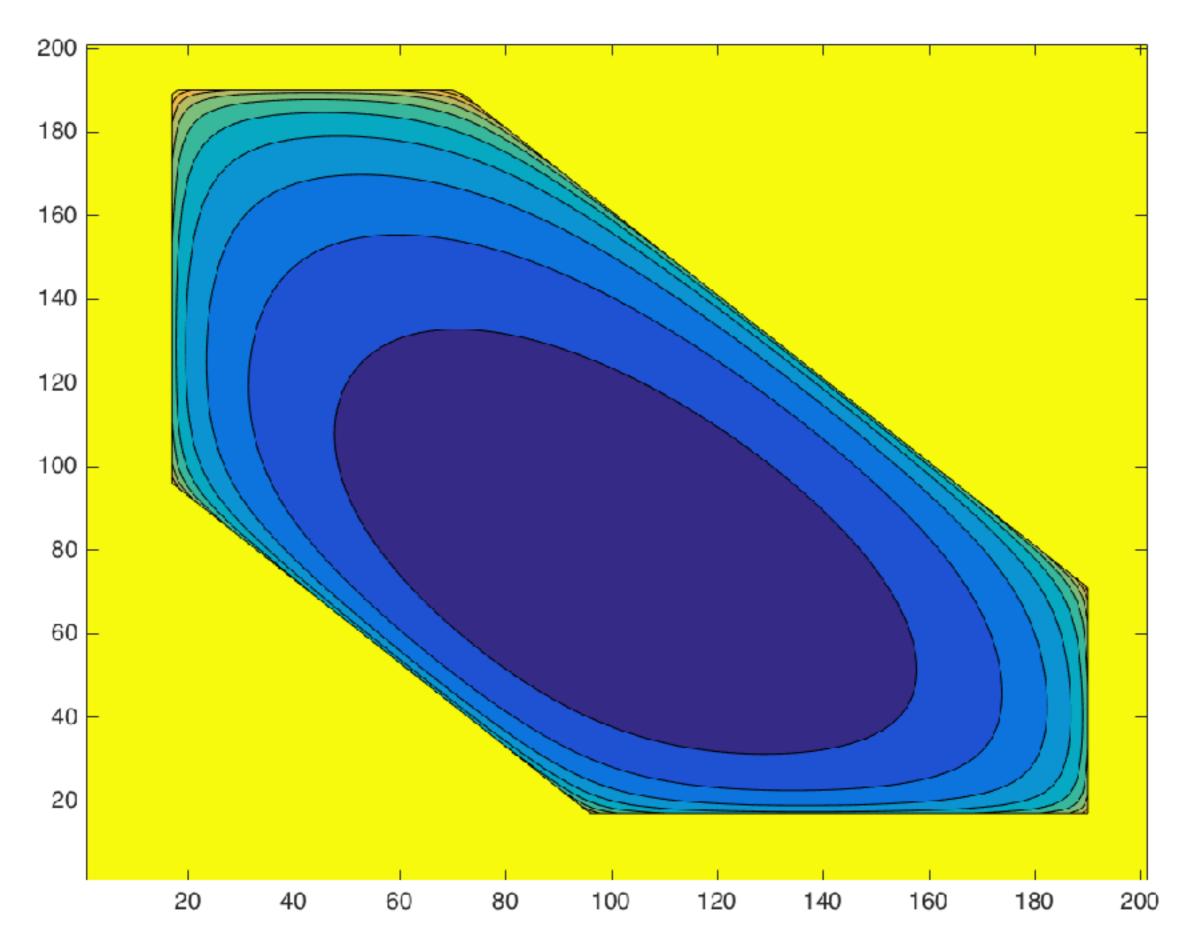
ALGORITHM: INTERIOR POINT PATH FOLLOWING METHOD

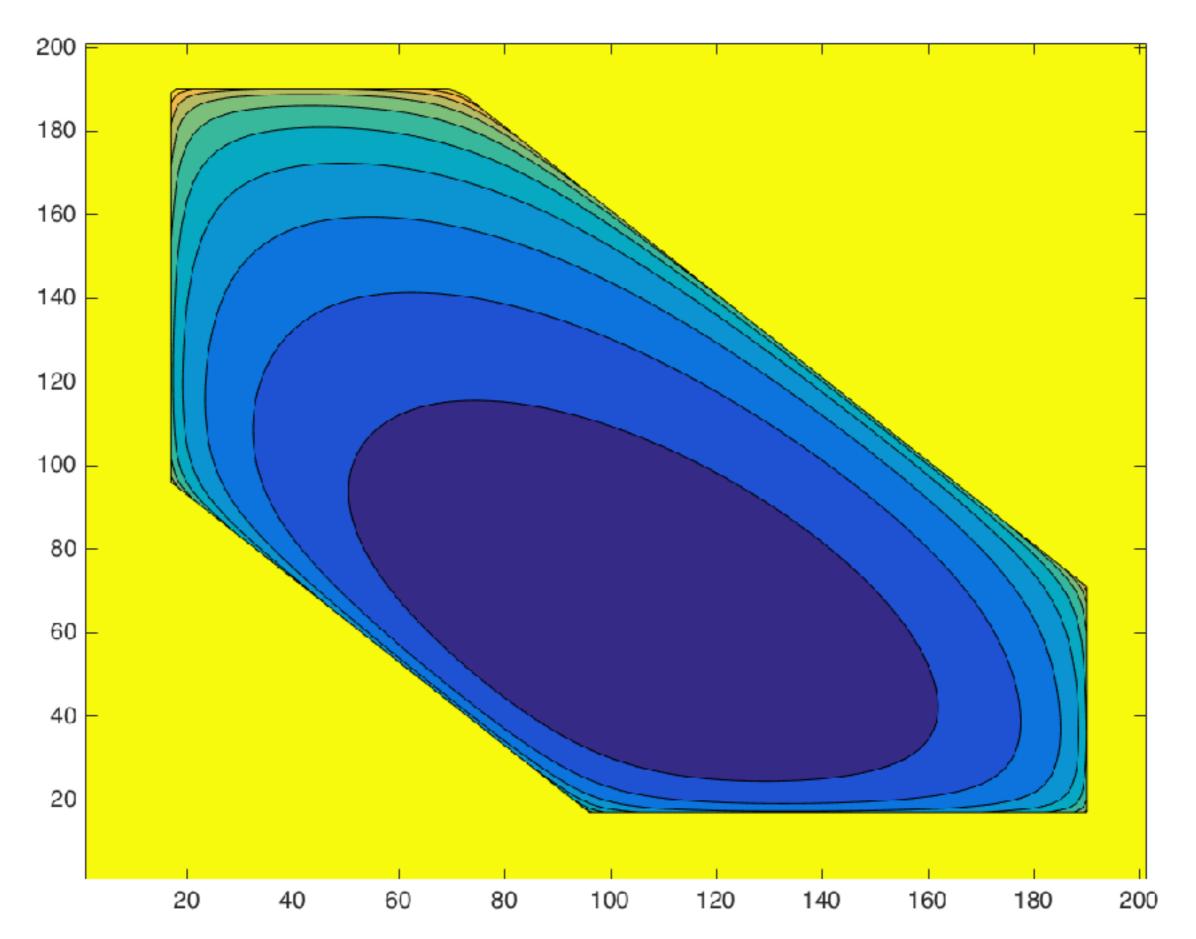
- Nesterov and Nemirovski developed the sequential "path following" method, described as follows:
- Let $\alpha = (1 + 1/\sqrt{\nu})$ the "inflation" rate
- For k=1,2,...
 - 1. Update temperature: $f_k(x) := \alpha^k(\theta^\top x) + \phi(x)$
 - 2. Newton update: $\hat{x} \leftarrow \hat{x} \frac{1}{1+c_k} \nabla^{-2} f_k(\hat{x}) \nabla f_k(\hat{x})$

