

# Learning and Testing Structured Distributions

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# This Talk

Algorithmic Framework for Distribution Estimation:  
Leads to *fast & robust* estimators  
for a *wide variety of statistical models*.

[Chan-D-Servedio-Sun, STOC'14]

[Chan-D-Servedio-Sun, NIPS'14]

[Acharya-D-Hegde-Li-Schmidt, PODS'15]

[Acharya-D-Li-Schmidt, manuscript'15]

**Key Idea:**

**Exploit piecewise polynomial approximation  
for structured model estimation**

# This Talk

A family of optimal estimators for hypothesis testing  
for a wide variety of structured models.

“Given samples from a statistical model does it satisfy a given property?”

[Daskalakis-D-Servedio-Valiant-Valiant, SODA'13]

[Chan-D-Valiant-Valiant, SODA'14]

[D-Kane-Nikishkin, SODA'15]

[D-Kane-Nikishkin, manuscript'15]

[Cannonne-D-Gouleakis-Rubinfeld, manuscript'15]

# Main Message of the Talk

**We can algorithmically exploit the underlying structure to perform statistical estimation efficiently.**

# Outline

- Learning via Piecewise Polynomial Approximation
  - Introduction
  - Framework Overview
  - Statistical Efficiency
  - Computational Efficiency
  - Empirical Results
- Applications to other Inference Tasks
- Future Directions and Concluding Remarks

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# Distribution Learning (Density Estimation)

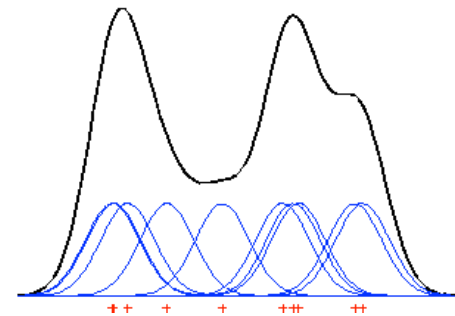
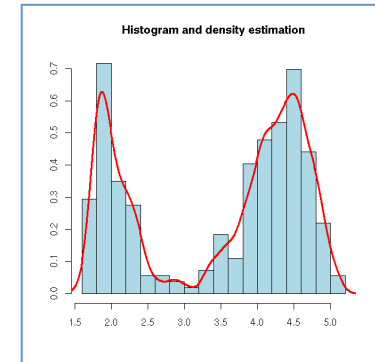
Given samples (observations) from an unknown probability distribution (model), construct an accurate estimate of the distribution.

- Classical Problem in Statistics
- Introduced by Karl Pearson (1891).
- Last fifteen years (TCS): computational aspects



# Distribution Learning: History

- Histograms [Pearson, 1895]
- Kernel methods [M. Rosenblatt, 1956]
- Metric Entropy [A.N. Kolmogorov, 1960]
- Wavelets  
[Donoho, Johnstone, Kerkyacharian, Picard, '90's]



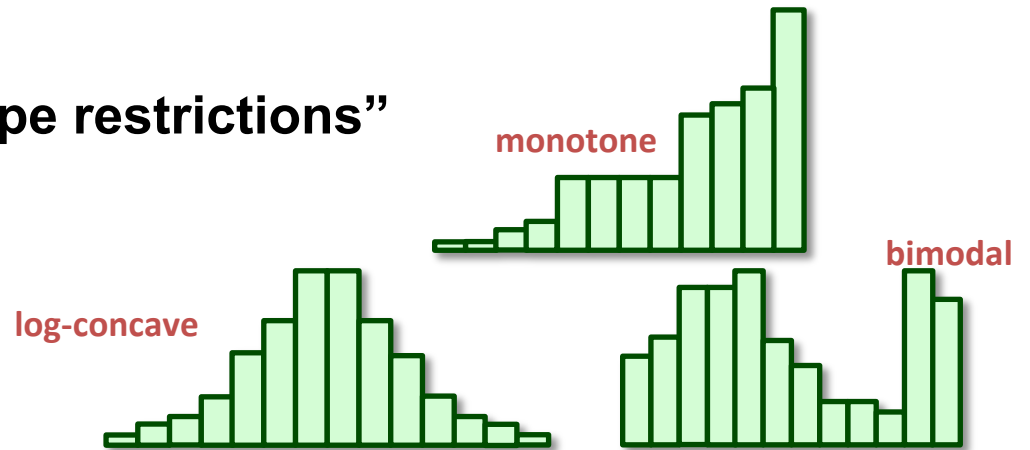
Many others: Nearest Neighbor, Orthogonal Series, ...

**Focus traditionally on sample size.**



# Types of Structured Distributions

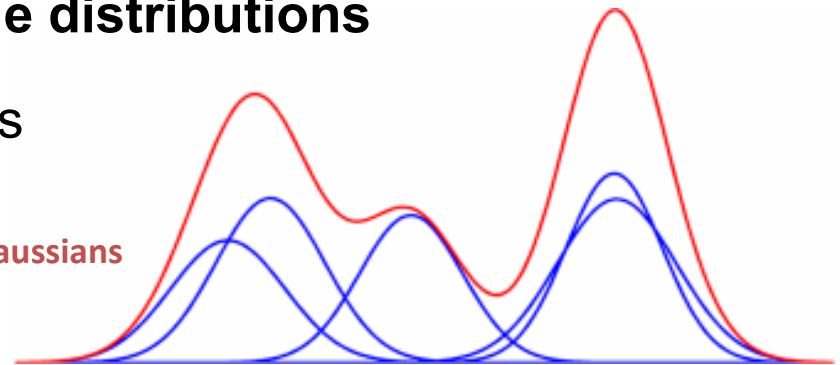
- Distributions with “shape restrictions”



