Extrapolating the profile of a finite population

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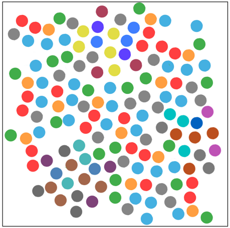
Bernoulli sampling model [Bunge and Fitzpatrick, 1993]



θ_1 Balls of color 1
θ_2 Balls of color 2
...
θ_k Balls of color k

- Setup: Population of k balls, each belonging to one of k types (color).
- Want to estimate: Profile of the urn [Orlitsky et al., 2005]:

$$\pi = \frac{1}{k}\sum_{j=1}^{k} \delta_{\theta_j}$$

  in total variation distance. Note that π_j gives us the proportion of color with exactly j balls.
- Data: X_j balls of color j, distributed as $\mathrm{Binom}(\theta_j, p)$. p might be vanishing, i.e. $p \xrightarrow{k\to\infty} 0$.
- Note that the empirical distribution of color contains more information, but requires more samples to learn. In particular, it cannot be estimated consistently in the sub-linear regime.

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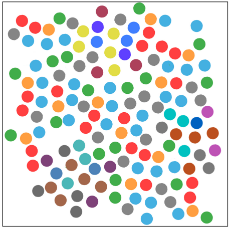

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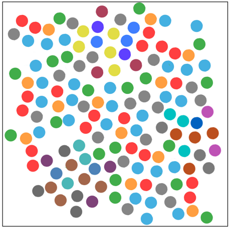

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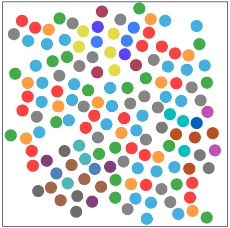

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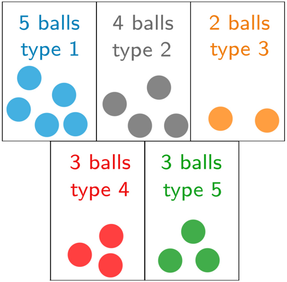
Example

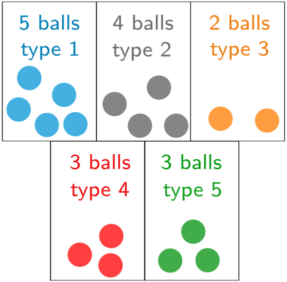


Urn of size 17. The distribution of color is

- 5 blue balls
- 4 gray balls
- 2 orange balls
- 3 red balls
- 3 green balls.

Then the empirical distribution of colors (μ) is given by

$$\mu(\text{blue}) = \frac{5}{17}, \mu(\text{gray}) = \frac{4}{17}, \mu(\text{orange}) = \frac{2}{17},$$
$$\mu(\text{red}) = \frac{3}{17}, \mu(\text{green}) = \frac{3}{17}.$$



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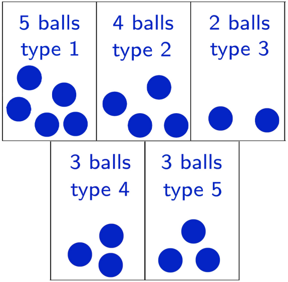
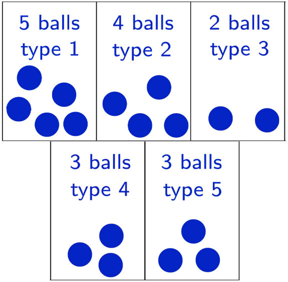


- The profile (π) depends on the color-deleted version of the urn.
- π is supported on $\{0, 1, \ldots, 17\}$ and is given by

$$\pi_m = \begin{cases} 1 - \frac{5}{17} & \text{if } m = 0 \\ \frac{1}{17} & \text{if } m = 2, 4, 5 \\ \frac{2}{17} & \text{if } m = 3 \\ 0 & \text{otherwise.} \end{cases}$$

- π_0 gives us total number of distinct colors (C)

$$\pi_0 = 1 - \frac{C}{k}.$$



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Usefulness

Usefulness of profile

[Orlitsky et al., 2005] Important label invariant properties (e.g. entropy, number of distinct species) are learnable through π.

Consider small sample regime (sample size vanishing fraction of k)

- Consistent estimation of μ is impossible.
- Consistent estimation of π is possible.
- Useful implication towards estimating label invariant properties from small sample.

