International Conference on
Automated Machine Learning
Sep 11, 2025
New York City

Tutorial 1

Limitations of State-of-the-Art and a New Principled Framework for HPO and Algorithm Selection

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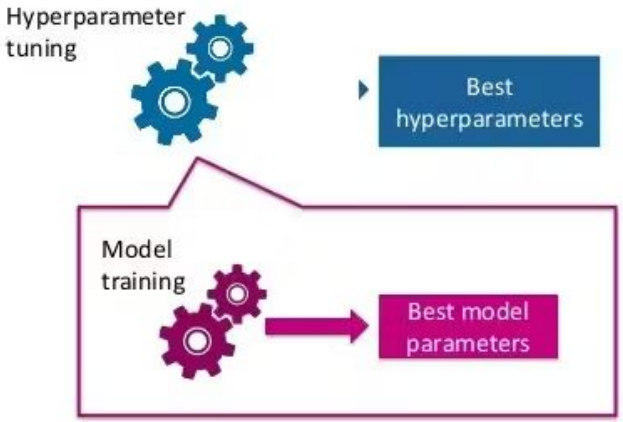
What is a hyperparameter?

HP tuning is a special case of algorithm selection in Machine Learning

Real or discrete values: each corresponding to an algorithm



Impacts everything!

1. Model accuracy
2. Training time
3. Model size/memory
4. Stability/adaptivity
5. …

Why so common in ML?

1. Hard problems ⇒ No single good algorithm
2. Role of data ⇒ Algorithms must adapt to domain-specific data

Hyperparameter tuning and transfer

HP tuning is important across ML

- Data prep + HP tuning take up most of the applied ML researcher hours
- Takes up to 90% of the compute
- Critical in high-stakes and large-scale applications

HP transfer is crucial today!

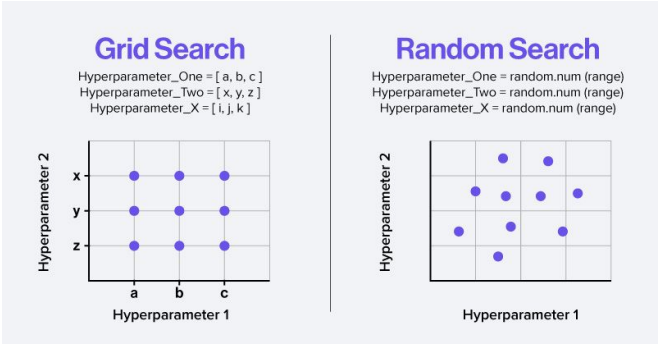
- Unavoidable in LLMs where each of the above is magnified multifold!

Roadmap

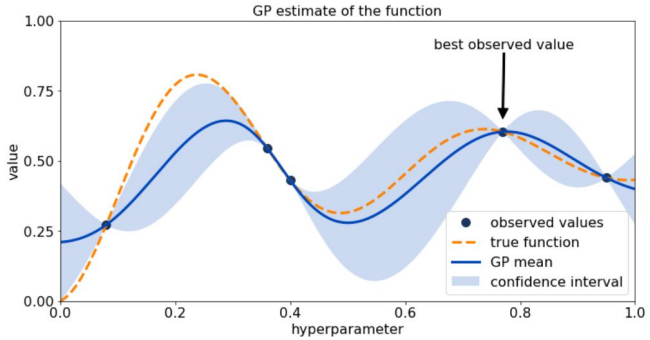
- Algorithm design for machine learning (aka HP tuning)
- **Current approaches in practice**
  - Bayesian Optimization and Bandit-based methods
- Machine learning for algorithm design
  - Learning-theoretic foundations
  - GJ algorithm framework
- Tuning core ML algorithms
  - Decision Trees
  - Neural networks
- Ongoing and future research directions

Existing approaches and their (theoretical) limitations

- Manual tuning, grid search, random search:
  - inefficient
  - unprincipled
  - no transfer across tasks
  - data-independent grids can be highly suboptimal
    [Balcan et al. BNVW (COLT'17), BDDKSV (JACM'24)]



- State-of-the-art:
  - Bayesian Optimization (BO);
    [e.g. Snoek et al. 2012]
  - Gradient-based;
  - Bandit-based



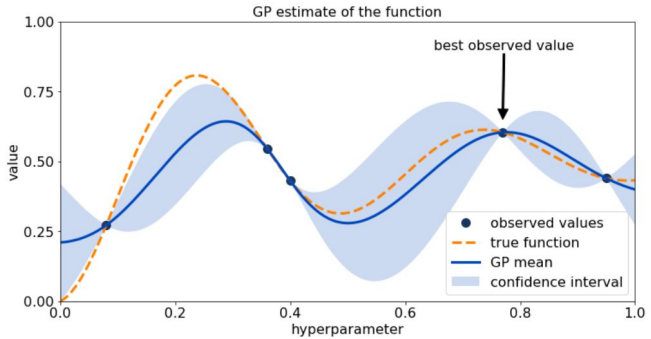
Gap: Limited <u>theoretical understanding</u>,
no guarantees for tuning <u>continuous hyperparameters</u>,
typically <u>no transfer</u> across tasks

But how does the model performance depend on its hyperparameters?

- **Short answer**: we don't really understand it!

- BO works with a crude approximation: Noisy evaluation of function with certain smoothness properties?
  - But how do we know what are the right smoothness priors?
  - Assumptions needed on noise correlations (kernel function)
  - How to search? (acquisition fns)

- But what is the **actual dependence**? Even on a fixed data instance?



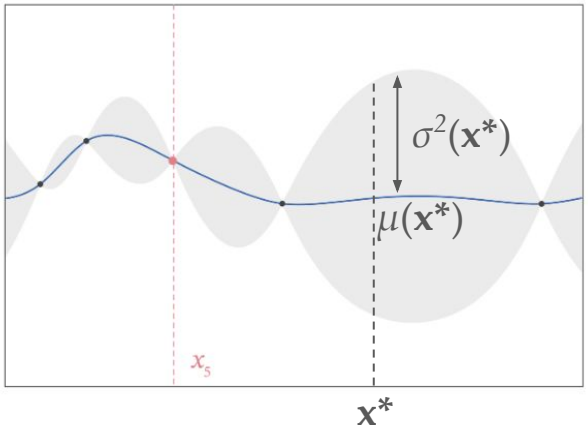
Bayesian Optimization

- **Gaussian Process**:
  - a collection of (infinitely many) random variables that are jointly Gaussian.
  - a distribution over functions – models noisy evaluation of some $f(\mathbf{x})$.
  - given by a mean function $m(\mathbf{x})$ and covariance $k(\mathbf{x}, \mathbf{x}')$.

$$\mathrm{E}[f(\mathbf{x})] = m(\mathbf{x}).$$
$$\mathrm{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))] = k(\mathbf{x}, \mathbf{x}').$$