- Simple combinations of simple distributions

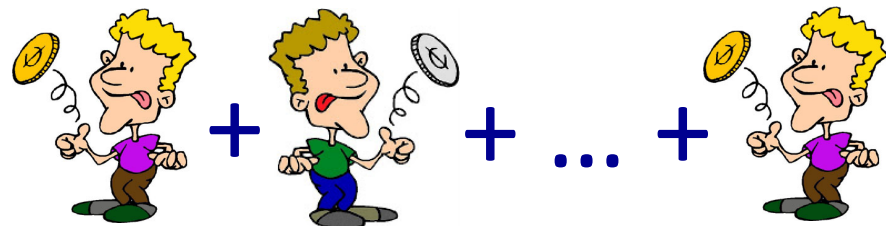
*Mixtures* of simple distributions

mixtures of Gaussians



*Sums* of simple distributions

Poisson Binomial Distributions



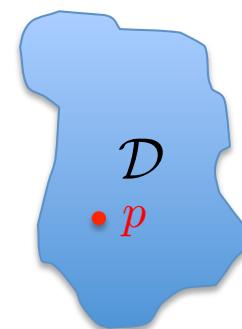
# History

## Nonparametric Estimation under “shape restrictions”

- Long line of work in statistics since the 1950's  
[Gre'56, Rao69, Weg70, Gro85, Bir87,...]
- Shape restrictions studied in early work: monotonicity, unimodality, concavity, convexity, Lipschitz continuity, ...
- Very active research area: log-concavity,  $k$ -monotonicity, ...  
[Balabdaoui-Wellner'07, Balabdaoui-Rufibach-Wellner'09, Walther'09, Dumbgen-Rufibach'09, Cule-Samworth'10, Koenker-Mizera'10, Guntuboyina-Sen'13, Doss-Wellner'13, Kim-Samworth'14]
- Standard tool in these settings: MLE

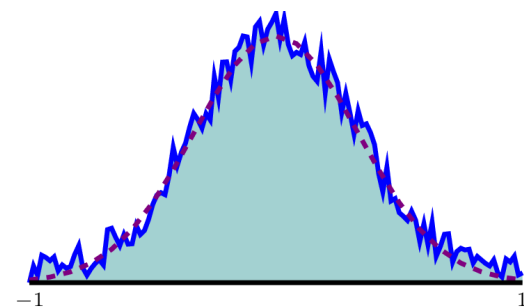
# Distribution Learning: Definition

- Learning problem defined by family  $\mathcal{D}$  of distributions
- Target distribution  $p \in \mathcal{D}$  unknown to learner.
- Learner given sample of IID draws from  $p$ .



**Output:** with probability  $\geq 9/10$  output  $h$  satisfying

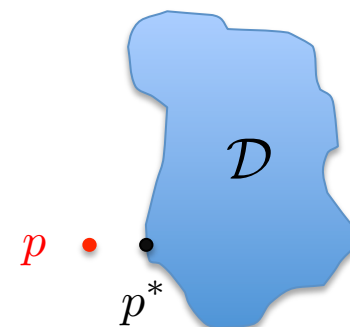
$$\|h - p\|_1 \leq \epsilon.$$



**Goal:** Sample optimal & computationally efficient algorithms

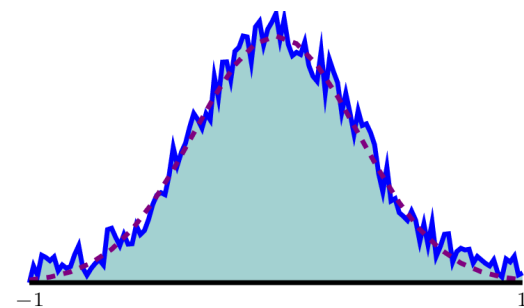
# Agnostic Learning: Definition

- Learning problem defined by class  $\mathcal{D}$  of distributions
- Target distribution  $p$  unknown to learner and let
$$\text{OPT} = \inf_{q \in \mathcal{D}} \|p - q\|_1$$
- Learner given sample of IID draws from  $p$



**Output:** with probability  $\geq 9/10$  output  $h$  satisfying

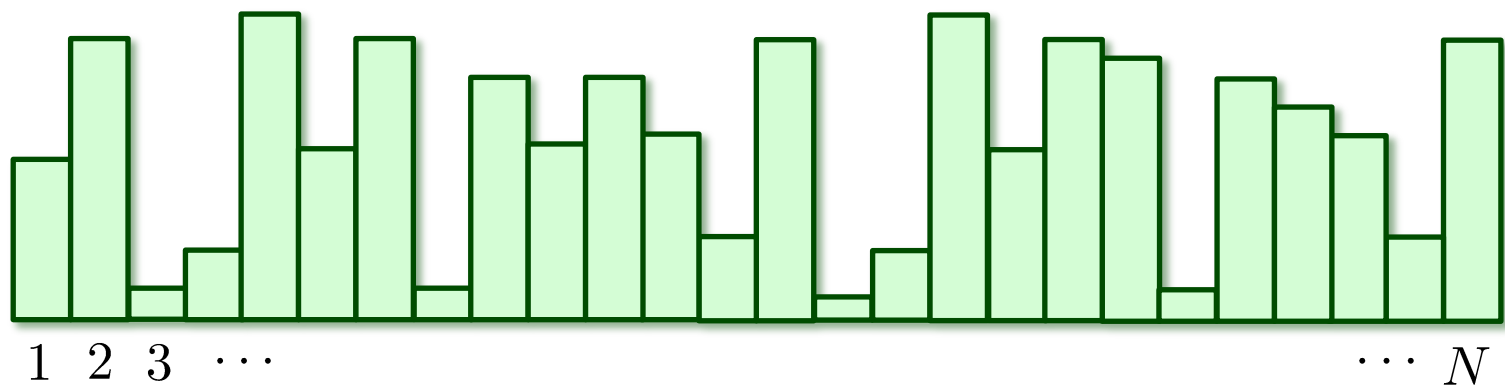
$$\|h - p\|_1 \leq \text{OPT} + \epsilon.$$