The problem of estimating π is part of the program of "empirical Bayes" [Robbins, 1951, Robbins, 1956].

- Want to estimate functional f of $\vec{\theta} = (\theta_1, \ldots, \theta_j)$.
- The goal is to compete with the oracle estimator $\hat{f}(\vec{X}, \pi)$ which one can compute when the true π is known.
- When π is unknown we get estimator $\hat{\pi}$ of π and then substitute to get $\hat{f}(\vec{X}, \hat{\pi})$.

Question : How well the estimation of π can be done?

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Existing literature

Distinct elements problem

Find estimator $\hat{\pi}_0$ such that

$$\max_{k \text{ ball urn}} \mathbb{E}|\hat{\pi}_0 - \pi_0| \xrightarrow{k\to\infty} 0.$$

- [Bunge and Fitzpatrick, 1993, Charikar et al., 2000, Raskhodnikova et al., 2009, Valiant and Valiant, 2011, Wu and Yang, 2018, ...]
- [Wu and Yang, 2018] If $\frac{1}{\log k} \lesssim p \lesssim 1$ the optimal rate of estimating π_0 is $k^{-\Theta(p)}$.
- [Valiant, 2012, Wu and Yang, 2018] Consistent estimation is not possible if $p = O\left(\frac{1}{\log k}\right)$.

Estimation of π_m, $m \geq 1$

- Our results refines the above for other atoms of π. We show that the polynomial rate $k^{-\Theta(p)}$ holds for all π_m with $m = o(\log k)$.
- For $m = \Theta(\log k)$ estimation is much harder, with rate $\Omega_p\left(\frac{1}{(\log k)^2}\right)$.

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- Want to evaluate (for possibly vanishing p)

$$R(k) = \inf \sup \mathbb{E}\left[\|\pi - \hat{\pi}\|_{\mathrm{TV}}\right].$$

- Sorted version of μ ($\mu^{\downarrow}$) and π are related

$$\|\pi^1 - \pi^2\|_{\mathrm{TV}} \le \|\mu^{1\downarrow} - \mu^{2\downarrow}\|_{\mathrm{TV}}.$$

- [Orlitsky et al., 2005, Valiant and Valiant, 2013, Han et al., 2018] studied estimation of $\mu^{\downarrow}$ for general population (might not be finite). There exists $\hat{\mu^{\downarrow}}$ based on sample of size $\Theta(k)$ such that

$$\mathbb{E}\left[\|\mu^{\downarrow} - \hat{\mu^{\downarrow}}\|_{\mathrm{TV}}\right] \le O\left(\frac{1}{\sqrt{\log k}}\right).$$

- This implies existence of $\hat{\pi}$ such that $\mathbb{E}\left[\|\pi - \hat{\pi}\|_{\mathrm{TV}}\right] \le O\left(\frac{1}{\sqrt{\log k}}\right)$.
- For finite population this upper bound is loose by a square root factor in view of our main result.

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Results

Main theorem

For all $k \geq \frac{d_0}{\bar{p}}$, where d_0 is some absolute constant, the following holds.

1. There exists absolute constant C such that

$$R(k) \leq \min\left\{\frac{C}{p \log k}, 1\right\}.$$

   The upper bound is achieved by minimum-distance estimator computable in polynomial time.

2. There exists absolute constant c such that

$$R(k) \geq \min\left\{\frac{\bar{p}}{p}, \sqrt{\log k}\right\} \frac{c}{\log k}$$

   where $\bar{p} = 1 - p$.

- This shows that in linear regime (i.e. constant p) the optimal TV rate is $\Theta\left(\frac{1}{\log k}\right)$.
- Consistent estimation is possible in vanishing regime $p = \omega\left(\frac{1}{\log k}\right)$.

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Connection to minimum distance estimator

General set up:

- Parameter space Θ.
- Distribution family $\{P_\theta : \theta \in \Theta\}$ with distance measure ρ.
- $\pi = \frac{1}{k}\sum_{i=1}^{k} \delta_{\theta_j}$.
- Want to analyze

$$R(k) = \inf_{\hat{\pi}} \sup_{\theta_1,\ldots,\theta_k} \mathbb{E}\left[d(\hat{\pi},\pi)\right]$$

under some cost constraint $\frac{1}{k}\sum_{j=1}^{k} c(\theta_j) \leq 1$.

Data: $X_j \sim P_{\theta_j}$ independently for $j = 1, \ldots, k$.