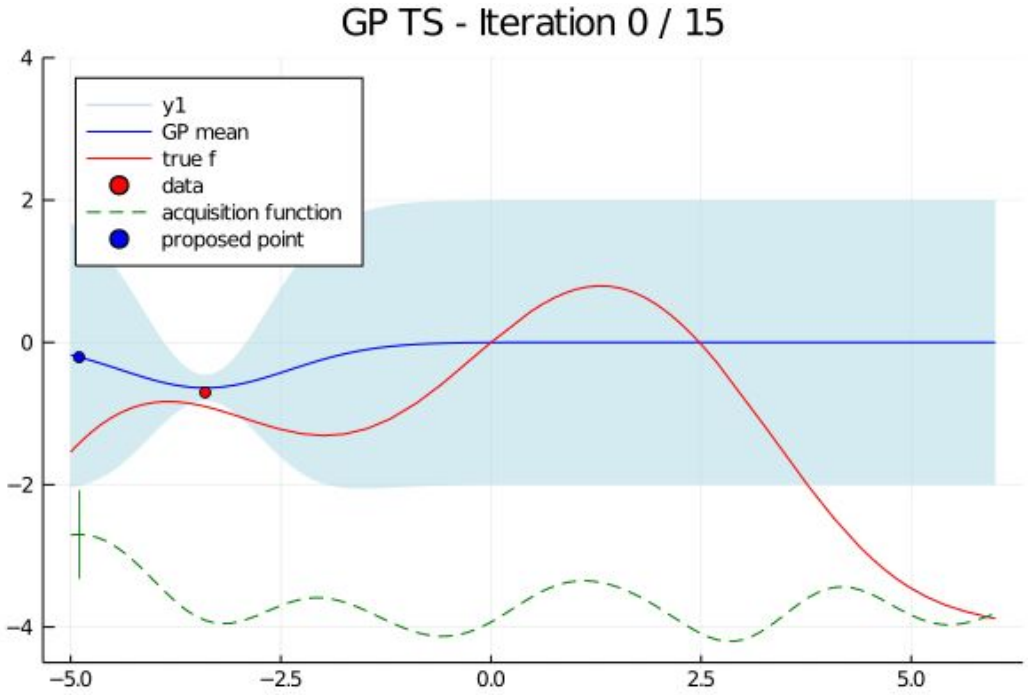
- Since all finite collections of function values are assumed jointly Gaussian, the conditional distribution of any new point given the observed points is also Gaussian, i.e. distribution of mean and variance at $\mathbf{x}^*$, given observed points $\mathbf{X}$ is

$$\mu(\mathbf{x}^*) = K(\mathbf{x}^*, \mathbf{X})K(\mathbf{X}, \mathbf{X})^{-1}f(\mathbf{X}).$$
$$\sigma^2(\mathbf{x}^*) = K(\mathbf{x}^*, \mathbf{x}^*) - K(\mathbf{x}^*, \mathbf{X})K(\mathbf{X}, \mathbf{X})^{-1}K(\mathbf{X}, \mathbf{x}^*).$$



$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5]$$

Bayesian Optimization



[Timothy Wolodzko github]

BO has its own hyperparameters!

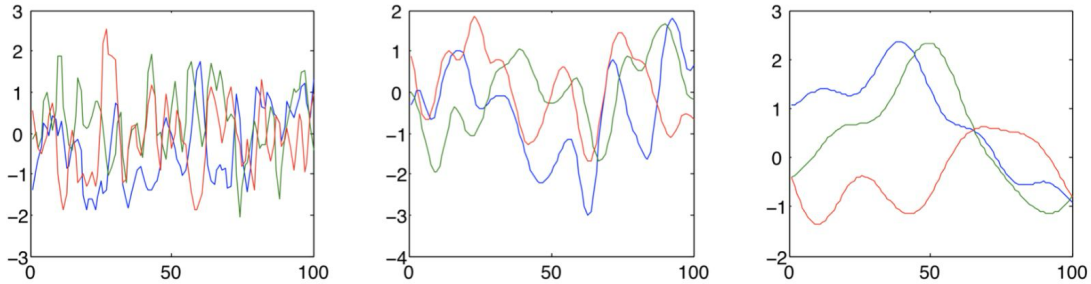


Figure 2: Random functions f drawn from a Gaussian process prior with a power exponential kernel. Each plot corresponds to a different value for the parameter α_1, with α_1 decreasing from left to right. Varying this parameter creates different beliefs about how quickly $f(x)$ changes with x.

[A Tutorial on Bayesian Optimization, Frazier 2018]

Some other great tutorials:

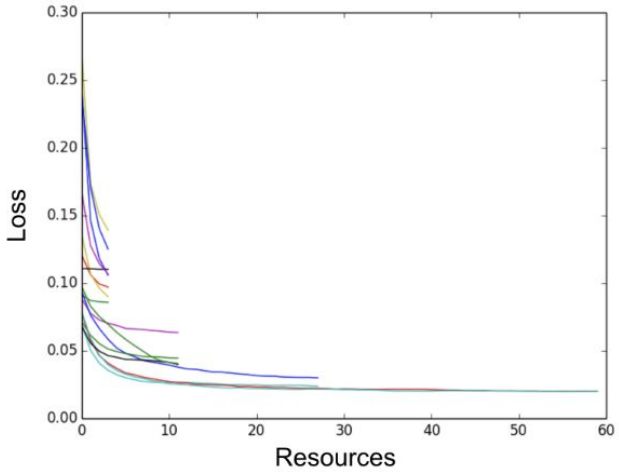
- GP regression [Schulz, Speekenbrink, Krause]
- Geometric probabilistic models, UAI 2024 [Borovitskiy, Terenin]

Exception *[Berkenkamp, Schoellig, Krause JMLR 2019]* ***But very slow convergence!***

Bandit-based approaches

Essentially bandit problems with additional HP-specific assumptions

1. **Hyperband**: Each arm has a noisy non-stationary reward that eventually converges to a limiting value [Li, Jamieson, DeSalvo, Rostamizadeh, & Talwalkar (JMLR 2018)]

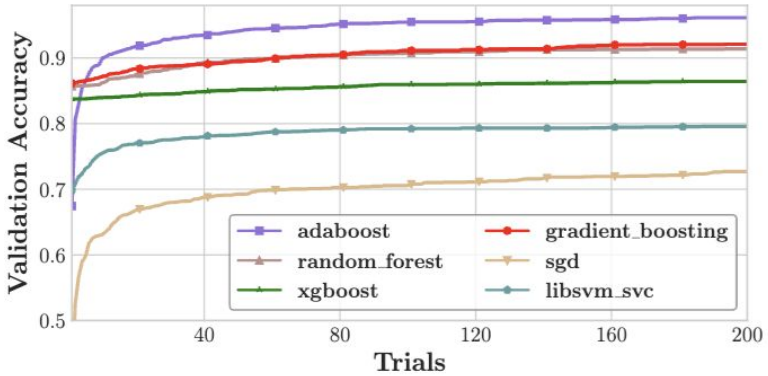


Bandit-based approaches

Essentially bandits problems with additional HP-specific assumptions

2. **Rising/improving bandits**: Arms have concave “learning curves”

[Heidari, Kearns, Roth (IJCAI 2016), Li et al. (AAAI 2020), Metelli et al. (ICML 2022), Mussi et al. (ICML 2024), Blum and Ravichandran (ALT 2025)]



Known guarantees (and lack thereof)

Approaches are black-box!!
(agnostic to structure)

Bayesian optimization

– Guarantees typically need strong prior assumptions

– Need design of kernels (with hyperparameters) and acquisition functions

Guarantees e.g. for GP-UCB assume you can magically do this!

[Srinivas, Krause, Kakade, Seegar (2010)]

Bandit-based methods

– Guarantees typically only over a finite subset of hyperparameter values (arms)

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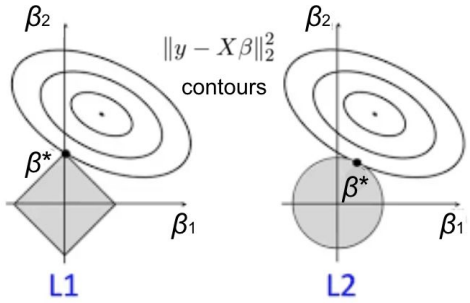
Data-driven algorithm design

[Gupta and Roughgarden, 2016] [Balcan, 2020] [Sharma, 2024]

★ **Algorithm families** occur frequently in machine learning

- Often as tunable “hyperparameters”
- One could smoothly “interpolate” good heuristics

Regularized linear regression



(sparse)