**Goal:** Sample optimal & computationally efficient algorithms

# Learning Arbitrary Discrete Distributions

Let  $\mathcal{D}$  be the set of all distributions over  $[N]$ .  
*What is the best learning algorithm?*

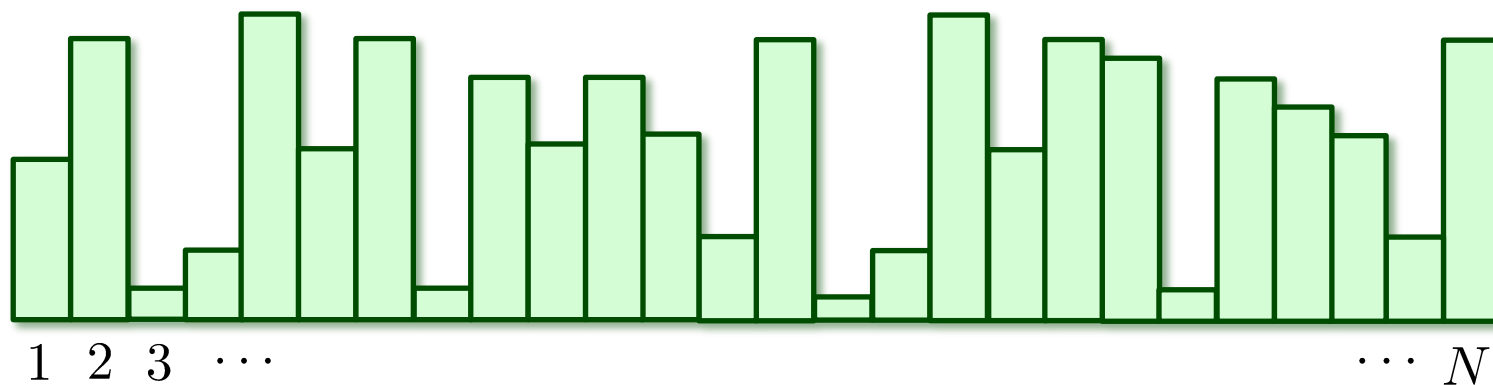


Simple answer (folklore):

- Algorithm with sample (and time) complexity  $O(N/\epsilon^2)$ .
- Information theoretic lower bound of  $\Omega(N/\epsilon^2)$ .

# Learning Arbitrary Discrete Distributions

Learning an *arbitrary* distribution over  $[N]$ :  
Sample size  $\Theta(N/\epsilon^2)$   
necessary and sufficient



When can we do better?

Which distributions are easy to learn, which are hard (and why)?

# Structure and Statistical Estimation

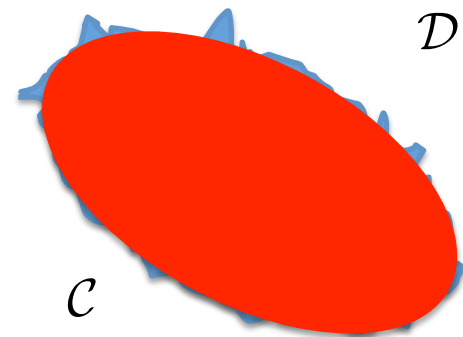
General Recipe for Statistical Estimation:

Given a “complex” distribution family  $\mathcal{D}$ .

1. Find a “canonical” class of distributions  $\mathcal{C}$  that approximates  $\mathcal{D}$  well.

(For every  $p \in \mathcal{D}$  there is  $q \in \mathcal{C}$  such that  $p \approx q$ .)