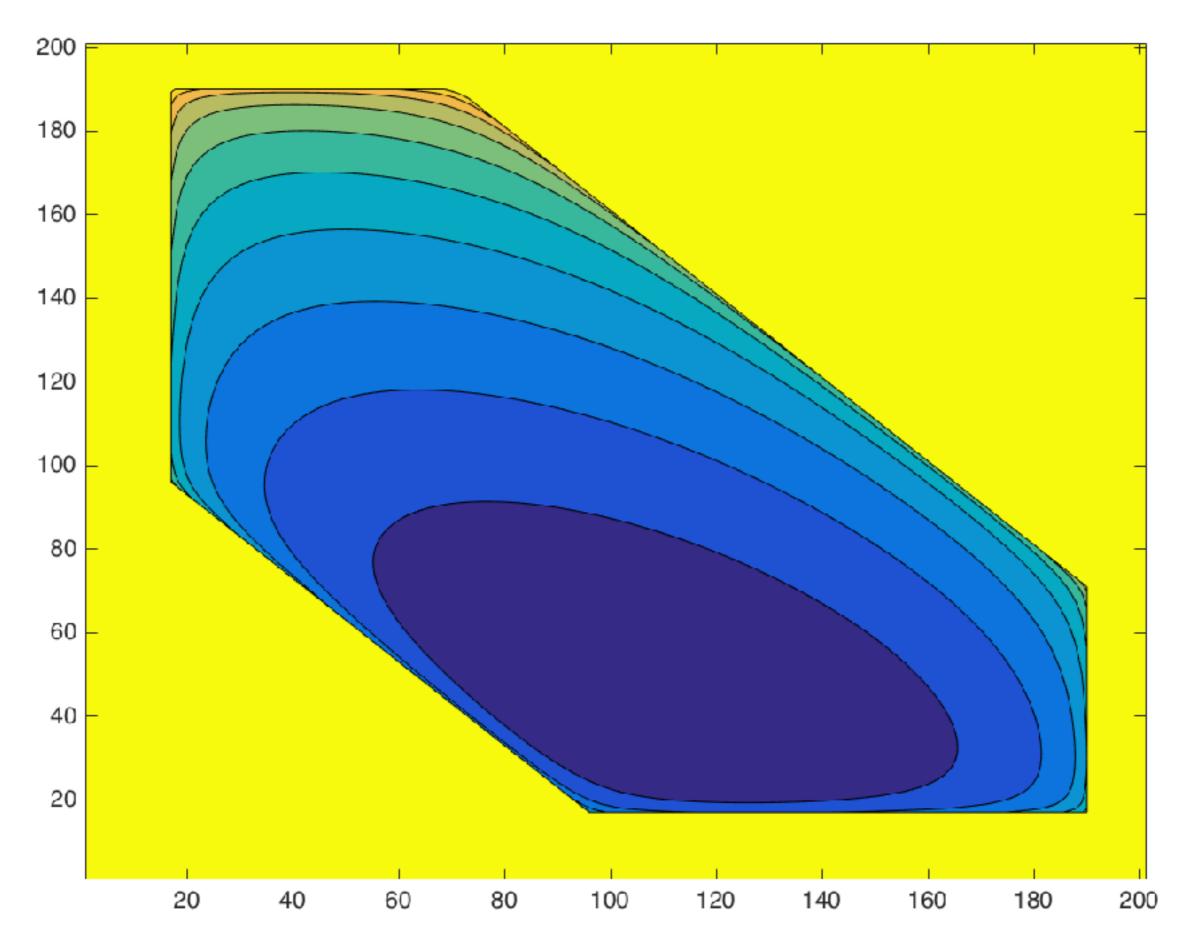
WHAT DOES THE SEQUENCE OF OBJECTIVES LOOK LIKE?

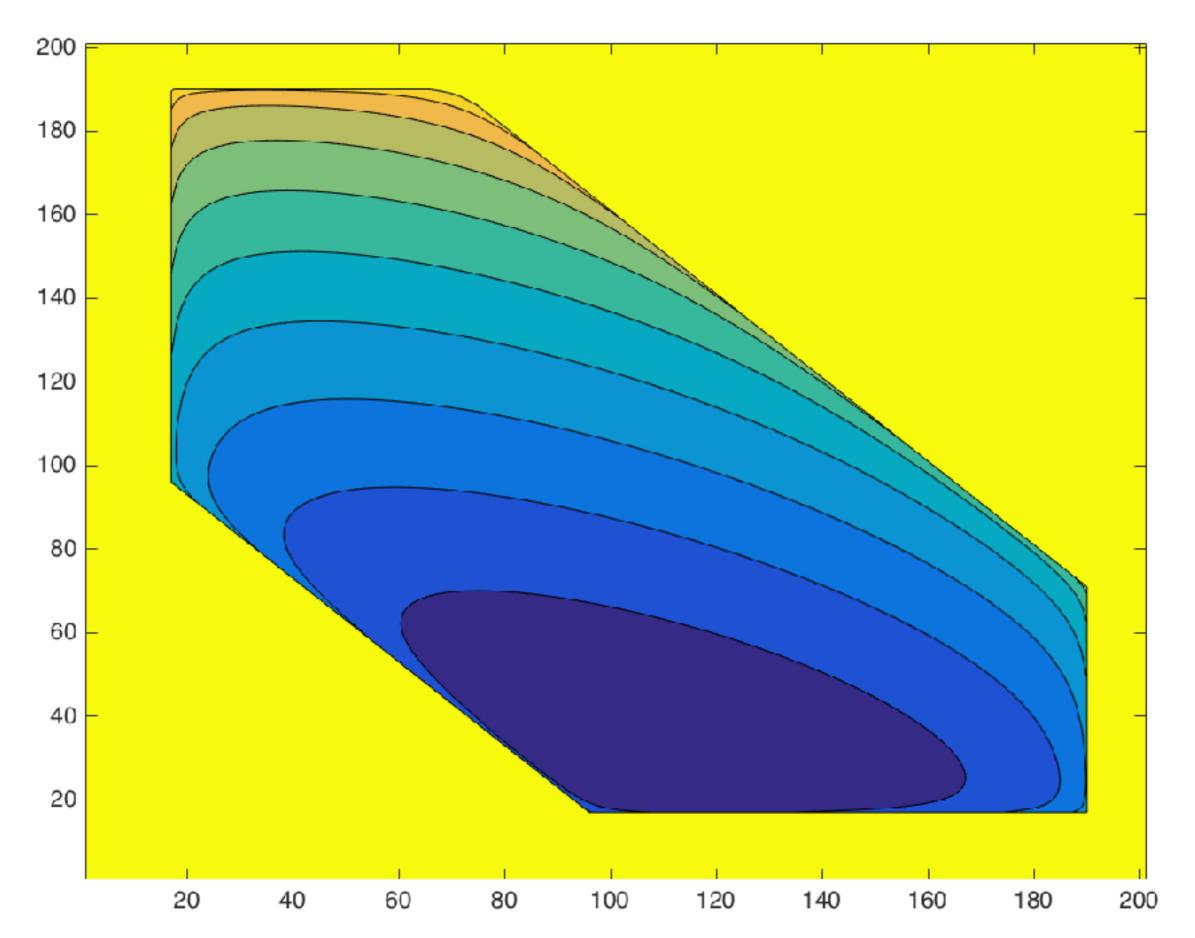
$$f_k(x) := \alpha^k(\theta^\top x) + \phi(x)$$

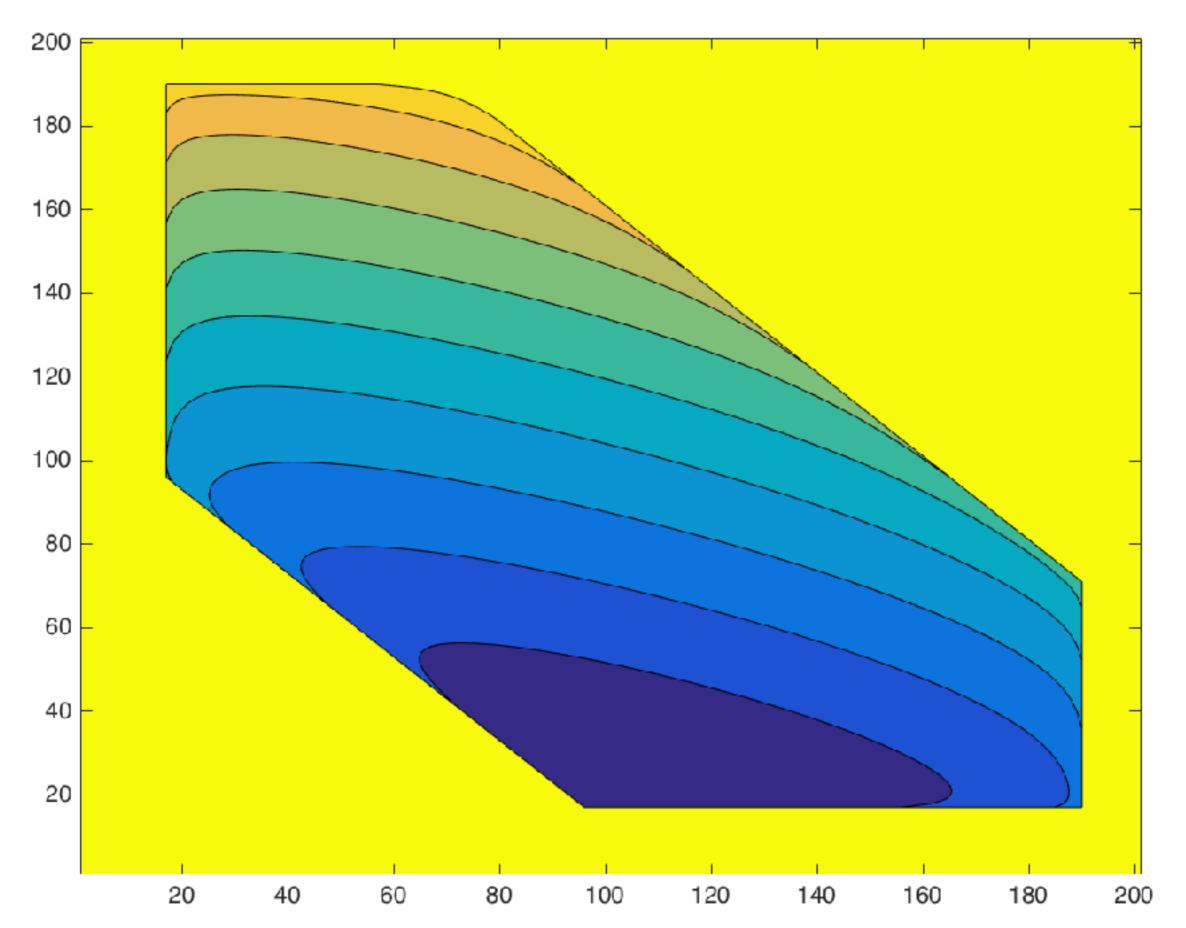
Let's show these objective function as we increase k!!