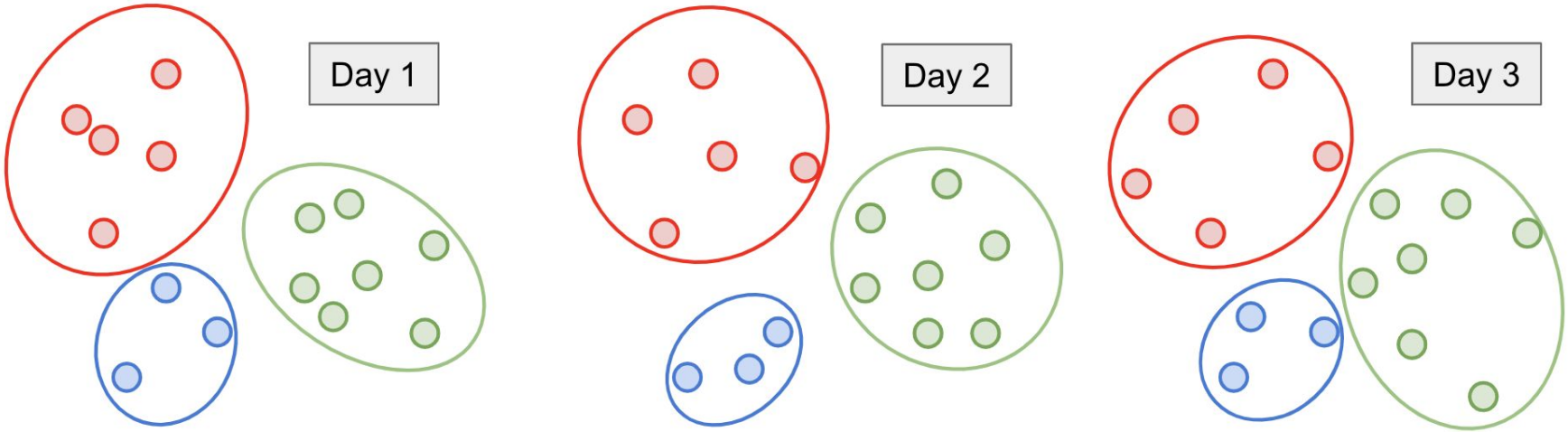
(handles overparameterization, multicollinearity well)

Interpolate: elastic net (best of both worlds!)

Data-driven algorithm design [GR16, Bal20, Sha24]

★ **Repeated problems** from the same problem domain

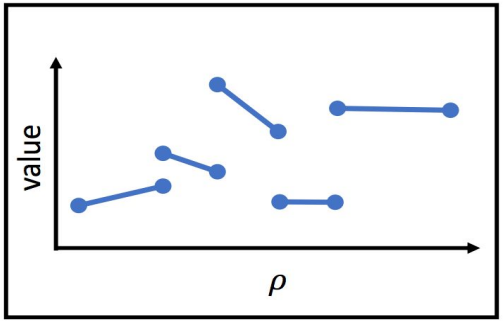
- Expected with regular use of ML
- May come *randomly* (optimistic) or in an *adversarial sequence* (pessimistic)

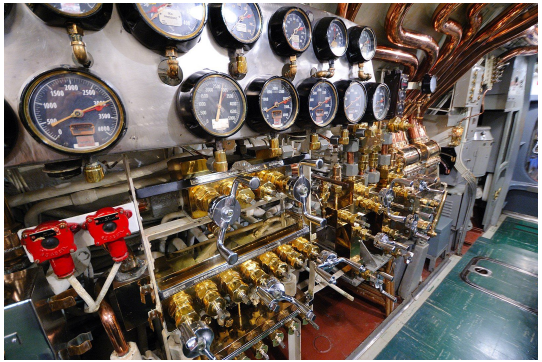


Data-driven algorithm design [GR16, Bal20, Sha24]

★ **Technical challenges**:

- Algorithms form an interesting “concept space”
- *Sharp transition boundaries* in optimization objective
- Particularly tricky to handle multiple “hyperparameters”





Data-driven algorithm design [GR16, Bal20, Sha24]

- Instead of tuning for one specific problem, we tune the **hyperparameter that generalizes** across **a collection of related problems**.
- Concretely:
  - x is a **problem instance** from a **problem set** $\mathcal{X}$, our (infinite) **algorithm family** A
  - D is a **problem distribution** over $\mathcal{X}$, representing the *application-specific domain*
  - We also study no-regret **online learning**, where instances arrive in a sequence
- E.g., academic email spam filter for Gmail, or electronic products sold on Amazon

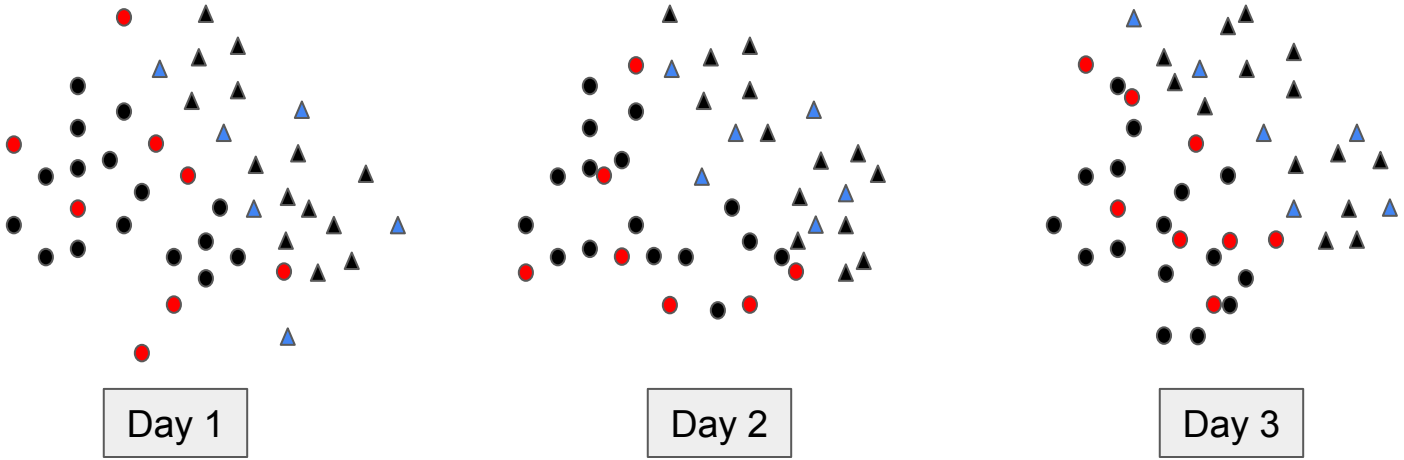
Example: Semi-Supervised Learning

[Balcan and Sharma (2021)];
Oral (55/9122, top 0.6%) at NeurIPS'2021

★ Repeated problems e.g. emails on an email server, spam vs. non-spam

Goal: learn how to connect points using a graph s.t. a (soft) min-cut yields accurate predictions

- **statistical learning**: tight upper+lower bounds on learning-theoretic complexity
- **online learning**: primal-dual style algorithms achieve no regret, under mild assumptions



Example: Decision Trees

[Balcan and Sharma, UAI 2024 **Outstanding Student Paper Award**]

Tuning different aspects of decision tree learning

- **Splitting criterion** (which node to split when building the tree?)
  - A **novel algorithmic family** which unifies entropy, Gini impurity and Kearns-Mansour criterion
  - Sample complexity of selecting best splitting algorithm
- **Bayesian methods** (Parameters to select initial tree skeleton)
- **Pruning** (Deleting nodes to avoid overfitting)
- **Interpretability** (Adding tree size to cost with tunable parameter)

Some related lines of work

Algorithm configuration [Kevin-Leyton Brown and Frank Hutter, ICML 2019 tutorial]

Meta-learning or learning to learn [Hutter and Vanschoren, NeurIPS 2018 tutorial], [Khodak, Balcan and Talwalkar, NeurIPS 2019]

Learning-augmented algorithms [Thodoris Lykouris and Sergei Vassilvitskii, ICML 2018; Piotr Indyk's Course 6.890 at MIT, 2019]

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Primal and dual utility functions

- Denote **input instance space** $\mathcal{X}$ and **Hyperparameter space** A

- Utility (performance) on any instance for any hyperparameter are given by a function:

$$u(x, \alpha) : \mathcal{X} \times A \rightarrow [0, H]$$

- Primal utility function class:

$$U = \{u_\alpha : \mathcal{X} \rightarrow [0, H] \mid \alpha \in A\}$$

- Dual utility function class:

$$U^* = \{u^*_x : A \rightarrow [0, H] \mid x \in \mathcal{X}\}$$

Statistical learning theory: sample complexity and pseudo-dimension

Given $\varepsilon > 0$ and $0 < \delta < 1$, what is the sample complexity $m(\varepsilon, \delta)$?