2. Use samples from  $p$  to estimate it **as if it was**  $q$ .



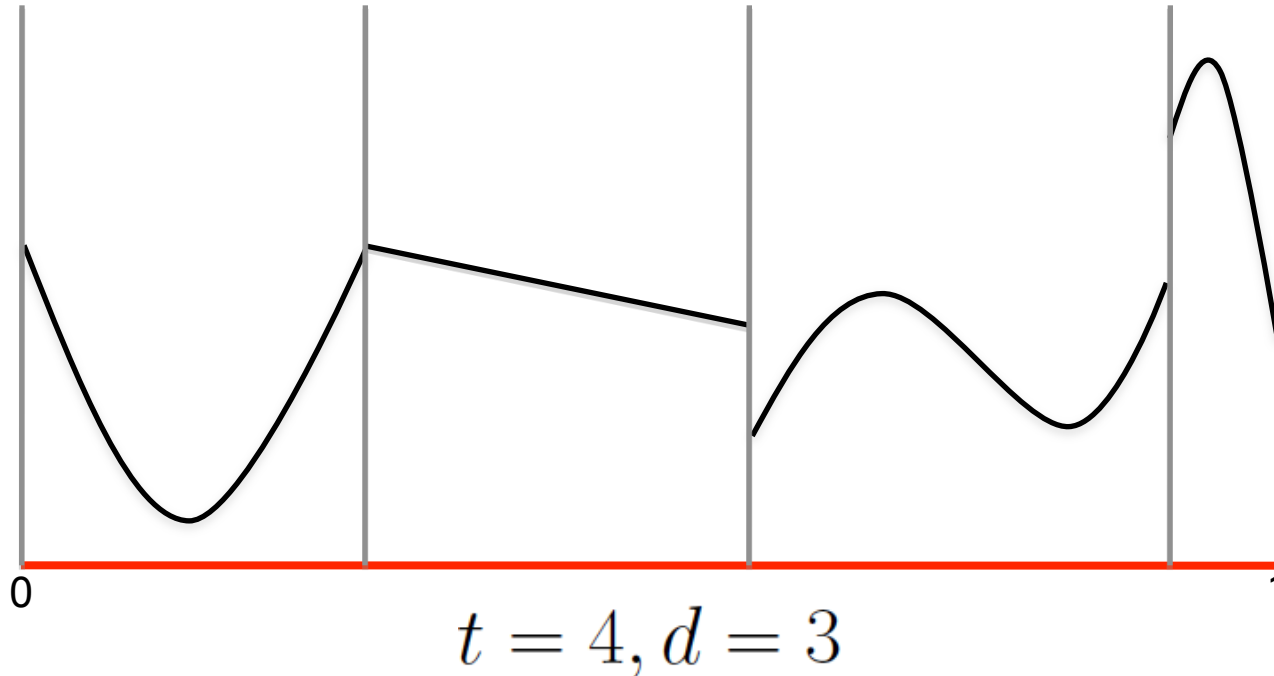
**Reduction-based approach.**

**Main difficulty:** Algorithm for  $\mathcal{C}$  should be **robust to error** in the data.

**Question:** Which “canonical” class should we use?

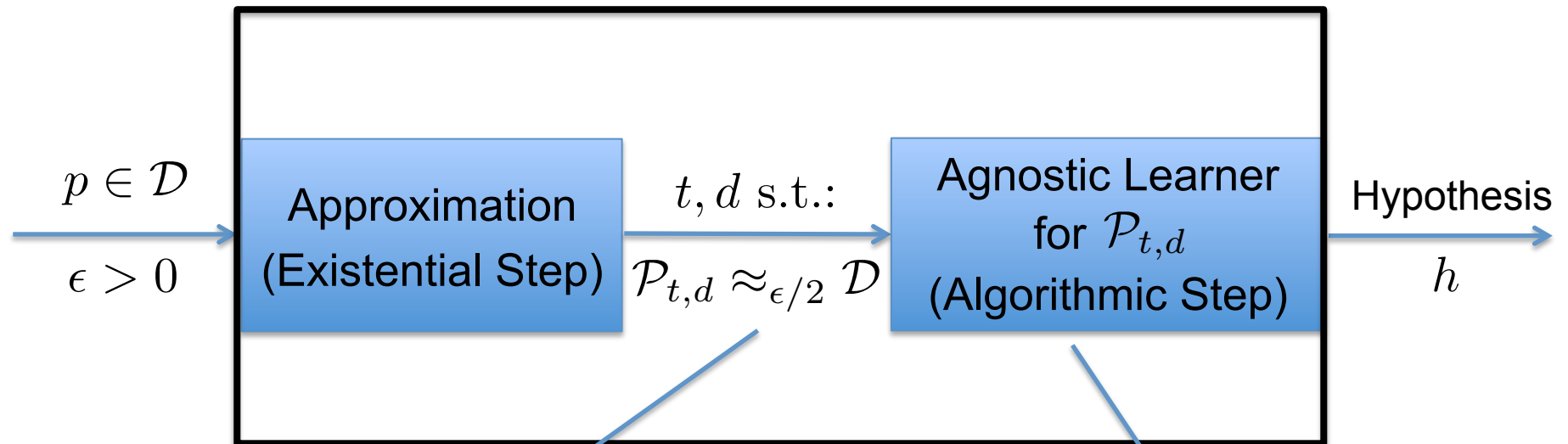
# Piecewise polynomial distributions

- Distribution  $p$  is  $t$ -**piecewise degree- $d$**  if there exists a partition of the domain into  $t$  intervals such that within each interval, the density of  $p$  is a degree- $d$  polynomial.
- Let  $\mathcal{P}_{t,d}$  be the family of all such distributions.





# Overview of Framework



$$\min t \cdot (d + 1) \text{ s.t.}$$

for each  $p \in \mathcal{D}$  there is  
 $q \in \mathcal{P}_{t,d}$  with

$$\|q - p\|_1 \leq \epsilon/2$$

$$\|h - p\|_1 \leq \text{OPT} + \epsilon/2$$

$$\leq \epsilon/2 + \epsilon/2$$

# Why Piecewise Polynomials?

- Analogy with PAC learning of Boolean functions  
[Linial-Mansour-Nisan'93]
- Common method in statistics: fitting splines to data  
[Wegman-Wright'83, Stone et al.'90's, Willet-Nowak'07]
- Gives sample optimal and computationally efficient estimators for wide range of distribution families