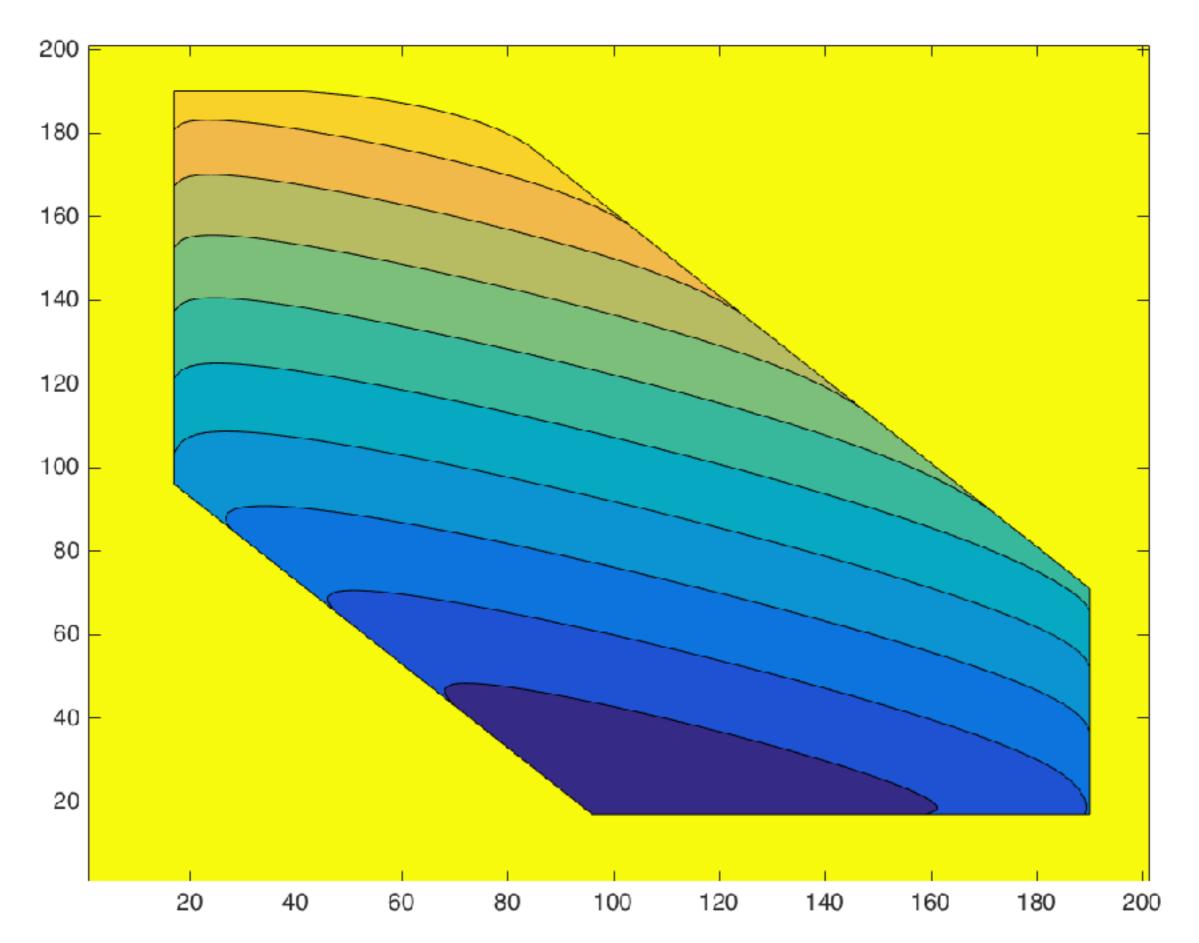


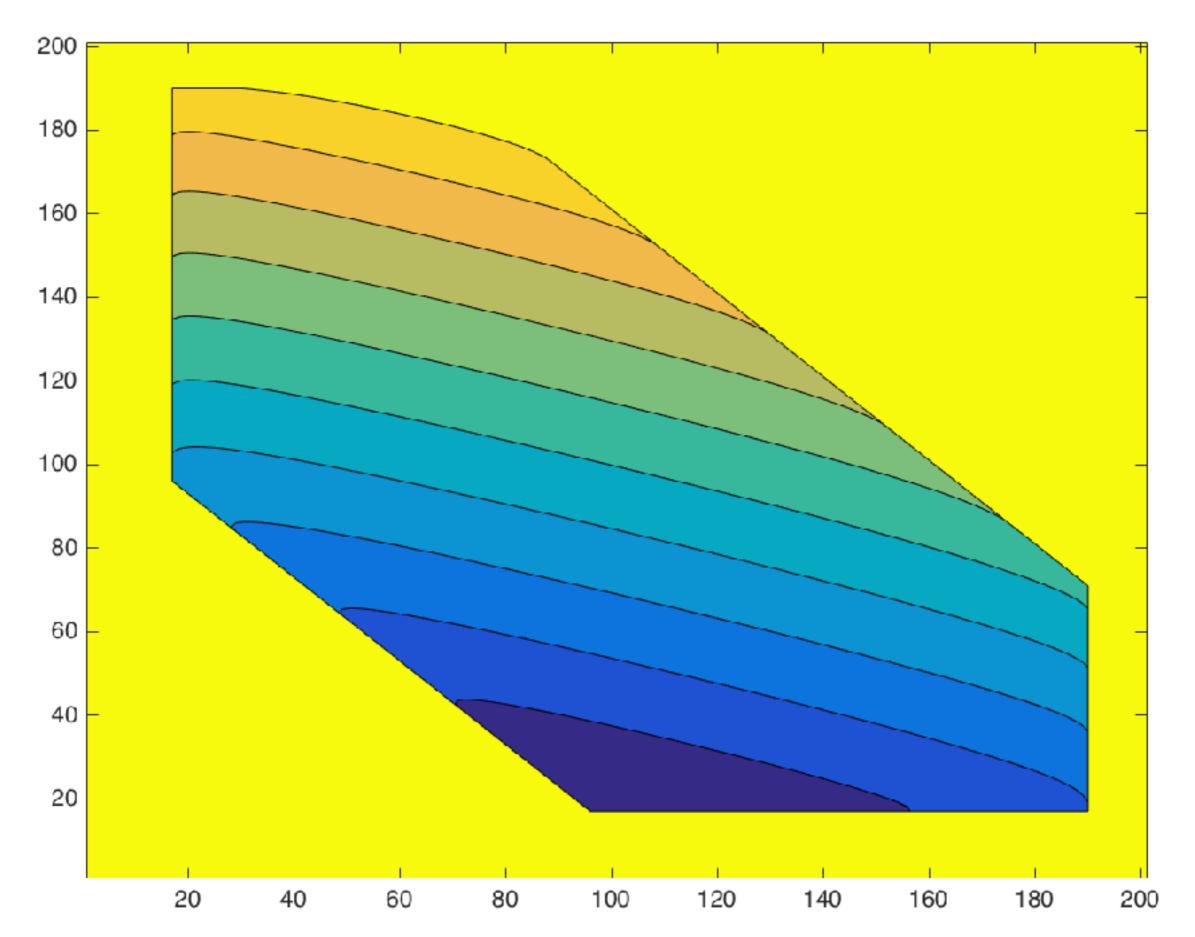


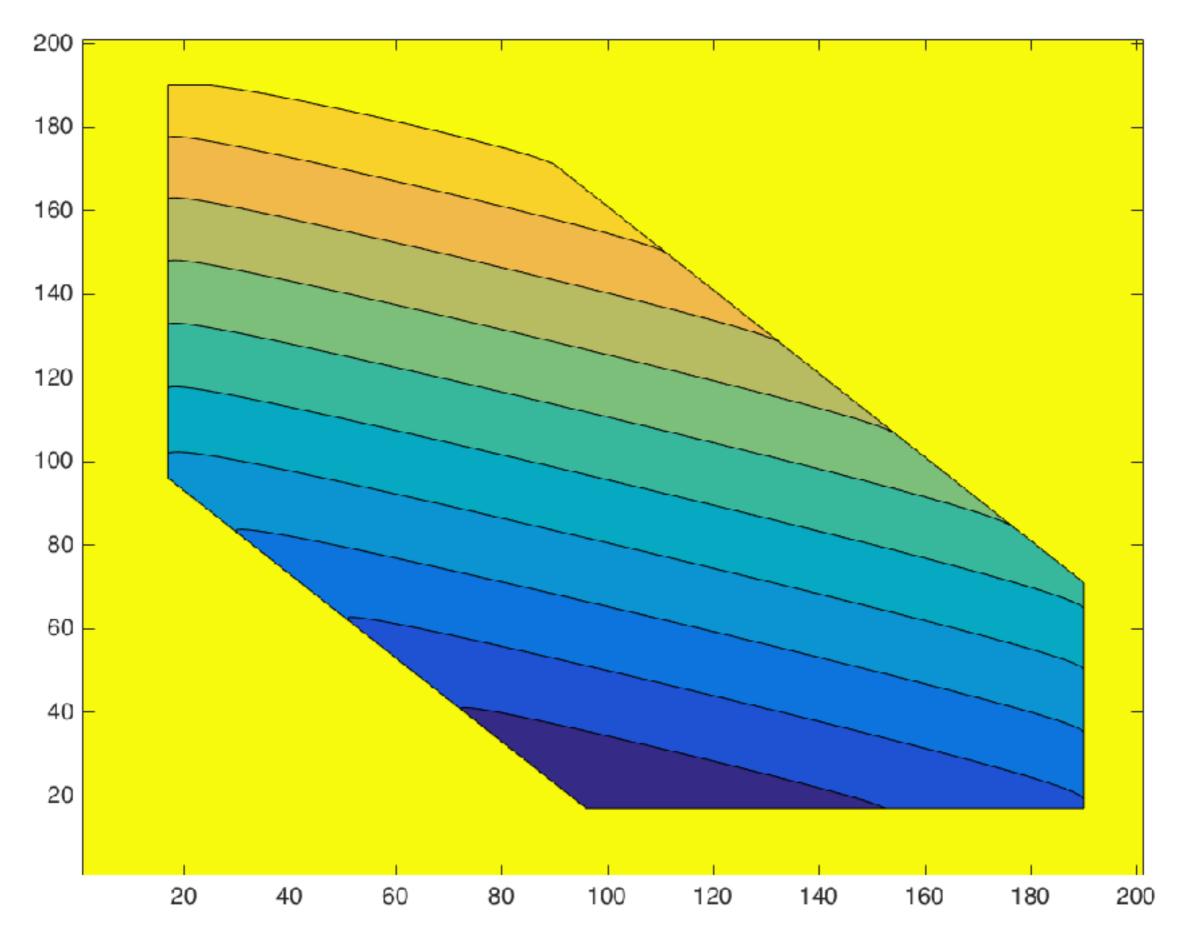








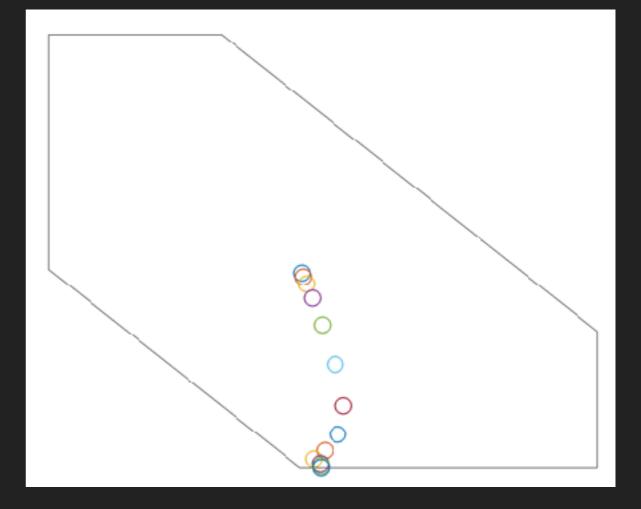




WHY IS THIS CALLED "PATH FOLLOWING"?

$$\Phi(\alpha) := \underset{x \in K}{\arg\min \alpha(\theta^{\top}x)} + \phi(x)$$

 As we increase inflation, the minimizer moves closer to the true desired minimum. We can plot this minimizer as α increases. This is known as the Central Path.



CONVERGENCE RATE OF PATH FOLLOWING

- Nesterov and Nemirovski showed:
 - 1. Best inflation rate is $\alpha_k = (1 + 1/\sqrt{\nu})^k$
 - 2. Approx error after k iter is $\epsilon = \frac{\nu}{(1+1/\sqrt{\nu})^k}$
 - 3. Hence, to achieve ϵ error, need $k = O(\sqrt{\nu} \cdot \log(\nu/\epsilon))$
- The barrier parameter v is pretty important. Nesterov and Nemirovski showed that every set has a self-concordant barrier with barrier parameter v = O(n)

KEY ANALYSIS ELEMENTS OF IPM PATH FOLLOWING

Define:

$$\begin{split} \|v\|_x &:= \sqrt{v^\top \nabla^2 \varphi(x) v}, \\ \|v\|_x^* &:= \sqrt{v^\top \nabla^{-2} \varphi(x) v}, \\ \Phi_k(x) &:= \alpha_k \hat{\theta}^\top x + \varphi(x) \\ \lambda(x, \alpha_k) &:= \|\nabla \Phi_k(x)\|_x^*, \end{split}$$

"local norm" of v w.r.t x;

dual norm of v,

the Newton decrement of x.