- Standard PAC-Learning approach: bound the learning-theoretic complexity of U

$$U = \{u_\alpha : \boldsymbol{\mathcal{X}} \to [0, H] \mid \alpha \in A\}$$

- Complexity measure: pseudo-dimension, Pdim(U)
  - The maximum size n such that U can "shatter" $\{\boldsymbol{x_1}, \ldots, \boldsymbol{x_n}\}$, using thresholds $\boldsymbol{t_1}, \ldots, \boldsymbol{t_n} \in \mathbb{R}$
  - by "shattering", we mean $|\{\text{sign}(u_\alpha(\boldsymbol{x_1}) - \boldsymbol{t_1}), \ldots, \text{sign}(u_\alpha(\boldsymbol{x_n}) - \boldsymbol{t_n}) \mid u_\alpha \in U\}| = 2^n$

- Classical learning theory: If Pdim(U) is finite, then $m(\varepsilon, \delta) = O(H/\varepsilon^2(\text{Pdim}(U) + \log 1/\delta))$

Analogue of VC dimension for real-valued functions

Statistical learning theory: sample complexity and pseudo-dimension

- Simple examples to illustrate pseudo-dimension

Straight lines in 2D, functions $f_{a,b,c}(x, y) = ax + by + c$ for real a, b, c.

$F = \{f_{a,b,c}\}$. $\mathrm{Pdim}(F) = ?$

Answer: 3

Primal and dual utility functions

- So we want to bound the pseudo-dimension of the primal function class U.

- But the structure of U is too complex!
- On the otherwise, it is often easier to establish the structure of the dual class U^*.

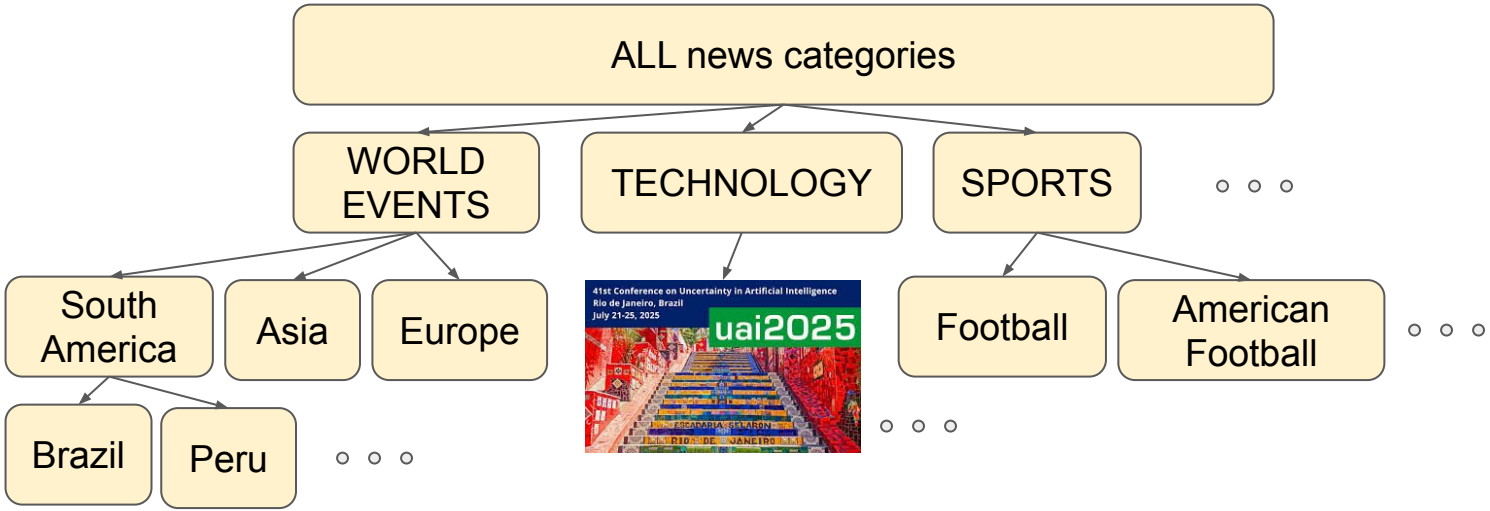
- A general tool (for bounding Pdim of primal using dual structure):

Theorem [BDDKSV STOC'21]: Suppose the dual function class has a piecewise-structure with k boundary functions coming from some function class F^*, and piece functions from class G^*. Then, $\text{Pdim}(U) = \tilde{O}((\text{VC}\tilde{\dim}(F^*) + \text{Pdim}(G^*))\log k)$.

Example: Linkage Clustering [BNVW COLT'17, BSS NeurIPS'24]

Example application: Linkage or hierarchical clustering.

Given a collection of n objects, organize them into hierarchy
e.g. "categories" of news articles



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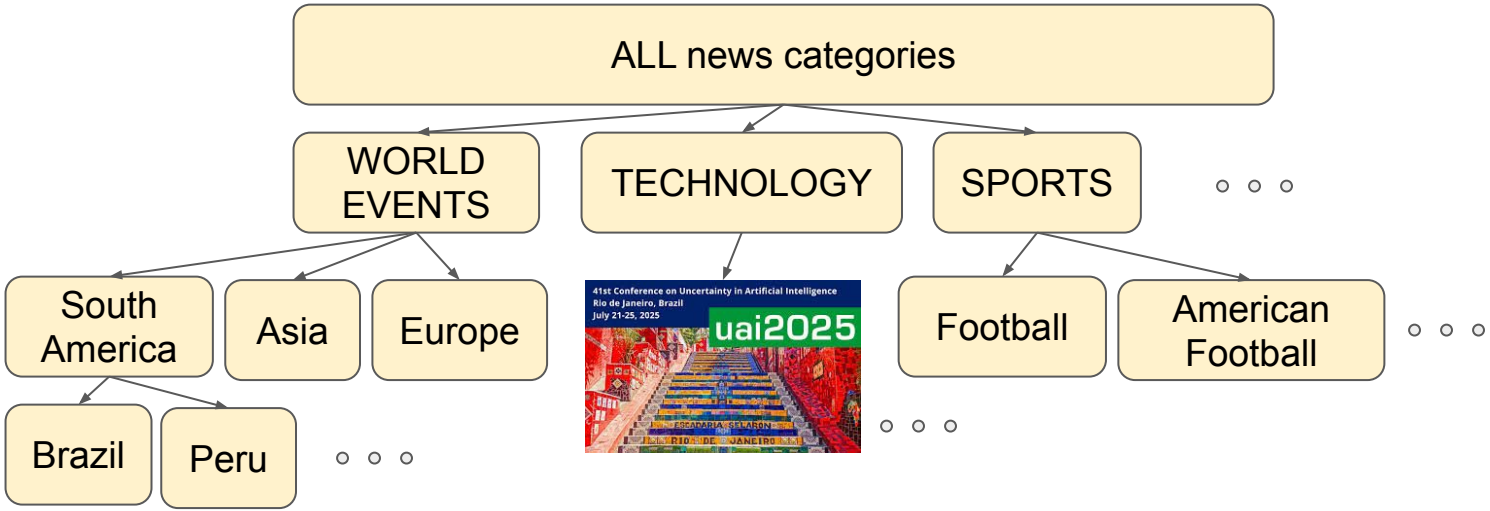
Example application: Linkage or hierarchical clustering.