# Results: Learning Structured Families

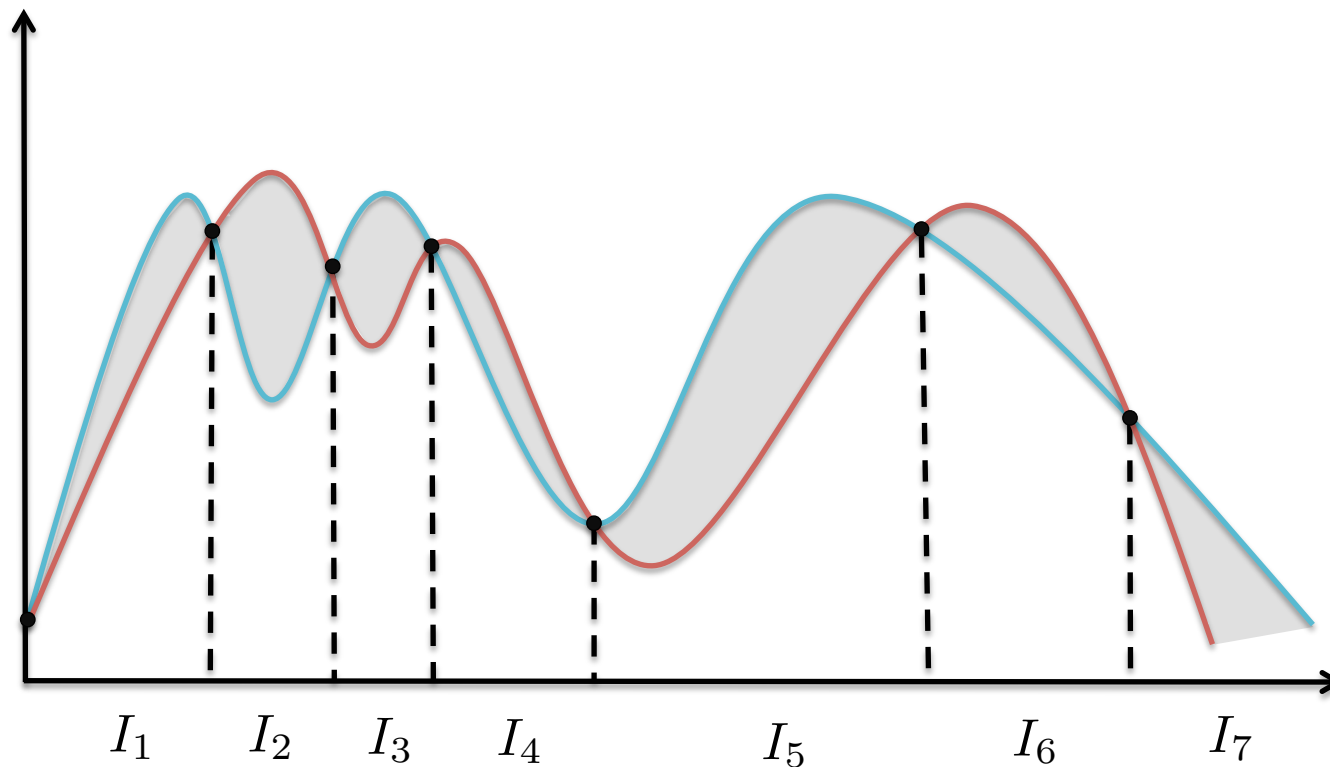
Distribution	Sample Size	Parameters	Reference
Exponential	$O(k/\epsilon^3)$	$t = \log n/\epsilon, d = 0$	Birgé'87
hazard rate	$O(k/\epsilon^3)$	$t = k \log n/\epsilon, d = 0$	Daskalakis-D-Servedio'12
log-concave $k$ -mixture	$O(\log(n/\epsilon)/\epsilon^3)$	$t = \log(n/\epsilon), d = 0$	Chan-D-Servedio-Sun'13
Gaussian $k$ -mixture	$O(k/\epsilon^{5/2})$	$t = k/\sqrt{\epsilon}, d = 1$	Chan-D-Servedio-Sun'14, D-Kane'15
Poisson/Binomial $k$ -mixture	$\tilde{O}(k/\epsilon^2)$	$t = k, d = \log(k/\epsilon)$	Chan-D-Servedio-Sun'14
Besov spaces	$\tilde{O}(k/\epsilon^2)$	$t = k, d = \log(k/\epsilon)$	Daskalakis-D-Stewart'15
$k$ -monotone	$O(1/\epsilon^{2+1/\alpha})$	$t = \epsilon^{-1/\alpha}, d = \lceil \alpha \rceil$	Devore'98
	$O(k/\epsilon^{2+1/k})$	$t = k, d = \epsilon^{-1/k}$	Konovalov-Leviatan'07

Previous work  
(parameter estimation):  
Moitra-Valiant'10  
 $(1/\epsilon)^{\Omega(k)}$

# Statistical Performance: Intuition (I)

**Question:** Let  $p$ ,  $q$  be probability density functions. How many samples are required to distinguish between them?

**Partial Answer:** If  $p$ ,  $q$  have a few “crossings”, distinguishing is easy.

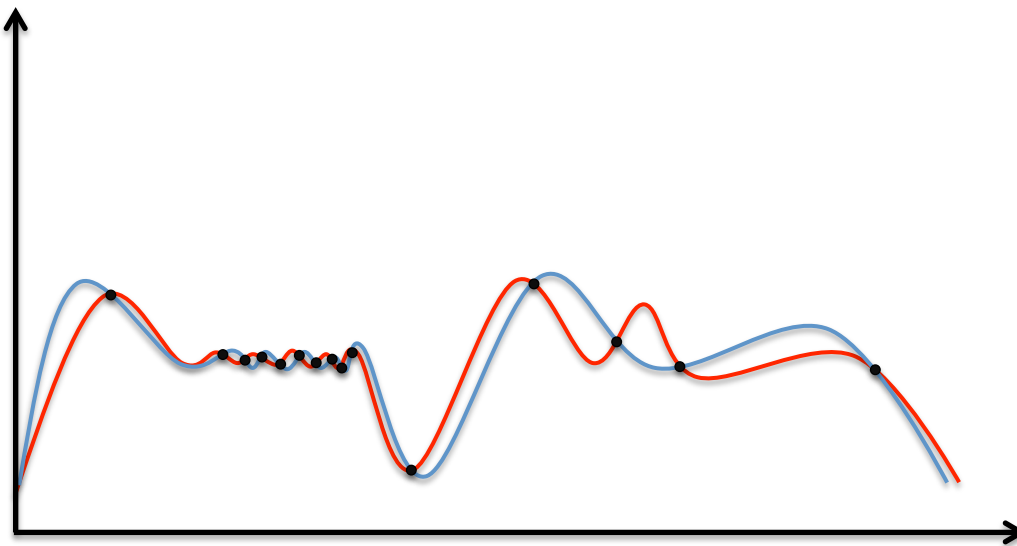


# Statistical Performance: Intuition (II)

**Question:** Let  $p$ ,  $q$  be probability density functions. How many samples are required to distinguish between them?

**Partial Answer:** If  $p$ ,  $q$  have a few “crossings”, distinguishing is easy.

Typically, unbounded many crossings, but only a few are important.