Lemma 1. Let $\alpha > 0$ be arbitrary and let $\alpha' = \alpha \left(1 + \frac{c}{\sqrt{\nu}}\right)$. Then for any $x \in int(\mathcal{K})$, we have $\lambda(x, \alpha') \leq (1 + c)\lambda(x, \alpha) + c$. **Lemma 2.** Let x be arbitrary. Then x', the newton update from x, satisfies $\lambda(x', \alpha) \leq 2\lambda^2(x, \alpha)$.

KEY ANALYSIS ELEMENTS OF IPM PATH FOLLOWING

With previous two lemmas, we can prove a very simple invariant. **Lemma 3.** Let c = 1/20. Then for all k we have $\lambda(\hat{x}_k, \alpha_k) < \frac{1}{3}$.

Proof. (By induction) The base case is satisfied since we assume that $\lambda(\hat{x}_0, \alpha_0) = 0$, as $\alpha_0 = 1$. Inductive step: assume $\lambda(\hat{x}_{k-1}, \alpha_{k-1}) < 1/3$. Then

$$\begin{aligned} \lambda(\hat{x}_k, \alpha_k) &\leq 2\lambda^2(\hat{x}_{k-1}, \alpha_k) \\ &\leq 2((1+c)\lambda(\hat{x}_{k-1}, \alpha_{k-1}) + c)^2 < 2(0.4)^2 < 1/3. \end{aligned}$$

The first inequality follows by Lemma 2 and the second by Lemma 1, hence we are done. $\hfill\square$

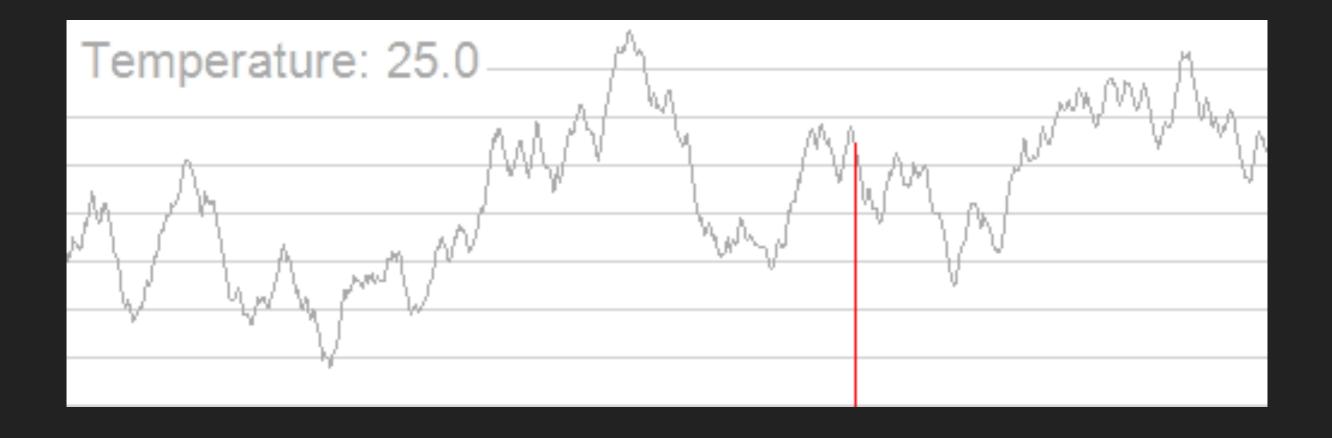
THE PROBLEM: EFFICIENT SELF-CONCORDANT BARRIER IN GENERAL?

- Given any convex set K, how can we construct a selfconcordant barrier for K?
- Polytopes are easy. So are L2-balls. We have barriers for some other sets also, e.g. the PSD cone.
- PROBLEM: Find an efficient universal barrier construction?
- Open problem for some time.