Algorithm:

1. Start with each object as its own cluster.
2. Repeatedly merge "most similar" clusters.



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Example application: Linkage or hierarchical clustering.
Algorithm:

1. Start with each object as its own cluster.
2. Repeatedly merge "most similar" clusters.

But what is "most similar"? Define a notion of distance between cluster pairs:

Single linkage: $D_{\min}(A, B) = \min_{a \in A, b \in B} d(a, b)$
Complete linkage: $D_{\max}(A, B) = \max_{a \in A, b \in B} d(a, b)$

How to tune α?

Interpolate linkage: $D_{\alpha}(A, B) = \alpha D_{\min}(A, B) + (1 - \alpha) D_{\max}(A, B)$

Piecewise constant structure with poly(n) pieces $\Rightarrow$ $\text{Pdim}(U) = O(\log n)$

Combined Algorithm and Hyperparameter Selection [A general tool]

What if we have multiple algorithms each with its own hyperparameters?

Algorithms: $A_1, A_2, \ldots, A_k$
Utility function classes (resp. Hyperparameters): $U_1, U_2, \ldots, U_k$

What is the sample complexity of algo+hyperparameter selection?

Theorem: Sample complexity of CASH is $O(H^2/\varepsilon^2(\log k + \max_i \text{Pdim}(U_i)))$.

[Balcan and Sharma, Arxiv'25]

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Goldberg-Jerrum (’95) Framework

Another general useful technique for bounding the pseudo-dimension of function classes based on algorithms with *real parameters* that perform *arithmetic operations*.

– Original results yield Pdim bounds in terms of the running time of the algorithm.

– The corresponding bounds are sub-optimal for data-driven algorithm design.

Recent works provide refined GJ frameworks for data-driven algorithm design.

[Bartlett, Indyk, Wagner, COLT’22], [Balcan, Nguyen, Sharma, TMLR’25]

Refined GJ Framework [Bartlett, Indyk, Wagner, COLT'22]

Takes in:

n real algorithm parameters

GJ (95) Algorithm

Two types of operations:

(1) Arithmetic (binary): +, –, ×, ÷

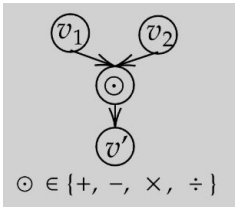
(2) Conditional: if .. then .. else ..

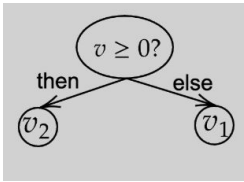
Output(s): E.g.

Cluster,

Matrix,

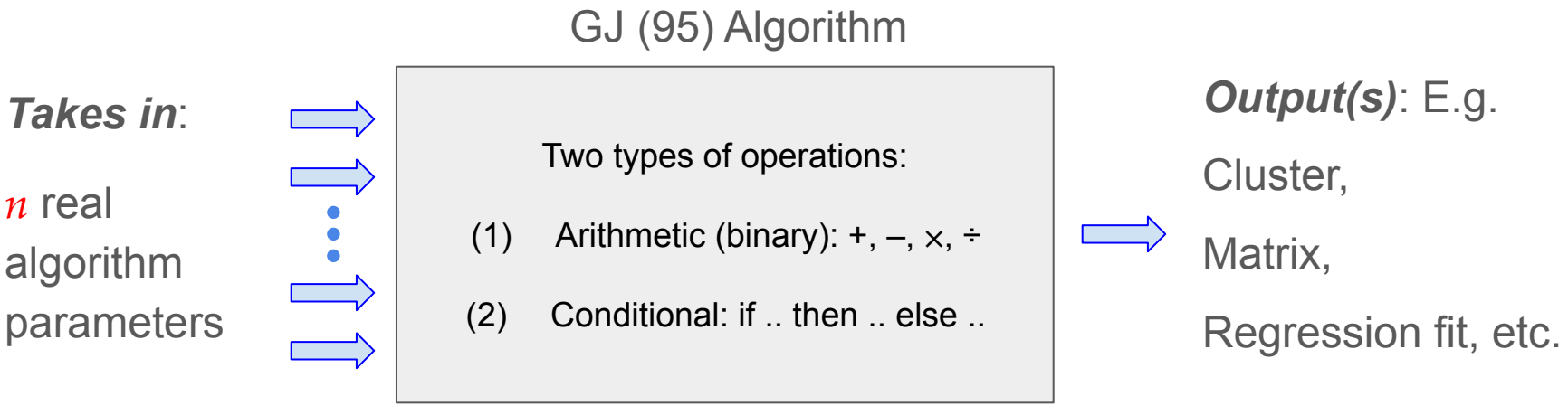
Regression fit, etc.





Note: All expressions computed by the GJ algorithm are rational functions (ratios of polynomials) of its inputs

Refined GJ Framework [Bartlett, Indyk, Wagner, COLT'22]

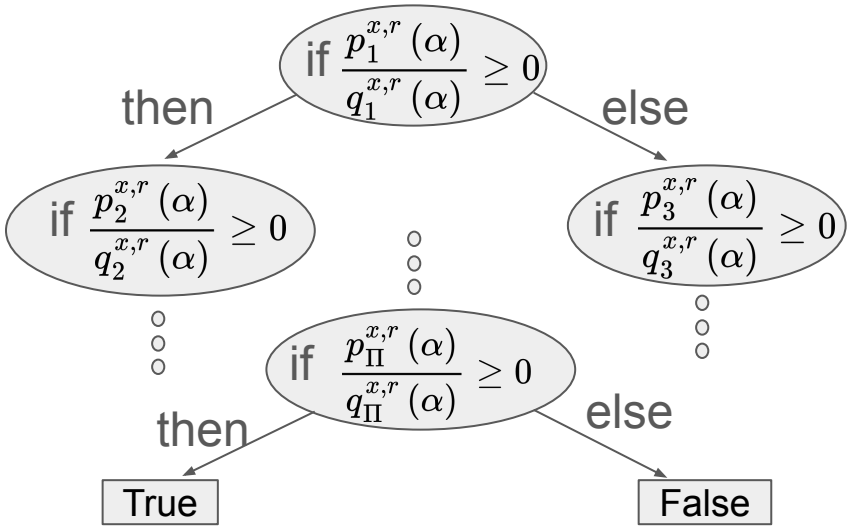


Theorem: Suppose the algorithm family has n real parameters. Also, for any problem instance x and real threshold r, there is a GJ algorithm $\Gamma_{x,r}$ that determines whether $u_x(\alpha) \geq r$ by evaluating at most $\mathbf{\Pi}$ distinct predicates (rational expressions) with maximum degree Δ. Then,

$$\mathrm{Pdim}(U) = O(n \log(\Delta \mathbf{\Pi})).$$

Refined GJ Framework [Bartlett, Indyk, Wagner, COLT'22]

$\Gamma_{x,r}$



Π : # distinct expressions

Δ : max degree of all p's and q's

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$$\mathrm{Pdim}(U) = O(n \log(\Delta\Pi)).$$

Refined GJ Framework [Balcan, Goyal, Sharma, Arxiv'25]

Example application: Tuning the ridge penalty λ in linear regression.

$$\min_w ||Xw - y||^2 + \lambda||w||^2$$

Input: Training data X, y and validation data X', y'.
Goal: Tune λ to minimize validation loss.

Applying GJ framework: Note that the ridge solution is $w_\lambda = (X^TX + \lambda I)^{-1}X^Ty$.

Lemma: $w_\lambda = (X^TX + \lambda I)^{-1}X^Ty$ is a rational function of lambda with degree at most d (#features).