Empirical estimate $\hat{\nu} = \frac{1}{k}\sum_{j=1}^{k} \delta_{X_j}$ satisfies

$$\mathbb{E}\left[\hat{\nu}\right] = \pi P.$$

This motivates estimation of π as

$$\hat{\pi} = \operatorname*{argmin}_{\pi'} \left\{\rho(\hat{\nu}, \pi' P) : \mathbb{E}_{\pi'}\left[c(\theta)\right] \leq 1\right\}.$$

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Connection to linear programming

Suppose additionally we have concentration of $\hat{\nu}$ around πP

$$\mathbb{P}\left[\rho(\pi P, \hat{\nu}) > t_k\right] \leq \epsilon_k$$

for some $t_k, \epsilon_k \to 0$. Then we can argue to get results of type

$$R(k) \lesssim \delta(2t_k)$$

where δ is the linear program given by

$$\delta(t) = \sup\left\{d(\pi, \pi') : \rho(\pi P, \pi' P) \leq t, \mathbb{E}_\pi\left[c(\theta)\right] \leq 1, \mathbb{E}_{\pi'}\left[c(\theta)\right] \leq 1\right\}.$$

Choice of total variation: Choosing $\rho(\cdot,\cdot) = \|\cdot - \cdot\|_{\mathrm{TV}}$ gives us

$$\delta(1/k) \lesssim R(k) \lesssim \delta(t_k).$$

When $\delta(1/k) \asymp \delta(t_k)$ we get the rate.

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$$\delta(1/k) \lesssim R(k) \lesssim \delta(t_k).$$

When $\delta(1/k) \asymp \delta(t_k)$ we get the rate.

Linear programming: BSM and the total variation case

- For Bernoulli sampling model the family is given by Markov kernel P

$$P_{im} = \binom{i}{m} p^m (1-p)^{i-m}, \quad i, m \geq 0.$$

- Note that profile has mean less than 1. Define linear program

$$\delta_{\mathrm{TV}}(t) \triangleq \sup \left\{ \|\pi - \pi'\|_{\mathrm{TV}} : \|\pi P - \pi' P\|_{\mathrm{TV}} \leq t; \mathbb{E}_\pi[\theta], \mathbb{E}_{\pi'}[\theta] \leq 1 \right\}.$$

- $\delta_{\mathrm{TV}}(t)$ is a modulus of continuity type linear program that appears in previous work of statistical estimation.

Theorem

There exist absolute constants C_1, C_2, d_0 such that for all $k \geq d_0$

$$\frac{1}{72}\delta_{\mathrm{TV}}\left(\frac{1}{6k}\right) - \frac{C_2}{\sqrt{k}} \leq R(k) \leq 2\delta_{\mathrm{TV}}\left(\sqrt{\frac{C_1 \log k}{k}}\right), \quad (1)$$

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Analyzing $\delta_{\rm TV}$

Lemma

1. *There exists absolute constant* $C_3 > 0$ *such that for all* p, t *we have*

$$\delta_{\rm TV}(t) \leq \min\left\{\frac{C_3}{p\log(1/t)}, 1\right\}. \tag{2}$$

2. *There exist absolute constants* $C_4, t_0 > 0$ *such that for any* $p \in (0,1)$, $t \leq t_0$,

$$\delta_{\rm TV}(t) \geq \min\left\{\frac{\bar{p}}{p}, \sqrt{\log(1/t)}\right\}\frac{C_4}{\log(1/t)}.$$

In view of previous theorem this gives us the rate.

Sketch of proof
($\delta_{\mathrm{TV}}(t)$ bounds)

- To bound $\delta_{\mathrm{TV}}(t)$ we first relate it to another linear program $\delta_*(t)$ in terms of generating functions.
- For any $g(z) = \sum_{n=0}^{\infty} a_n z^n$ define its $\|\cdot\|_A$ norm as

$$\|g\|_A = \sum_{n=0}^{\infty} |a_n|.$$

- Define the new linear program

$$\begin{aligned}\delta_*(t) &\triangleq \sup_{\Delta} \left\{ \sum_{m=0}^{\infty} |\Delta_m| : \|\Delta P\|_1 \le t, \sum_{m=0}^{\infty} m|\Delta_m| \le 1 \right\}. \\ &= \sup_f \left\{ \|f\|_A : \|f_p\|_A \le t, \|f'\|_A \le 1 \right\}\end{aligned}$$

where $f_p(z) = f(\bar{p} + pz)$ and the sup is over all analytic functions f.