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SIMULATED ANNEALING FOR OPTIMIZATION



From Wikipedia: Optimization of a 1-dimensional function

INTRODUCTION TO SIMULATED ANNEALING

Your goal is to solve the optimization

$$\min_{x \in K} f(x)$$

Maybe it is easier to sample from the distribution

$$P_t(x) = \frac{\exp(-f(x)/t)}{\int_K \exp(-f(x')/t)dx'}$$

for a temperature parameter t

INTUITION BEHIND SIMULATED ANNEALING HEURISTIC

$$P_t(x) = \frac{\exp(-f(x)/t)}{\int_K \exp(-f(x')/t)dx'}$$

- Why is sampling easier? And why would it help anyway?
- First, when t is very large, sampling from P_t() is equivalent to sampling from the uniform distribution on K. Easy(ish)!
- Second, when t is very small, all mass of P_t() is concentrated around minimizer of f(x). That's what we want!
- Third, the successive distributions P_t() and P_{t+1}() are all very close, so we can "warm start" from previous samples

HIT-AND-RUN FOR LOG-CONCAVE DISTRIBUTIONS

$$P_t(x) = \frac{\exp(-f(x)/t)}{\int_K \exp(-f(x')/t)dx'}$$

- Notice that f() convex in $x ==> \log P_t$ is concave in x
- Lovasz/Vempala showed that problem of sampling logconcave dists is **poly-time** using **Hit-And-Run random walk** IF you have a warm start (more on this later)
- Hit-And-Run is an interesting randomization procedure to sample from a convex body, with an interesting history

HIT-AND-RUN

Inputs: distribution P, #iter N, initial $X_0 \in K$. For i = 1, 2, ..., N

1. Sample random direction $u \sim N(0, I)$

2. Compute line segment $R = \{X_{i-1} + \rho u : \rho \in \mathbb{R}\} \cap K$

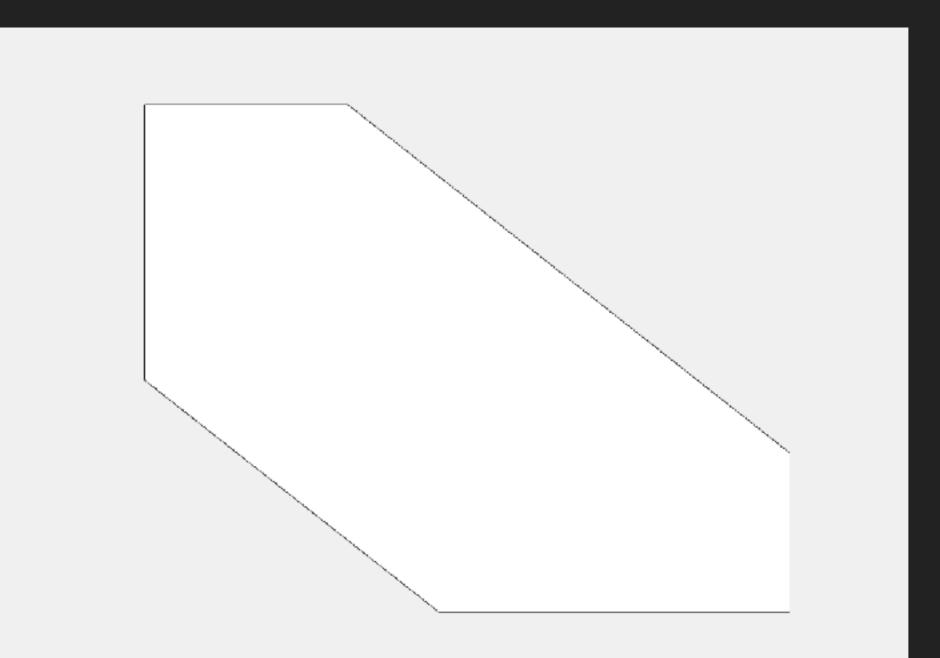
3. Sample X_i from P restricted to R

Return X_N

Claim: Hit-And-Run walk has stationary distribution P

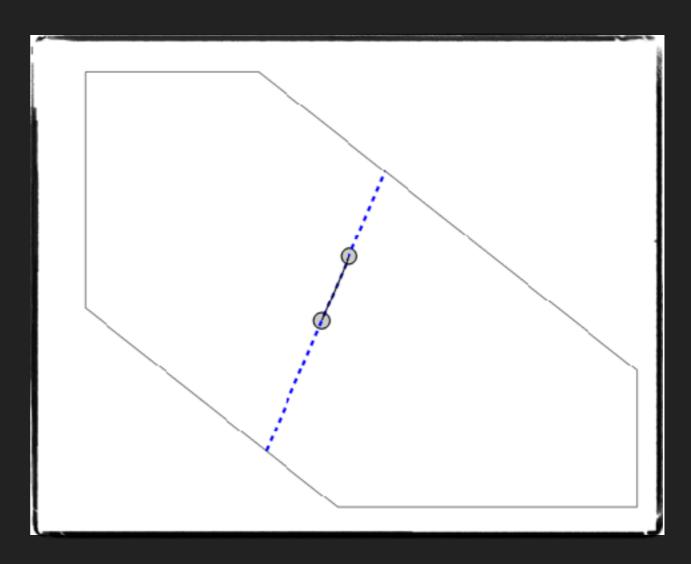
Question: In what way does K enter into this random walk?

HIT-AND-RUN



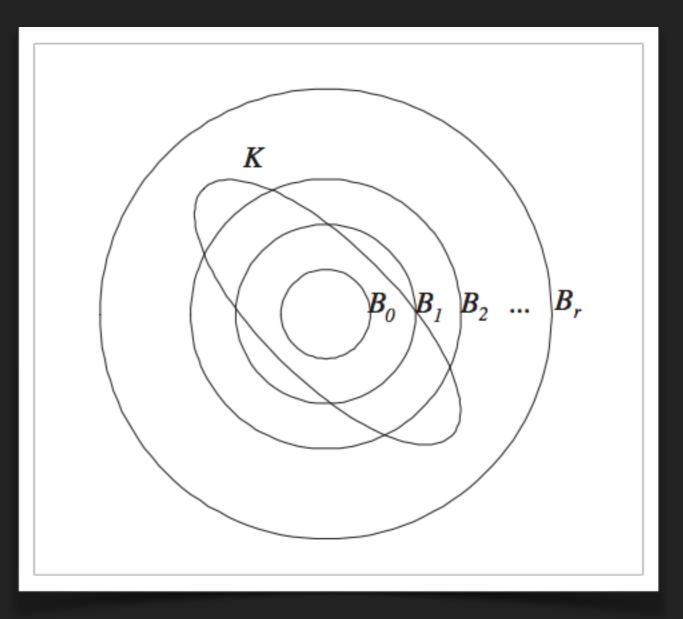
HIT-AND-RUN REQUIRES ONLY A MEMBERSHIP ORACLE

- Notice: a single update of Hit-And-Run required only computing the endpoints of a line segment.
- Can be accomplished using binary search with a *membership oracle*



ASIDE: VOLUME COMPUTATION THROUGH RANDOM WALKS

- If you can uniformly sample from a convex body with a membership oracle, you can approximately compute it's volume!
- Requires computing a sequence of volume ratios between smaller and smaller regions of the body.