⇒ Validation loss is a rational function with degree at most $2d$.
⇒ GJ algorithm to check $u_x(\lambda) \geq r$ has degree $2d$ and predicate complexity 1.

Theorem: Sample complexity of tuning λ is $O(\log(d)/\varepsilon^2)$.

Refined GJ Framework [Balcan, Nguyen, Sharma, NeurIPS'23]

Example application: Tuning Elastic Net coefficients.

$$\min_w ||Xw - y||^2 + \lambda||w||^2 + \lambda'||w||_1$$

Input: Training data X, y and validation data X', y'.
Goal: Tune λ, λ' to minimize validation loss.

Lemma: The validation loss is piecewise decomposable in the λ, λ' space with
– at most $d3^d$ algebraic boundaries of degree at most d,
– at most 3^d distinct piece functions, each a rational function with degree at most $2d$.

Idea: we can reduce Elastic Net to Lasso for a fixed λ + analyze the piecewise structure for Lasso solution (for each λ) as λ'. is varied.
⇒ GJ algorithm to check $u_x(\lambda, \lambda') \geq r$ has degree $2d$ and $\leq (d+1)3^d$ predicates.

Theorem: Sample complexity of tuning λ is $O(d/\varepsilon^2)$.

Refined GJ Framework [Bartlett, Indyk, Wagner, COLT'22]

Example application: Low-rank approximation.

Input: Given a sparse matrix $A \in \mathbb{R}^{n \times n}$ with $||A||_F = 1$, target rank $k < n$.
Goal: Sparse matrix $\tilde{A}$ with rank k that minimizes $\quad$ (approximates A well).

Exact algorithm based on SVD (singular value decomposition) is inefficient!

Faster algorithm IVY [Indyk, Vakilian, Yuan '19] is family of parameterized heuristics uses a m x n auxiliary matrix (runtime nearly linear in #non-zero entries!).

Theorem: Sample complexity of tuning IVY is $O(mn/\varepsilon^2)$.

Pfaffian functions

Pfaffian function chain: A sequence of multivariate functions $f_1, f_2, \ldots, f_q$ with arguments $a_1, \ldots, a_n$, if all partial derivatives can be expressed via polynomials of the arguments or previous functions in the chain, i.e.

$$\frac{\partial f_j}{\partial a_i} = P_{i,j}\left(a_1, \ldots, a_n, f_1, \ldots, f_j\right)$$

Pfaffian function: Polynomial fn of the Pfaffian chain $Q\left(a_1, \ldots, a_n, f_1, \ldots, f_q\right)$

Chain length, q: number of functions in the sequence

Pfaffian degree, M: Maximum degree of a derivative polynomials

Degree, Δ: Maximum degree of a polynomial of a chain of Pfaffian functions, Q

Pfaffian functions

Examples:

1. $e^{2a} + a^3$: Chain length ? Pfaffian degree ? degree ?

2. $\log \sqrt{a}$: Chain length ? Pfaffian degree ? degree ?

3. $a^{1/2} + a^{2/3}$: Chain length ? Pfaffian degree ? degree ?

Pfaffian functions

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1. $e^{2a} + a^3$: Chain length ? Pfaffian degree ? degree ?

Pfaffian functions

1. $e^{2a} + a^3$: Chain length ? Pfaffian degree ? degree ?

   $f_1(a) = e^{2a} + a^3$; $f_1'(a) = 2e^{2a} + 3a^2 = 2f_1(a) - 2a^3 + 3a^2 = P(a, f_1(a))$; $Q(a, f_1(a)) = f_1(a)$

   Chain length = 1, Pfaffian degree = 3, degree = 1

   $f_1(a) = e^a$; $f_1'(a) = f_1(a) = P(a, f_1(a))$; $Q(a, f_1(a)) = (f_1(a))^2 + a^3$

   Chain length = 1, Pfaffian degree = 1, degree = 3

Pfaffian functions

Pfaffian function chain: A sequence of multivariate functions $f_1, f_2, \ldots, f_q$ with arguments $a_1, \ldots, a_n$, if all partial derivatives can be expressed via polynomials of the arguments or previous functions in the chain, i.e. $\frac{\partial f_j}{\partial a_i} = P_{i,j}(a_1, \ldots, a_n, f_1, \ldots, f_j)$

Pfaffian function: Polynomial fn of the Pfaffian chain $Q(a_1, \ldots, a_n, f_1, \ldots, f_q)$

Chain length, q: number of functions in the sequence

Pfaffian degree, M: Maximum degree of a derivative polynomials

Degree, Δ: Maximum degree of a polynomial of a chain of Pfaffian functions, Q

2. $\log \sqrt{a}$: Chain length ? Pfaffian degree ? degree ?

Pfaffian functions

2. $\log \sqrt{a}$: Chain length ? Pfaffian degree ? degree ?

$f_1(a) = \log a$; $f_1'(a) = 1/a$

Not a polynomial in $\log a$ and a!

$f_1(a) = 1/a$; $f_2(a) = \log a$;

$f_1'(a) = -a^{-2} = P(a, f_1(a))$; $f_1'(a) = 1/a = P(a, f_1(a), f_2(a))$; $Q(a, f_1(a)) = ½ f_2(a)$

Chain length = 2, Pfaffian degree = 2, degree = 1

Pfaffian functions

3. $a^{1/2} + a^{2/3}$: Chain length ? Pfaffian degree ? degree ?

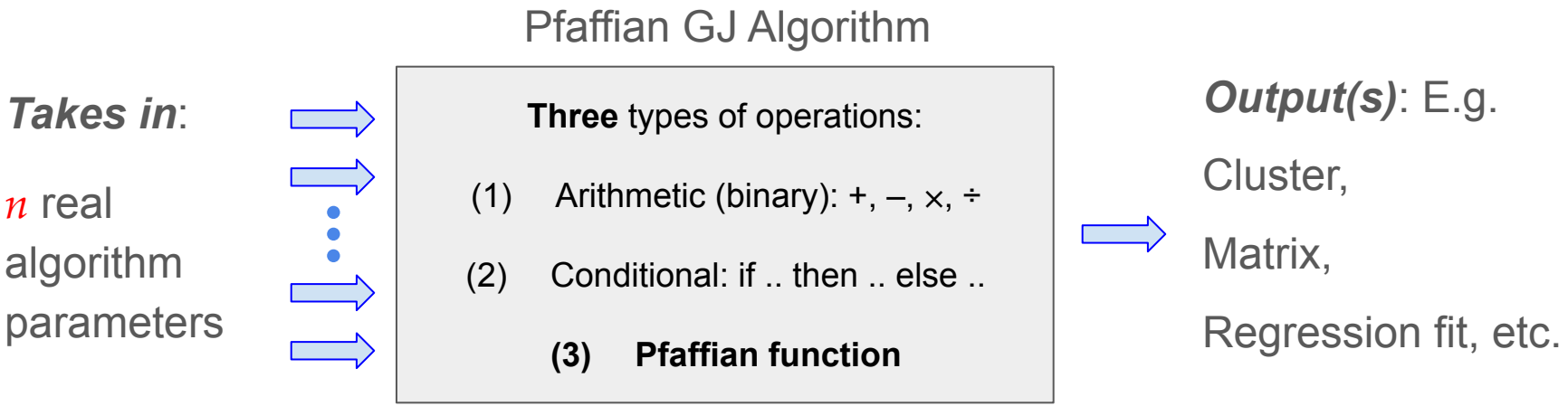
$f_1(a) = 1/a$; $f_2(a) = a^{1/2}$; $f_3(a) = a^{2/3}$

$f_1'(a) = -a^{-2} = -(1/a)^2$; $f_2'(a) = a^{-1/2}/2 = \frac{1}{2} \cdot 1/a \cdot a^{1/2}$; $f_3'(a) = 2a^{-1/3}/3 = \frac{2}{3} \cdot 1/a \cdot a^{2/3}$