# “Complexity measure” for learning a distribution family

**Definition.** For  $p, q : \mathbb{R} \rightarrow \mathbb{R}_+$  and  $k \geq 1$ , we define the  $\mathcal{A}_k$  - distance between  $p, q$  as follows:

$$\|p - q\|_{\mathcal{A}_k} = \sup_{\mathcal{I}=(I_i)_{i=1}^k} \sum_{i=1}^k |p(I_i) - q(I_i)|$$



**Upper Bound on Sample Complexity:** For a family of one-dimensional distributions  $\mathcal{D}$  and  $\epsilon > 0$ , let  $k = k(\mathcal{D}, \epsilon)$  be the smallest integer such that for any  $p, q \in \mathcal{D}$  it holds

$$\|p - q\|_1 \approx_\epsilon \|p - q\|_{\mathcal{A}_k}.$$

Then, the parameter  $k$  is an upper bound on the sample complexity of agnostic learning for  $\mathcal{D}$ .

# Statistical Estimator

**Lemma.** For any  $\mathcal{D}$  and  $\epsilon > 0$ , let  $k = k(\mathcal{D}, \epsilon)$  be such that for any  $p, q \in \mathcal{D}$  it holds  $\|p - q\|_1 \leq \|p - q\|_{\mathcal{A}_k} + \epsilon$ . Then there exists an agnostic learning algorithm for  $\mathcal{D}$  using  $O(k/\epsilon^2)$  samples.

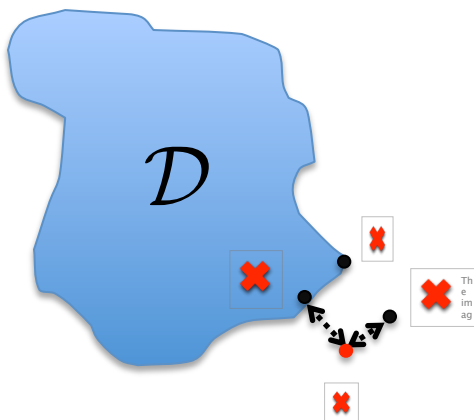
## Proof Sketch.

Consider the following procedure:

1. Draw  $m = \Omega(k/\epsilon^2)$  samples from  $p$  and let  $\hat{p}_m$  be the empirical distr.
2. Compute  $h \in \mathcal{D}$  that minimizes  $\|h - \hat{p}_m\|_{\mathcal{A}_k}$ .

## Analysis:

Empirical Process Theory (Vapnik, Chervonenkis, Dudley ~70's)



# Difficulties in Implementing Estimator

For any  $\mathcal{D}$  and  $\epsilon > 0$ , let  $k = k(\mathcal{D}, \epsilon)$  be such that for any  $p, q \in \mathcal{D}$  it holds  $\|p - q\|_1 \leq \|p - q\|_{\mathcal{A}_k} + \epsilon$ .

## Algorithm:

1. Draw  $m = \Omega(k/\epsilon^2)$  samples from  $p$  and let  $\hat{p}_m$  be the empirical distr.
2. Compute  $h \in \mathcal{D}$  that minimizes  $\|h - \hat{p}_m\|_{\mathcal{A}_k}$ .

## Main Issues:

1. How do we bound the value of  $k = k(\mathcal{D}, \epsilon)$ ?
2. How do we efficiently perform the “projection” step?  
(**Non-convex optimization problem**)

**Solution:** Replace  $\mathcal{D}$  by  $\mathcal{P}_{t,d}$  such that  $\mathcal{D} \approx_{\epsilon/2} \mathcal{P}_{t,d}$



# Agnostically Learning Piecewise Polynomials

Application of general framework for  $\mathcal{C} = \mathcal{P}_{t,d}$  and  $k = O(t(d+1))$ .

1. Draw  $m = \Omega(t(d+1)/\epsilon^2)$  samples from  $p$ .
2. Compute  $h \in \mathcal{P}_{t,d}$  that minimizes  $\|h - \hat{p}_m\|_{\mathcal{A}_k}$ .

Still non-convex optimization problem...