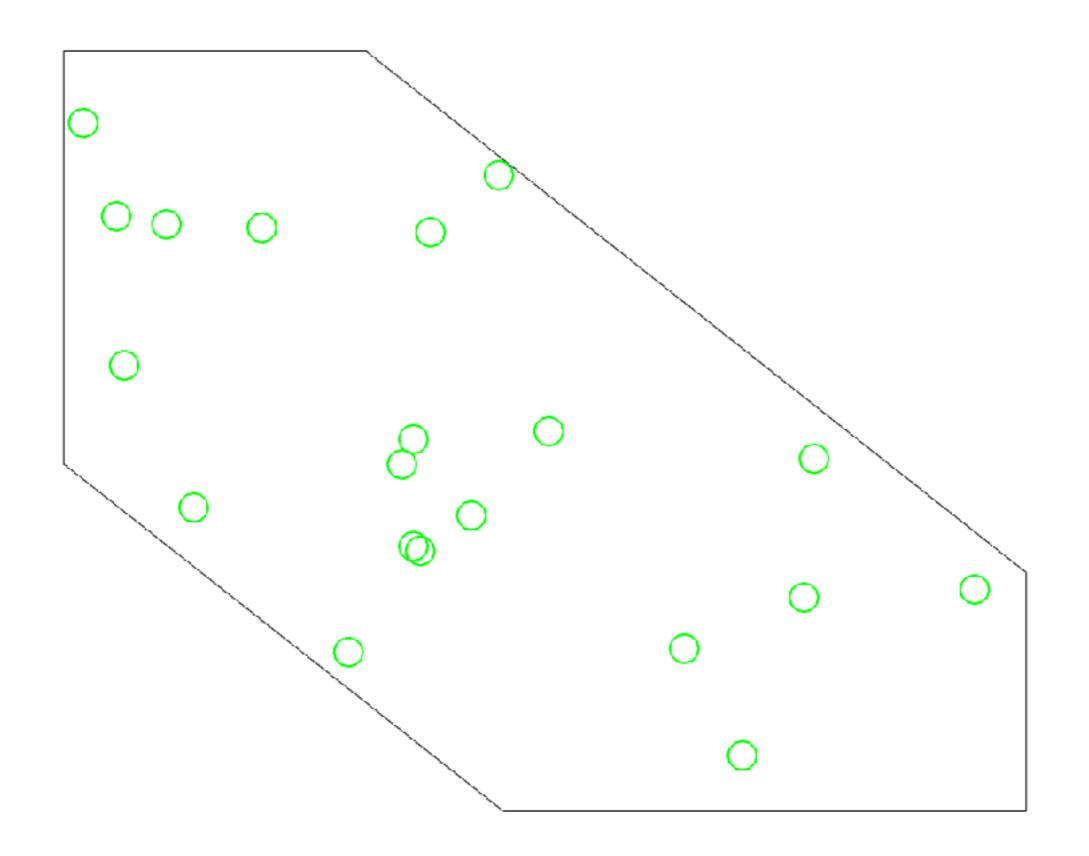


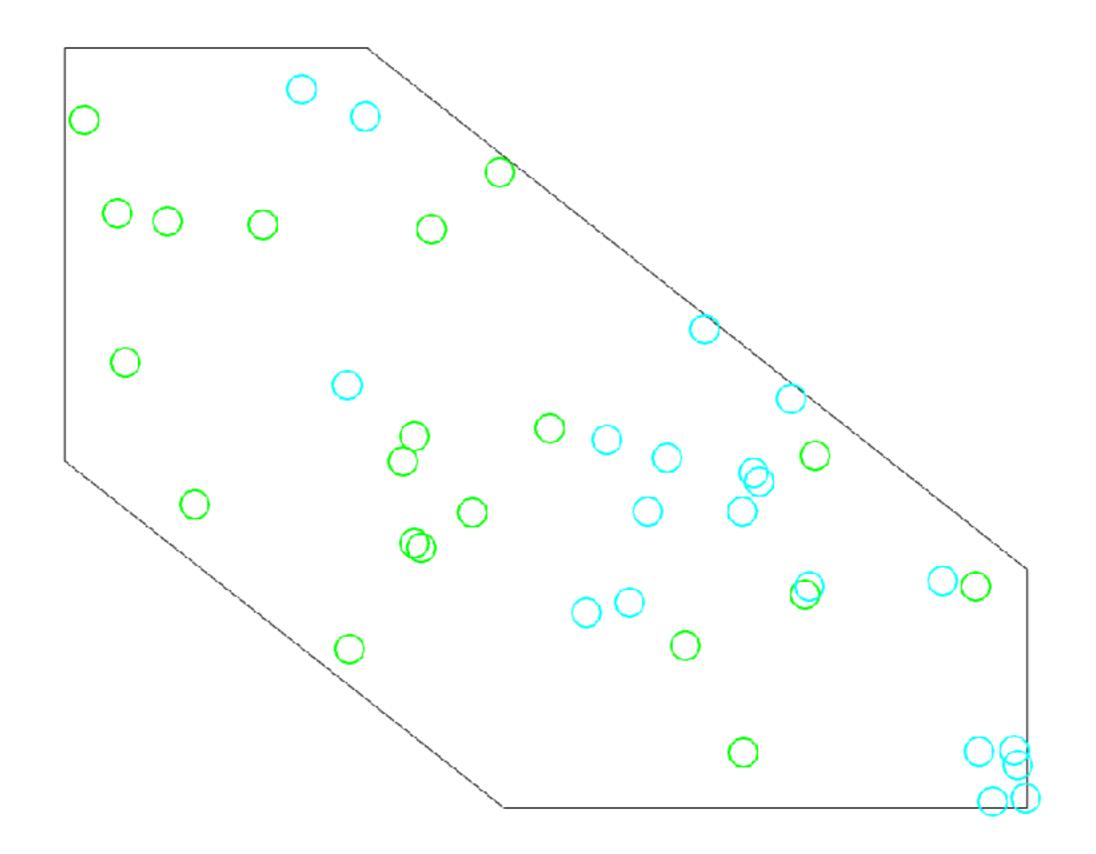
POLYTIME SIMULATED ANNEALING CONVERGENCE RESULT

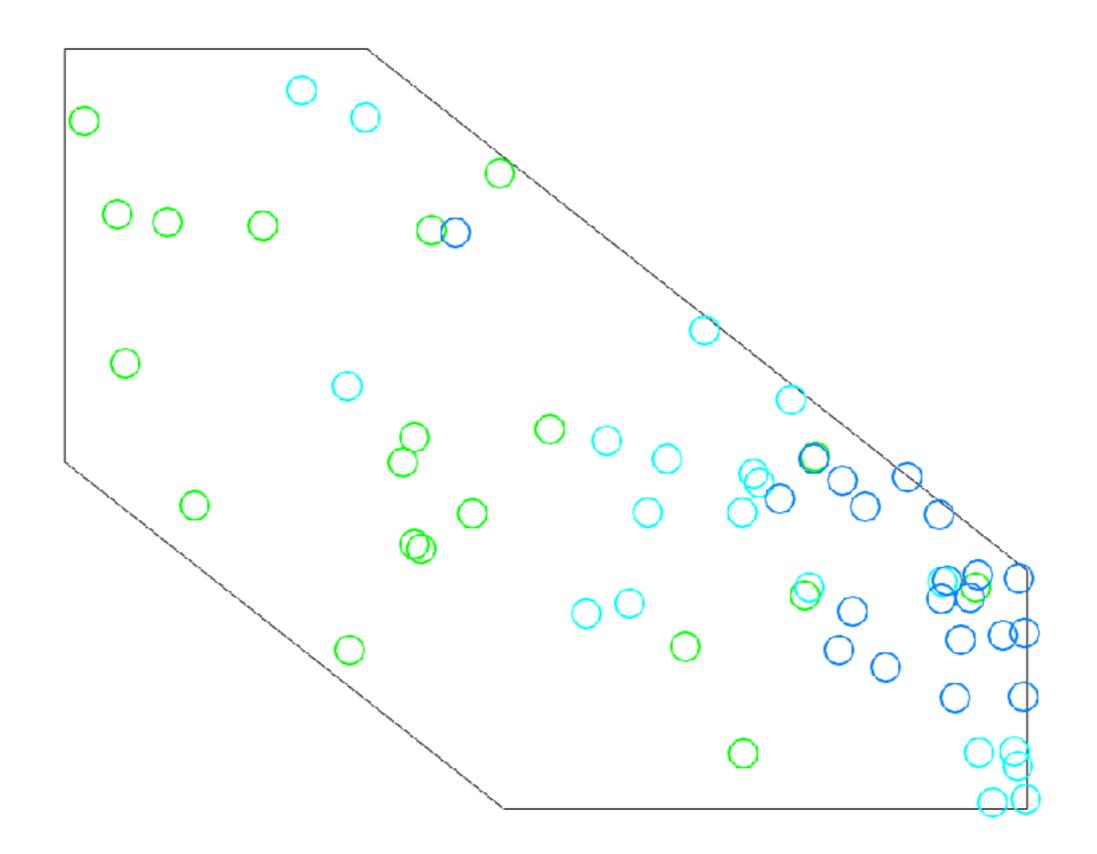
- Kalai and Vempala (2006) gave a poly-time guarantee for annealing using Hit-and-Run (membership oracle only!)
- 1. Sample from $P_k(x) \propto \exp(-\theta^{\top} x/t_k)$
- 2. Successive dists are "close enough" if $KL(P_{k+1}(x)||P_k(x)) \leq 1/2$
- 3. The closeness is guaranteed as long as $t_k \approx (1 1/\sqrt{n})^k$
- 4. Roughly $O(\sqrt{n} \log 1/\epsilon)$ phases needed, $O(n^3)$ Hit-and-Run steps needed for mixing, and O(n) samples needed per phase
- Needed: n^3 steps to mix, n samples per phase, n^0.5 phases. Hence, total running time is O(n^{4.5})