$Q(a, f_1(a), f_2(a), f_3(a)) = a^{1/2} + a^{2/3}$

Chain length = 3, Pfaffian degree = 2, degree = 1

Pfaffian GJ Framework [Balcan, Nguyen, Sharma (TMLR 2025)]



Theorem: Suppose the algorithm family has n real parameters. Also, for any problem instance x and real threshold r, there is a **Pfaffian** GJ algorithm $\Gamma_{x,r}$ that determines whether $u_x(\alpha) \geq r$ by evaluating Π distinct predicates with Pfaffian chain length q, degree Δ, and Pfaffian degree M. Then,

$$\mathrm{Pdim}\left(\mathcal{U}\right) = O\left(n^2q^2 + nq\ln\left(\Delta + M\right) + n\ln\Pi\right)$$

Pfaffian GJ Framework Example: Linkage Clustering [BN**S** TMLR'25]

Algorithm:

1. Start with each object as its own cluster.
2. Repeatedly merge "most similar" clusters.

But what is "most similar"? Define a notion of distance between cluster pairs:

Single linkage: $\mathrm{D}_{\min}(A, B) = \min_{a \in A,\, b \in B} \mathrm{d}(a, b)$

Complete linkage: $\mathrm{D}_{\max}(A, B) = \max_{a \in A,\, b \in B} \mathrm{d}(a, b)$

Also, what if we have multiple distances $d_1, d_2, \ldots, d_L$?

How to tune α, $\boldsymbol{\beta}$?

1. Interpolate distances: $\mathrm{d}_{\boldsymbol{\beta}} = \beta_1 \mathrm{d}_1 + \beta_2 \mathrm{d}_2 + \ldots + \beta_L \mathrm{d}_L$
2. Interpolate linkage: $\mathrm{D}_{\alpha,\boldsymbol{\beta}}(A, B) = (\min_{a \in A,\, b \in B} (\mathrm{d}_{\boldsymbol{\beta}}(a, b))^{\alpha} + \min_{a \in A,\, b \in B} (\mathrm{d}_{\boldsymbol{\beta}}(a, b))^{\alpha})^{1/\alpha}$

Pfaffian GJ Framework Example: Linkage Clustering [BN**S** TMLR'25]

Algorithm:

1. Start with each object as its own cluster.
2. Repeatedly merge "most similar" clusters.

$$\mathrm{D}_{\alpha,\boldsymbol{\beta}}(A, B) = (\min_{a \in A,\, b \in B} (\mathrm{d}_{\boldsymbol{\beta}}(a, b))^{\alpha} + \min_{a \in A,\, b \in B} (\mathrm{d}_{\boldsymbol{\beta}}(a, b))^{\alpha})^{1/\alpha}$$

The algorithm uses exponents:
so arithmetic operations not enough to compute the clusters!
But Pfaffian GJ framework applies!

Theorem: Sample complexity of tuning α, $\boldsymbol{\beta}$ is $\mathrm{O}(n^4 L^2/\varepsilon^2)$.

Pfaffian GJ Framework Example: Linkage Clustering [BNS TMLR'25]

Algorithm:

1. Start with each object as its own cluster.
2. Repeatedly merge "most similar" clusters.

$$D_{\alpha,\boldsymbol{\beta}}(A, B) = (\min_{a \in A,\, b \in B} (d_{\boldsymbol{\beta}}(a, b))^{\alpha} + \min_{a \in A,\, b \in B} (d_{\boldsymbol{\beta}}(a, b))^{\alpha})^{1/\alpha}$$

What are the Pfaffian chains?

Merge decisions are governed by boundaries given by following inequation in α, $\boldsymbol{\beta}$

$$D_{\alpha,\boldsymbol{\beta}}(A, B) \gtrless D_{\alpha,\boldsymbol{\beta}}(A', B')$$

for some clusters A, B, A', B'

Equivalently, the boundaries are given by (at most n^8 equations)

$$(d_{\boldsymbol{\beta}}(a_1, b_1))^{\alpha} + (d_{\boldsymbol{\beta}}(a_2, b_2))^{\alpha} - (d_{\boldsymbol{\beta}}(a_3, b_3))^{\alpha} - (d_{\boldsymbol{\beta}}(a_4, b_4))^{\alpha} \gtrless 0$$

for some points $a_1, b_1, a_2, b_2, a_3, b_3, a_4, b_4$

Pfaffian GJ Framework Example: Linkage Clustering [BNS TMLR'25]

$$(\mathrm{d}_{\boldsymbol{\beta}}(a_1, b_1))^{\alpha} + (\mathrm{d}_{\boldsymbol{\beta}}(a_2, b_2))^{\alpha} - (\mathrm{d}_{\boldsymbol{\beta}}(a_3, b_3))^{\alpha} - (\mathrm{d}_{\boldsymbol{\beta}}(a_4, b_4))^{\alpha} \gtrless 0$$

What are the Pfaffian chains?

For each pair of points (a, b), define 3 functions

$f_{a,b}(\boldsymbol{\beta}) = 1/\mathrm{d}_{\boldsymbol{\beta}}(a, b)$;
$g_{a,b}(\boldsymbol{\beta}) = \ln \mathrm{d}_{\boldsymbol{\beta}}(a, b)$;
$h_{a,b}(\boldsymbol{\beta}) = (\mathrm{d}_{\boldsymbol{\beta}}(a, b))^{\alpha}$

Pfaffian chain: $\{f_{a,b}(\boldsymbol{\beta})\}_{a,b}$, $\{g_{a,b}(\boldsymbol{\beta})\}_{a,b}$, $\{h_{a,b}(\boldsymbol{\beta})\}_{a,b}$

Chain length < $3n^2$, degree 1, Pfaffian degree 2
Number of parameter = $L + 1$
Number of distinct predicates < n^8
Our result implies $\mathrm{Pdim}(U) = O(n^4 L^2)$

Roadmap

- Algorithm design for machine learning (aka HP tuning)
- Current approaches in practice
  - Bayesian Optimization, Gradient-based and Bandit-based methods
- Machine learning for algorithm design
  - Learning-theoretic foundations
  - GJ algorithm framework
- **Tuning core ML algorithms**
  - Decision Trees
  - Neural networks
- Ongoing and future research directions

Applications [ML, stats, optimization]

Low-rank approximation [Bartlett, Indyk, Wagner, COLT 2022]

Regularizing linear (Elastic Net) and logistic regression [BK**S**T NeurIPS 2022, BN**S** NeurIPS 2023, BG**S** 2025]

Simulated Annealing [Blum, Dan, Seddighin, AISTATS 2021]

Learning to branch and cut [Balcan, Dick, Sandholm, Vitercik, ICML 2018, JACM 2024]

Clustering (both k-center and hierarchical) [BNVW COLT 2017, BDW NeurIPS 2018, BDL ICLR 2020]

Gradient descent [Gupta and Roughgarden, ITCS 2016]

Integer and Linear Programming [Balcan et al., Khodak et al., Cheng and Basu, Sakaue and Oki (2024)]

More applications [CS theory, Comp bio, Mech design, Energy …]

Knapsack, Maximum Weighted Independent Set [Gupta and Roughgarden, ITCS 2016, Balcan et al., FOCS 2018, Sun et al. 2022]

Max cut, Max 2-SAT [Balcan et al., COLT 2017]

Dynamic Programming, Sequence Alignment [Balcan et al., COLT 2017, STOC 2021, NeurIPS 2024]

Mechanism and game design [Balcan et al., EC18, NeurIPS 24, Jin et al. NeurIPS 24, Dütting et al. EC 2025]

Energy and climate science [Mathioudaki et al., 2023, Bostandoost et al. 2024]

Open questions and research directions

- Provable tuning of hyperparameters in other fundamental algorithms and areas, E.g.
  - Causal inference algorithms
  - Constraint Satisfaction e.g. algorithms for SAT
  - Graph Algorithms
  - Bayesian Optimization itself! (e.g. [Sharma and Suggala (AAAI 25)] tune GP bandits)
  - …
- Computational efficiency and complexity of hyperparameter tuning
- Lower bounds on sample complexity
  - Tight bounds known only in some cases

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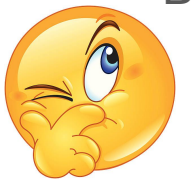
  - Neural networks
- Other aspects, ongoing and future research

ML needs to be interpretable!