Lemma

For all $t \in [0,1]$ we have

$$\frac{1}{2}(\delta_*(t) - t) \le \delta_{\mathrm{TV}}(t) \le \delta_*(t).$$

We bound $\delta_*(t)$ using complex analytic techniques.

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Upper bound on $\delta_*(t)$

- Note that the objective function in $\delta_*(t)$ can be written as

$$\|f\|_A = \sum_{m=0}^{\infty} \frac{\left|f^{(m)}(0)\right|}{m!}.$$

- The contribution from $\sum_{m \geq \log(1/t)} \frac{|f^{(m)}(0)|}{m!}$ is at most $\frac{C_p}{\log(1/t)}$ from the derivative constraint.
- For each other terms we use the LP's

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$$\delta_*(t) \leq \sum_{m=0}^{\log(1/t)} \delta_m(t) + \frac{C_p}{\log(1/t)}.$$

- We then show that each of $\delta_m(t)$ is negligible by using Hadamard three line theorem.

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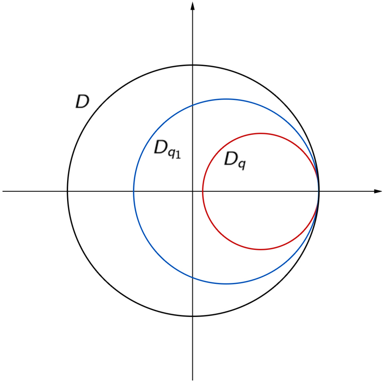
Hadamard's three line theorem



- For any analytic function f define its $\|\cdot\|_{H^\infty(C)}$ norm over set C

$$\|f\|_{H^\infty(C)} = \sup_{z\in C} |f(z)|.$$

Denote by D the unit disc on $\mathbb{C}$ and let $D_p = \bar{p} + pD$.

- Consider $0 < q < q_1 < 1$
- Then Hadamard's three line theorem says that

$$\|f\|_{H^\infty(D_{q_1})} \leq \|f\|_{H^\infty(D)}^{1-\frac{q\bar{q}_1}{\bar{q}q_1}} \|f\|_{H^\infty(D_q)}^{\frac{q\bar{q}_1}{\bar{q}q_1}}.$$

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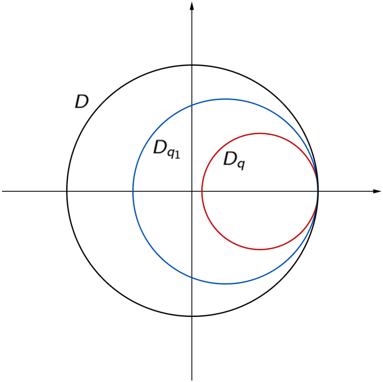

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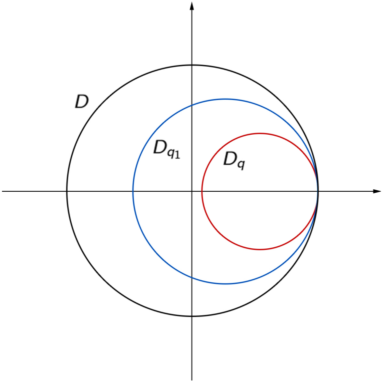

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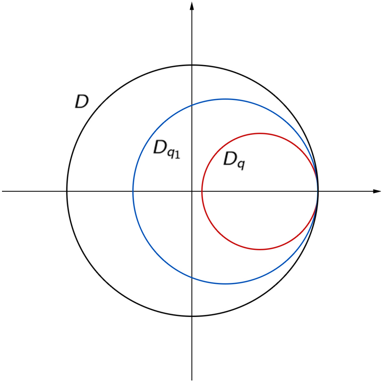

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Upper bounding $\delta_m(t)$ using Hadamard's theorem

- Using ordering between A norm and $H^\infty(D)$ norm, the constraints on $\delta_m(t)$, and Cauchy integral formula we get bounds on $\|f\|_{H^\infty(D)}$ and $\|f\|_{H^\infty(D_p)}$.
- Cauchy's integral formula also implies

$$\frac{|f^{(m)}|}{m!} \le 2^m \|f\|_{H^\infty(D_{1/2})}.$$

- For $p < \frac{1}{2} < 1$ we get $D_p \subset D_{1/2} \subset D_1$. So we can bound $\|f\|_{H^\infty(D_{1/2})}$ in terms of $\|f\|_{H^\infty(D)}$ and $\|f\|_{H^\infty(D_p)}$ by Hadamard's theorem.
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Lower bound on $\delta_*(t)$