**Main Algorithmic Contribution:**

**Polynomial time algorithm for Step 2.**

# Agnostically Learning Piecewise Polynomials

**Theorem** [Chan-D-Servedio-Sun, STOC'14]

There exists an agnostic learning algorithm for  $\mathcal{P}_{t,d}$  that uses

$$\tilde{O}(t(d+1)/\epsilon^2)$$

samples and runs in time

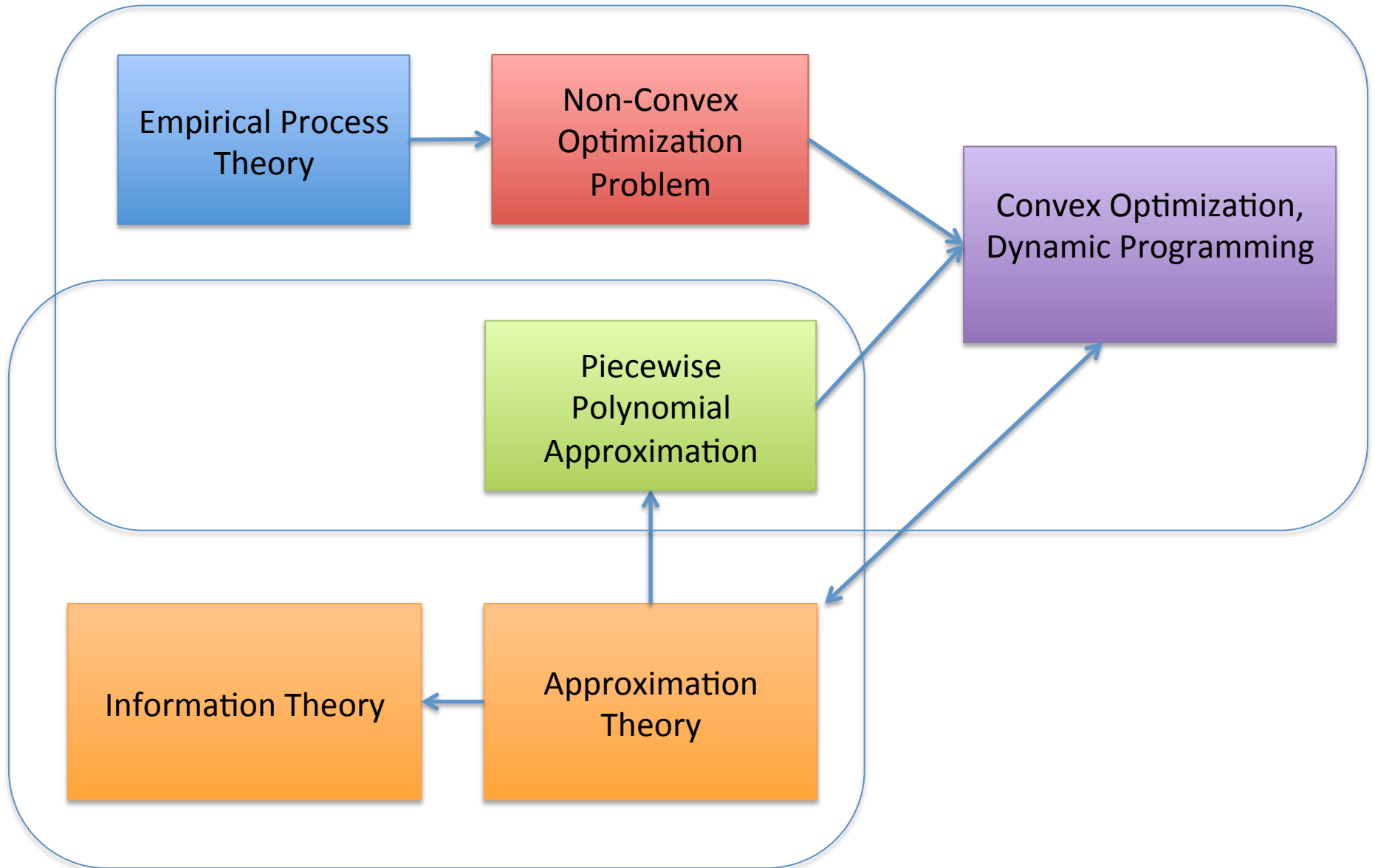
$$\text{poly}(t, d+1, 1/\epsilon).$$

Moreover,  $\Omega(t(d+1)/\epsilon^2)$  samples are information-theoretically necessary.

## Recent Progress:

- Piecewise constant: near-linear time [Chan-D-Servedio-Sun, NIPS'14]
- **General Case:**  $O(t(d+1)/\epsilon^2)$  samples and  $(t/\epsilon^2) \cdot \text{poly}(d)$  time.  
[Acharya-D-Li-Schmidt'15]

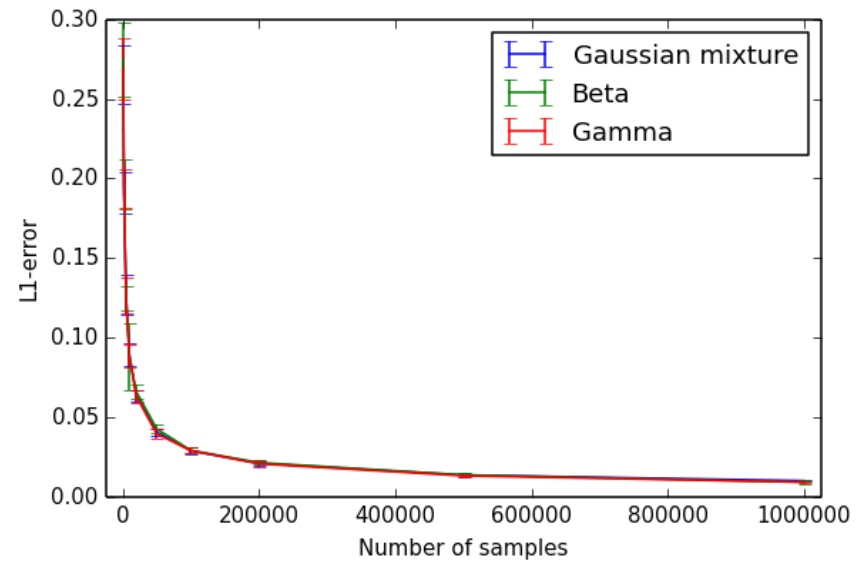
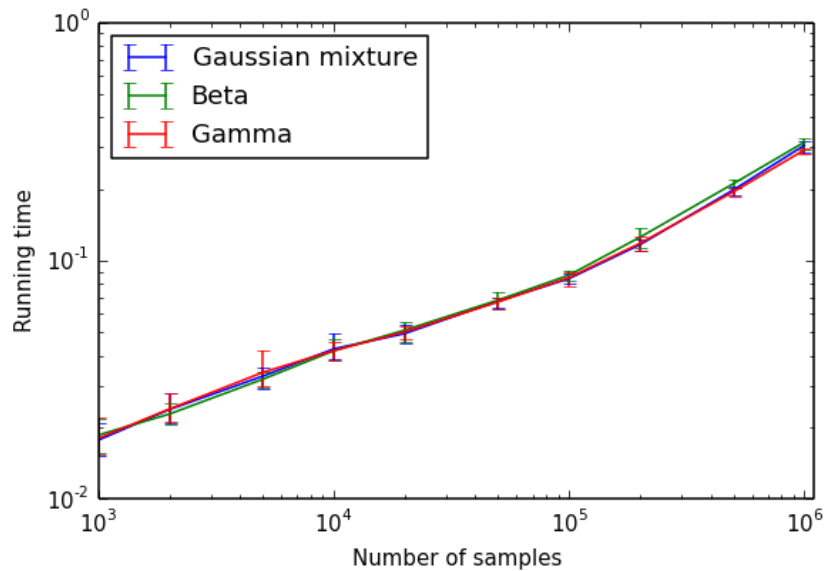
# Overview of Techniques



# Illustrative Empirical Results

## [Acharya-D-Li-Schmidt '15]

**Predictive performance of straightforward implementation:**  
speed-up over recent implementations of the MLE.



# Application in Databases: Succinct Representation of Data

[Acharya-D-Hegde-Li-Schmidt, PODS'15]: **Approximating Data Distributions by Histograms**

Classical problem in databases

[Gibbons-Matias-Poosala' 97, Jagadish et al. '98, Chaudhuri-Motwani-Narasayya '98, Thaper-Guha-Indyk-Koudas '02, Gilbert et al. '02, Guha-Koudas-Shim '06, Indyk-Levi-Rubinfeld'12.]