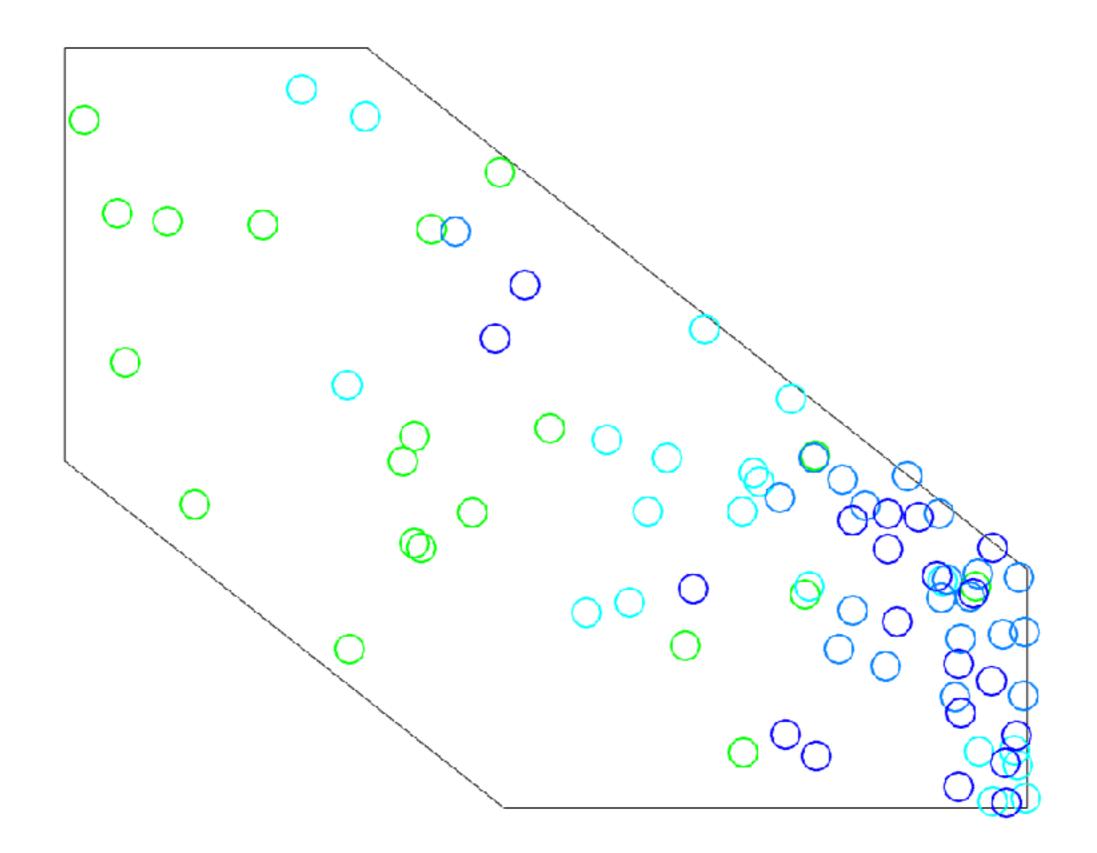
TWO DIFFERENT CONVEX OPTIMIZATION TECHNIQUES

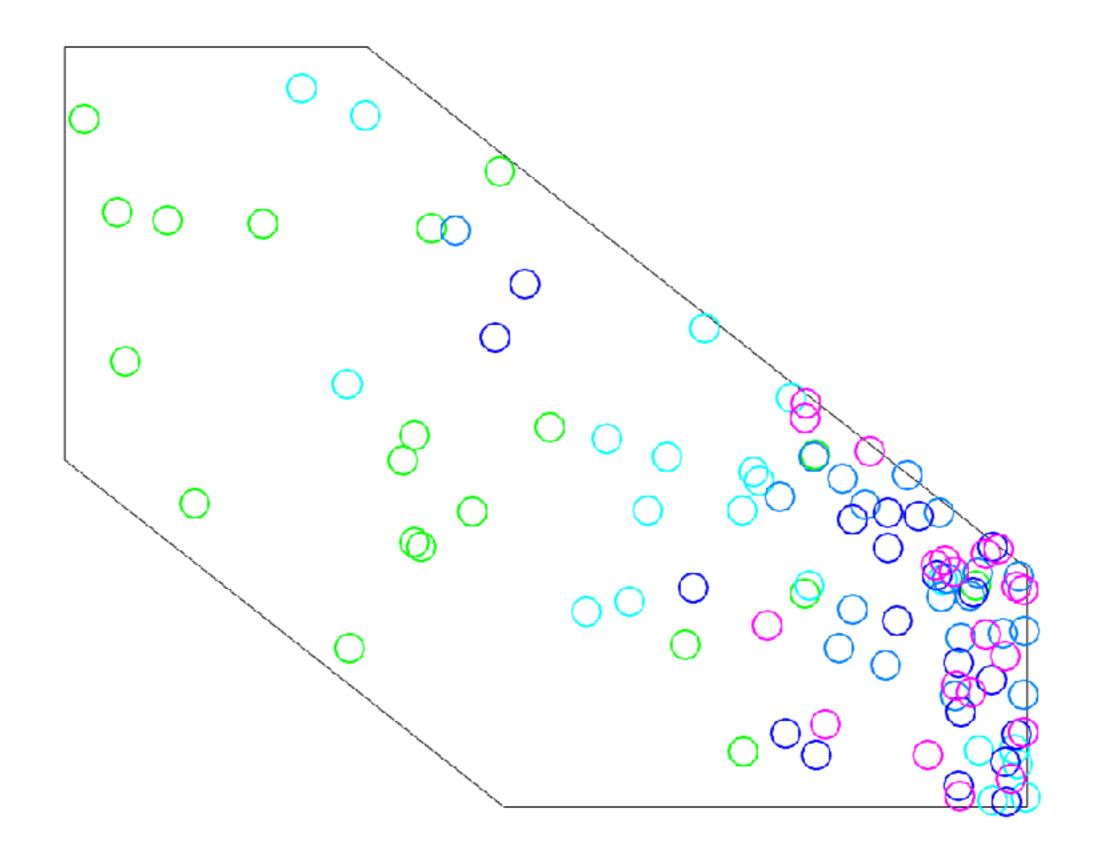
Simulated Annealing via Hit-and-Run Interior Point Methods via Path Following