- Using $\|\cdot\|_{H^\infty(D)} \le \|\cdot\|_A$ we relax the constraints and objective functions of $\delta_*(t)$ to get related linear program

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$$f(z) = \frac{c_p}{\log(1/t)}(1-z)^2 t^{\frac{p}{p}\frac{1+z}{1-z}}.$$

- We modify $f(z)$ by further dilation $z \to \alpha z$ to get feasible solution to $\delta_*(t)$.
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Summary

- The profile of population gives us information about many important label invariant properties.
- In small sample regime of $p = \omega\left(\frac{1}{\log k}\right)$ we can consistently estimate the profile in total variation distance..
- When $p = \Theta(1)$ the optimal rate is $\Theta\left(\frac{1}{\log k}\right)$.
- The estimator which achieves optimal rate is based of minimum distance type and can be computed in polynomial time.
- We device a single infinite dimensional linear program that characterizes the estimator and also proves its minimax optimality. We solve the LP using complex analytic techniques.

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Proof of upper bound: Connection of risk and $\delta_{\mathrm{TV}}(t)$

- $\hat{\nu}$ concentrates around $\mathbb{E}[\hat{\nu}] = \pi P$

$$\mathbb{E}[\|\hat{\nu} - \nu\|_{\mathrm{TV}}] = \left(\sqrt{\frac{C_1 \log k}{k}}\right).$$

- Using McDiarmid's inequality we get

$$\mathbb{P}[|\|\hat{\nu} - \nu\|_{\mathrm{TV}} - \mathbb{E}[\|\hat{\nu} - \nu\|_{\mathrm{TV}}]| \geq \epsilon] \leq exp\left(C_0 k \epsilon^2\right)$$

which implies

$$\mathbb{P}\left[\|\hat{\nu} - \nu\|_{\mathrm{TV}} \geq \sqrt{\frac{C_1 \log k}{k}}\right] \leq \frac{1}{k}.$$

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- Linear program

$$\delta_{\mathrm{TV}}(t) \triangleq \sup\left\{\|\pi - \pi'\|_{\mathrm{TV}} : \|\pi P - \pi' P\|_{\mathrm{TV}} \le t; \mathbb{E}_{\pi}[\theta], \mathbb{E}_{\pi'}[\theta] \le 1\right\}.$$

- The minimum distance estimator $\hat{\pi} = \mathrm{argmin}_{\pi}\left\{\|\hat{\nu} - \pi P\|_{\mathrm{TV}} : \mathbb{E}_{\pi}[\theta] \le 1\right\}$ satisfies

$$\|\hat{\pi} P - \pi P\|_{\mathrm{TV}} \le \|\pi P - \hat{\nu}\|_{\mathrm{TV}} + \|\hat{\pi} P - \hat{\nu}\|_{\mathrm{TV}} \le 2\|\pi P - \hat{\nu}\|_{\mathrm{TV}}.$$

- This implies

$$\mathbb{E}\left[\|\hat{\pi} - \pi\|_{\mathrm{TV}}\right] \le \mathbb{E}\left[\delta_{\mathrm{TV}}\left(2\|\pi P - \hat{\nu}\|_{\mathrm{TV}}\right)\right] + \frac{1}{k}$$

and hence

$$R(k) = \inf_{\hat{\pi}} \sup_{\pi} \mathbb{E}\left[\|\hat{\pi} - \pi\|_{\mathrm{TV}}\right] \le \mathbb{E}\left[\delta_{\mathrm{TV}}\left(2\|\pi P - \hat{\nu}\|_{\mathrm{TV}}\right)\right] \le \delta_{\mathrm{TV}}\left(\sqrt{\frac{C_1 \log k}{k}}\right) + \frac{1}{k}.$$

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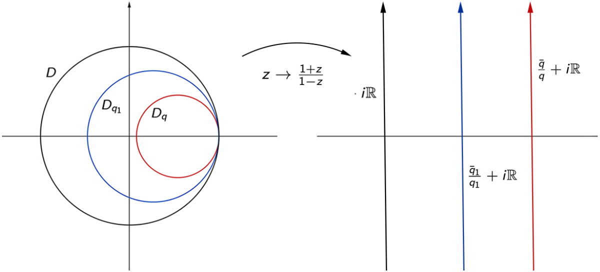
Proof of lower bound: Solution to auxiliary program $\delta_{H^\infty(t)}$