**Goal:** Given data distribution, construct a succinct approximation (histogram). Minimize **computation time**, **approximation error**.

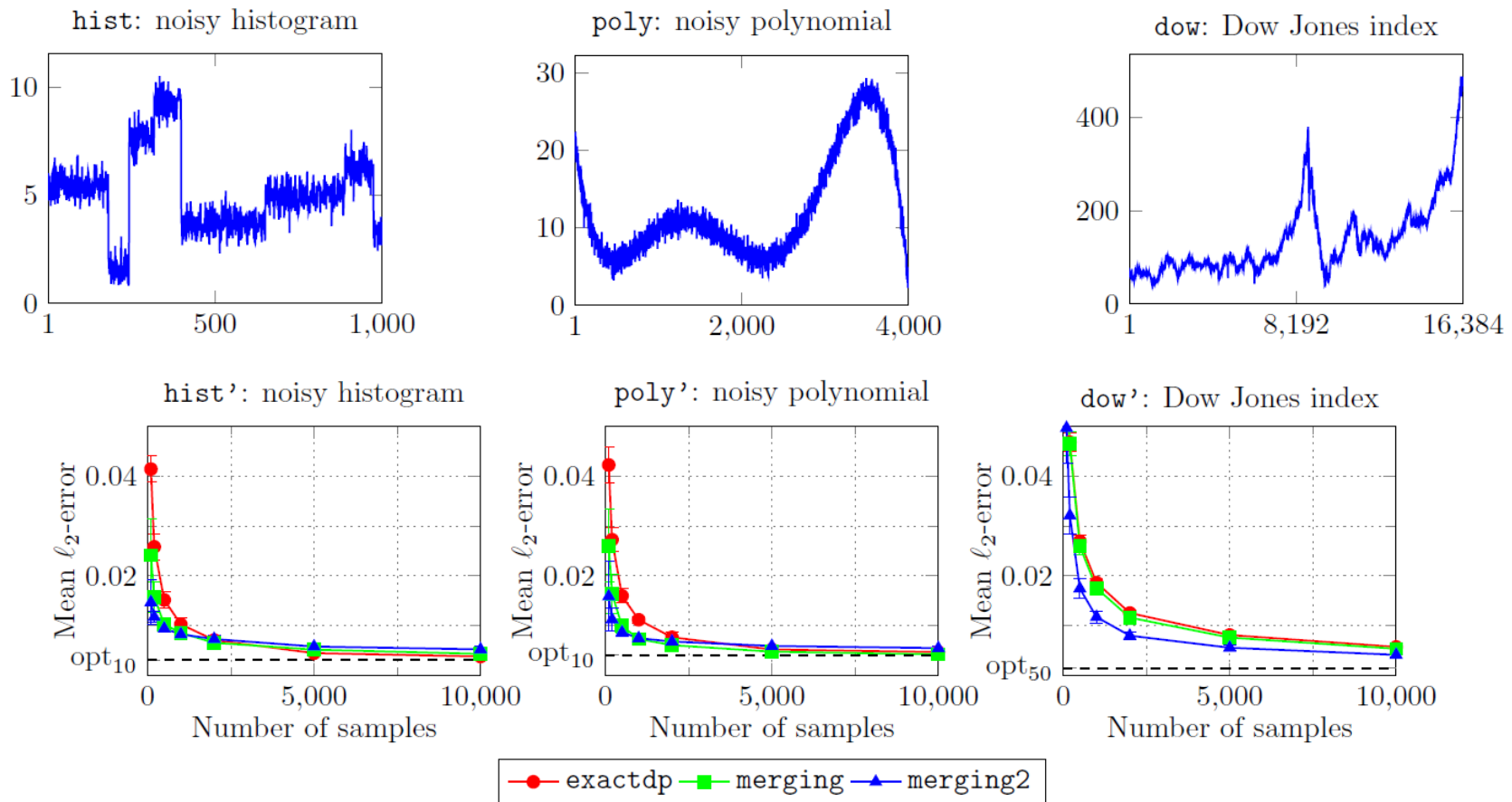
**Our Result:** Sample optimal, sample-linear time algorithm with optimal error (up to small constant factor).

**Experimental Evaluation:** Outperforms all previous algorithms for the problem by one to two orders of magnitude.

# Empirical Results (I)

[Acharya-D-Hegde-Li-Schmidt, PODS'15]

- Two synthetic and one real-word data set (same as [Guha-Koudas-Shim'06])



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# Additional Applications of Framework

## Hypothesis Testing (Property Testing)

- Testing Identity of Structured Distributions [D-Kane-Nikishkin'15a, '15b]

“Given samples from a **structured** distribution, is it uniform?”

“Given samples from two **structured** distributions, are they the identical?”

- Testing Shape Restrictions [Canonne-D-Gouleakis-Rubinfeld'15]

“Given samples from a (potentially arbitrary) distribution, is it **structured**?”



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# Future Directions

Broad Context:

## **Complexity theory for statistical estimation**

Specific Challenges:

- Agnostic proper learning
- “Instance optimal” (adaptive) algorithms
- Tradeoffs between sample size and computational efficiency

*Thank you for your attention!*