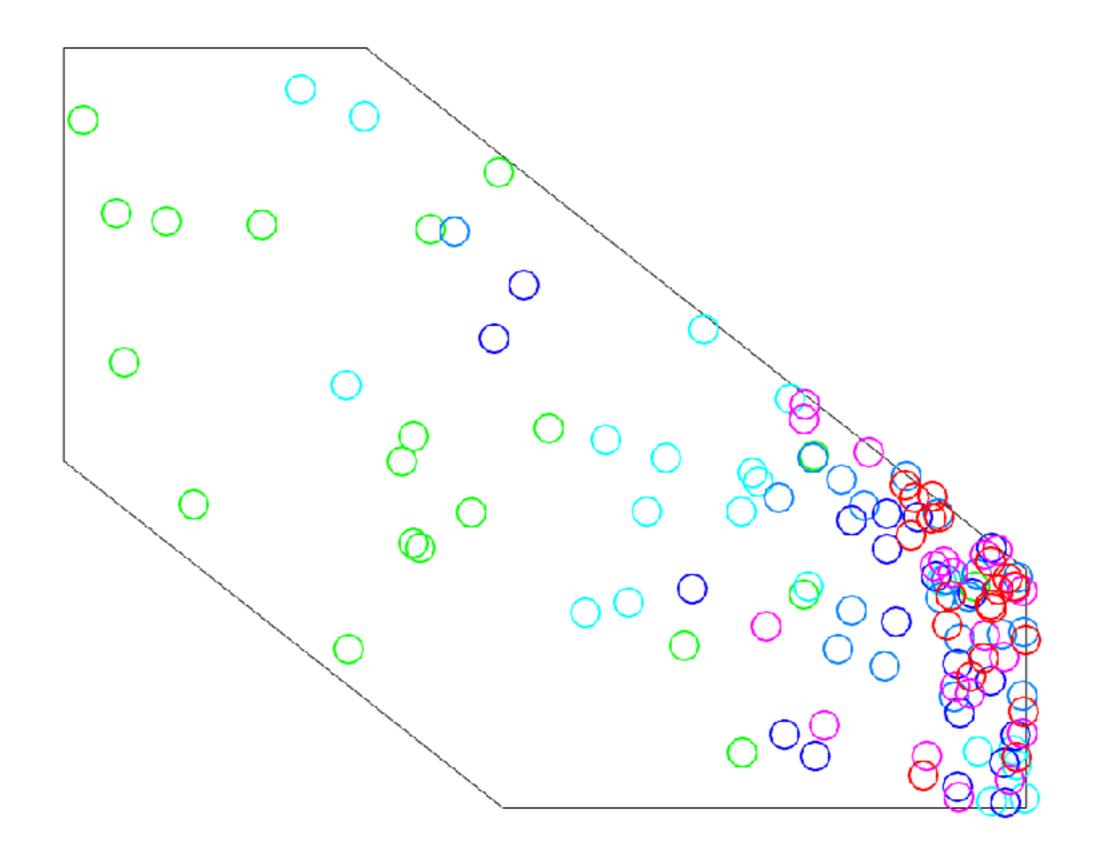


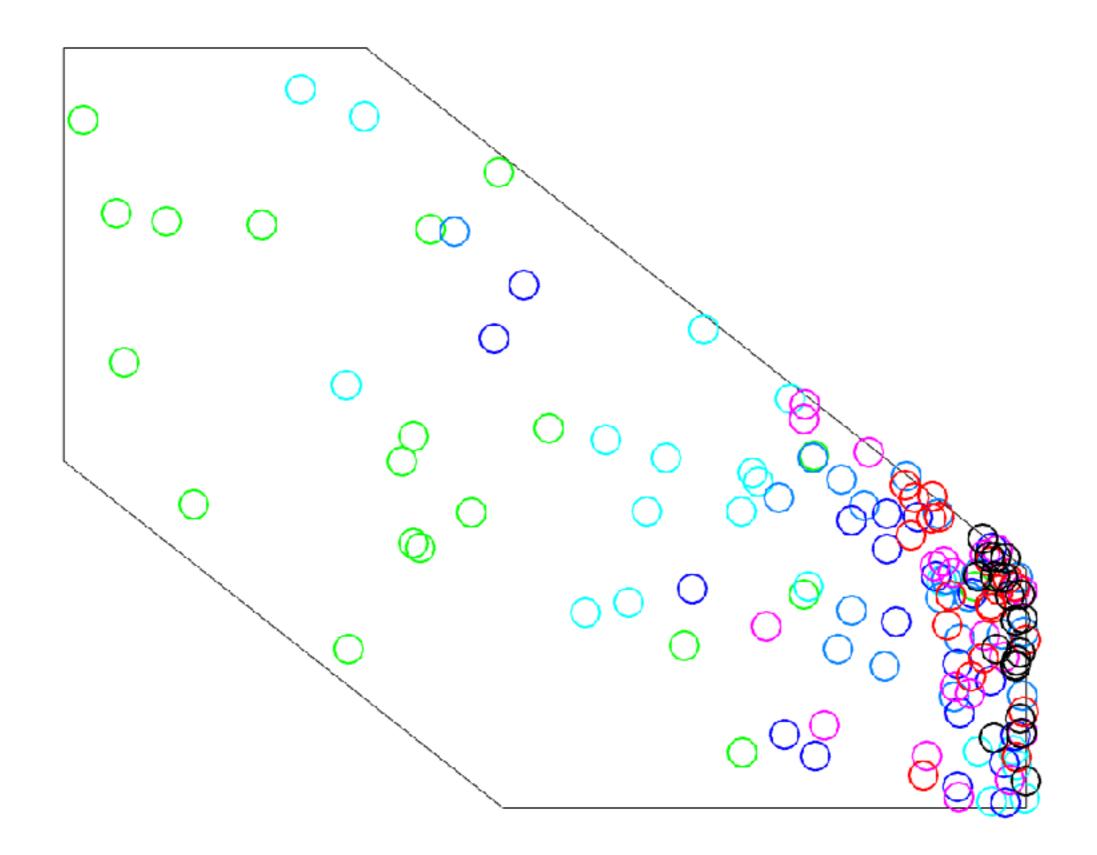










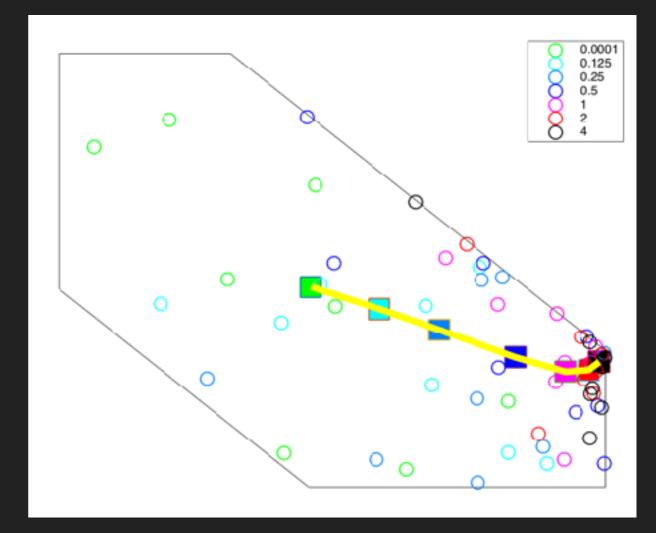


THE HEATPATH

 We can define a path according to the sequence of means one obtains as we turn down the temperature. Let

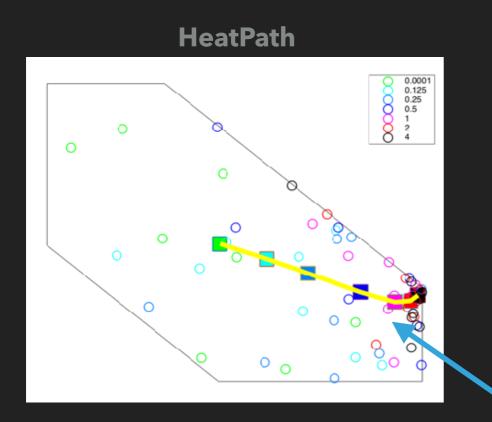
$$\chi(t) := \mathop{\mathbb{E}}_{X \sim \exp(-\theta^\top x/t)/Z} [X]$$

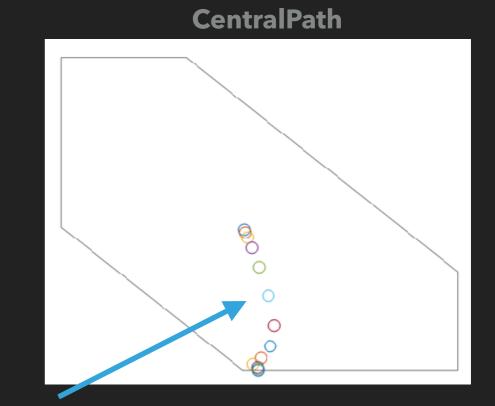
be the **HeatPath**.



THE EQUIVALENCE OF THE CENTRAL PATH AND THE HEAT PATH

Key result of A./Hazan 2016: there exists a barrier function φ() such that the CentralPath (for φ()) is *identically* the HeatPath for the sequence of annealing distributions





These are the same object

WHAT IS THE SPECIAL BARRIER?

- The barrier \u03c6() corresponds to the "differential entropy" of the exponential family distribution. Equivalently, it's the Fenchel conjugate of the log-partition function.
 - Let $A(\theta) = \log \int_K \exp(\theta^\top x) dx$
 - Let $A^*(x) = \sup_{\theta} \theta^\top x A(\theta)$
 - A fact about exponential families: $\nabla A(\theta) = \mathbb{E}_{X \sim P_{\theta}}[X]$
 - A fact about Fenchel duality: $\nabla A(\theta) = \arg \max_{x \in K} \theta^{\top} x A^*(x)$
- Guler 1996 showed this function is a barrier for cones. Bubeck and Eldan 2015 showed this in general, and gave an optimal parameter bound of n(1 + o(1)).

SIMULATED ANNEALING <=> IPM PATH FOLLOWING

Define:
$$\left\| \frac{\mu}{\pi} \right\| \equiv \mathbb{E}_{x \sim \mu} \left(\frac{\mu(x)}{\pi(x)} \right) = \int_{x \sim \mu} \left(\frac{\mu(x)}{\pi(x)} \right) d\mu(x).$$

Let $\gamma > 0$ be a parameter

Lovasz/Vempala: Properties of log-concave distributions imply that, given a warm start from P_{θ} , Hit-and-Run mixes quickly (in $\tilde{O}(n^3)$ steps) to $P_{(1+\gamma)\theta}$ as long as $\left\|\frac{P_{(1+\gamma)\theta}}{P_{\theta}}\right\| = O(1)$

Nesterov/Nemirovski: Properties of self-concordant barrier functions imply that, for the iterative path following scheme, a single newton step suffices to maintain the invariant $\lambda(x_k, (1 + \gamma)^k) < 1/3$.

SIMULATED ANNEALING <=> IPM PATH FOLLOWING

Question: How to bound
$$\left\|\frac{P_{(1+\gamma)\theta}}{P_{\theta}}\right\|$$
 using IPM analysis?

Consider the log of the L2-distance between distributions:

$$\log \left\| \frac{P_{(1+\gamma)\theta}}{P_{\theta}} \right\| = \operatorname{KL}(P_{(1+\gamma)\theta} || P_{\theta}) + \operatorname{KL}(P_{(1-\gamma)\theta} || P_{\theta})$$
$$= D_{A}((1+\gamma)\theta, \theta) + D_{A}((1-\gamma)\theta, \theta)$$
$$\approx \underbrace{2\lambda^{2}(x((1+\gamma)\theta), 1)}_{\text{exact quantity of interest in IPM}}$$

CONCLUSIONS

- Observation: Interior Point Path Following follows the same analytical framework as Simulated Annealing
- Benefit 1: This unifies two rich research areas, and lets one borrow tricks from barrier methods to understand annealing, and vice versa
- Benefit 2: The connection allows us to get a speedup on annealing using barrier methods, improving Kalai/ Vempala's rate of O(n^{4.5}) to O(v^{1/2}n⁴)

FUTURE DIRECTIONS

- Annealing + RandomWalk methods suffer due to the cost of the Markov chain procedure (although very generic!)
- Interior Point Methods suffer because it's hard to construct an efficient barrier (although great if you have one!)
- Question: can we rely on a weaker oracle than a SCBF gradient/hessian oracle? What is the weakest object that could be used to get a better rate?