- $\delta_{H^\infty}(t) = \sup_f \left\{ \|f\|_{H^\infty}(D) : \|f_p\|_{H^\infty(D)} \le t, \|f'\|_{H^\infty(D)} \le 1 \right\}$
- We use the transform $w : z \to \frac{1+z}{1-z}$



and re-parameterize $f(z) = g(w)$.

- Then we have $g'(w) = \frac{2}{(1+w)^2} f'\left(\frac{w-1}{w+1}\right)$ and using constraints get the bound

$$\|g'\|_{H^\infty(\Re=\epsilon)} \le 2C_p t^{\min\left\{\frac{\epsilon p}{2\bar{p}}, 1\right\}}, \quad \epsilon \in \left(0, \frac{\bar{p}}{p}\right).$$

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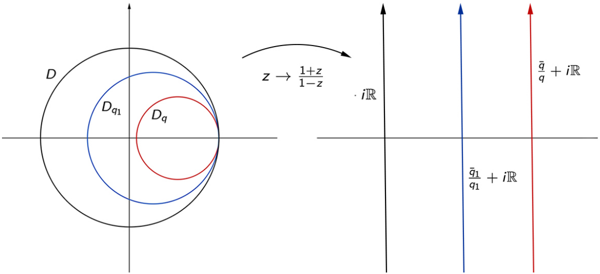

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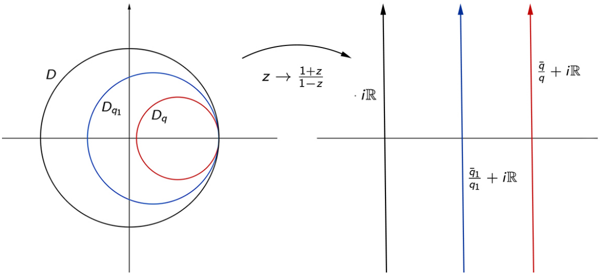

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- Using this we integrate the derivatives to get bound

$$\left|g(iw) - g\left(iw + \frac{\bar{p}}{p}\right)\right| \le C_p \int_0^{\frac{\bar{p}}{p}} t^{\frac{\epsilon p}{2\bar{p}}} \le \frac{C_p}{\log\left(\frac{1}{t}\right)}.$$

- As $\|g\|_{H^\infty(\Re=\bar{p}/p)} \le t$ we get $\|g\|_{H^\infty(\Re=0)} = \|f\|_{H^\infty}(D) \le C_p \frac{1}{\log(1/t)}$.
- As exponential function saturates the Hadamard three line theorem, the guess is to choose exponential function for lower bound. The choice

$$f(z) = \frac{c_p}{\log(1/t)}(1-z)^2 t^{\frac{p}{\bar{p}}\frac{1+z}{1-z}}$$

comes from modifications to satisfy the constraints.

Solving $\delta_*(t)$

- For $\beta > 0, 0 < \alpha < 1$ to be chosen later define

$$h(z) = \exp\left(-\beta \frac{1+\alpha z}{1-\alpha z}\right) = \exp(-\beta)\exp\left(-2\beta \frac{\alpha z}{1-\alpha z}\right).$$

- We use the Laguerre polynomial relation

$$h(z) = \exp(-\beta)\exp\left(-2\beta \frac{\alpha z}{1-\alpha z}\right) = e^{-\beta}\sum_{n=0}^{\infty} \alpha^n L_n^{-1}(2\beta).$$

- Denote $\Delta_m = e^{-\beta}\alpha^n L_n^{-1}(2\beta)$ and show that for sufficiently large β

$$|\Delta_m| + |\Delta_{m+1}| \geq \alpha^{3\beta/2}\beta^{-1/2}.$$

- We bound $\|h\|_A$ from below by $\sum_{\beta \leq m \leq 3\beta/2} |\Delta_m|$.
- For the choice $\beta = \max\left\{\frac{4p}{\bar{p}}\log(1/t), \sqrt{\frac{\log(1/t)}{p}}\right\}$ and $\alpha = \frac{1}{\beta}$ we get desired lower bound.

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