Trustworthy?
Biased?



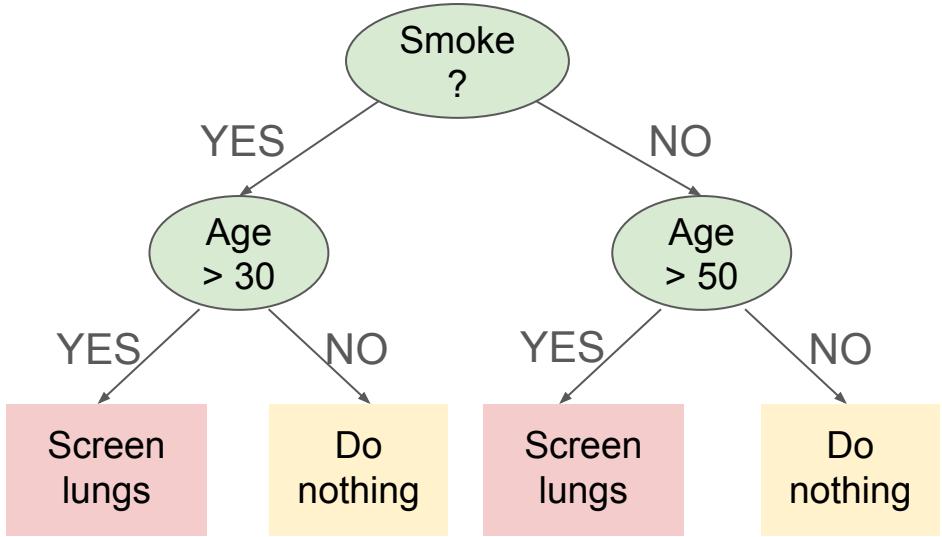
Decision Trees

Trees for classification:

- Each internal node ⇔ Splitting rule
- Each leaf node ⇔ Single Class

Interpretable ML models

- axis-parallel decision boundaries
- Neural nets are hard to interpret



Hard to learn optimal trees, but several useful heuristics!

Learning optimal decision trees is hard!

Hardness of DT learning

- NP-complete. [Laurent and Rivest (1976)]
- *Superconstant Inapproximability of Decision Tree Learning*.

  [Koch et al. COLT 2024] [Koch and Strassle FOCS 2023, FOCS 2024]

Faster optimal decision trees (speed up the exp time branch-and-bound algorithm)

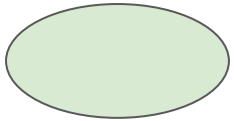
- [Hu et al. NeurIPS 2019]
- [McTavish et al. AAAI 2022]
- [Babbar et al. ICML 2025] (combines greedy with branch-and-bound)

Splitting criterion (a greedy approach)

Top-down decision tree learning

Inputs: Node function class $\mathcal{F}$, tree size **t**,
splitting criterion **G**

Splitting criterion

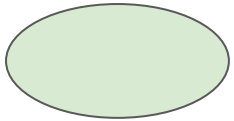


Top-down decision tree learning

Inputs: Node function class $\mathcal{F}$, tree size **t**,
splitting criterion **G**

- Start with leaf node

Splitting criterion



Top-down decision tree learning

Inputs: Node function class $\mathcal{F}$, tree size **t**,
splitting criterion **G**

- Start with leaf node
- While at most **t** leaf nodes
  - Split leaf node **l** using node function **f** which maximizes “splitting criterion”

Splitting criterion

Top-down decision tree learning

Inputs: Node function class $\mathcal{F}$, tree size **t**, splitting criterion **G**

- Start with leaf node
- While at most **t** leaf nodes
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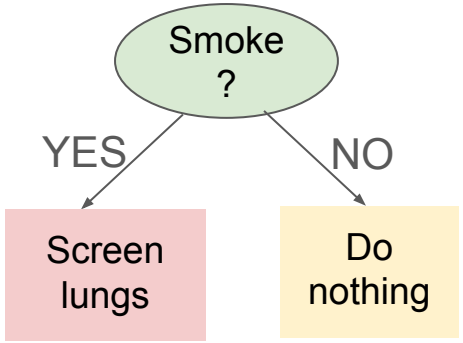


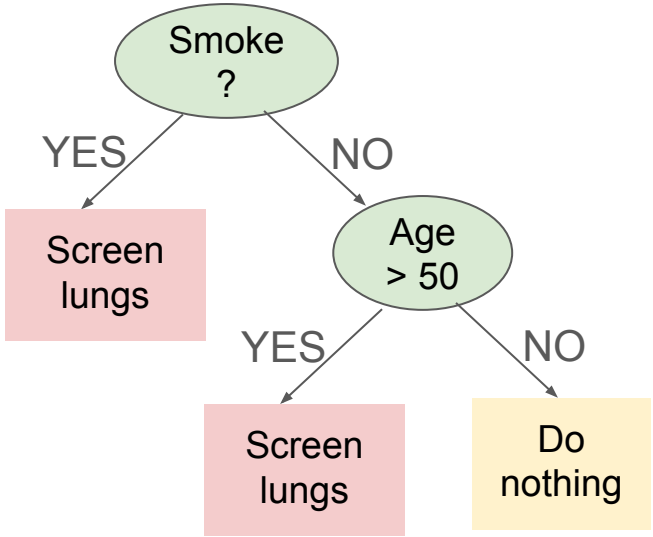
$\mathcal{F}$ = {Smoke, Age >30, Age >50}

Splitting criterion

Top-down decision tree learning

Inputs: Node function class $\mathcal{F}$, tree size **t**, splitting criterion **G**

- Start with leaf node
- While at most **t** leaf nodes
  - Split leaf node **l** using node function **f** which maximizes “splitting criterion”



Key decision: Which node to split next and how?

$\mathcal{F}$ = {Smoke, Age >30, Age >50}

Splitting criterion

DecisionTreeClassifier

```
class sklearn.tree.DecisionTreeClassifier(*, criterion='gini',
splitter='best', max_depth=None, min_samples_split=2, min_samples_leaf=1,
min_weight_fraction_leaf=0.0, max_features=None, random_state=None,
max_leaf_nodes=None, min_impurity_decrease=0.0, class_weight=None,
ccp_alpha=0.0, monotonic_cst=None)                                    [source]
```

A decision tree classifier.

Read more in the User Guide.

Parameters:

criterion : *{"gini", "entropy", "log_loss"}, default="gini"*

Splitting criterion

Empirical research suggests different criteria work best on different data [Mingers 1989]

- Entropy criterion
- Gini impurity
- Kearns Mansour 96

Algorithm selection via hyperparameter tuning

(α, β)-Tsallis entropy

A single criterion which interpolates all three!

$$g_{\alpha,\beta}^{\text{TSALLIS}}(P) := \frac{C}{\alpha - 1}\left(1 - \left(\sum_{i=1}^{c} p_i^{\alpha}\right)^{\beta}\right)$$

Splitting criterion

$g_{2,1}^{\text{TSALLIS}}(P)$ Gini impurity

$g_{\frac{1}{2},2}^{\text{TSALLIS}}(P)$ KM96

$\lim_{\alpha \to 1} g_{\alpha,1}^{\text{TSALLIS}}(P)$ Entropy

Splitting criterion

$g_{2,1}^{\text{TSALLIS}}(P)$

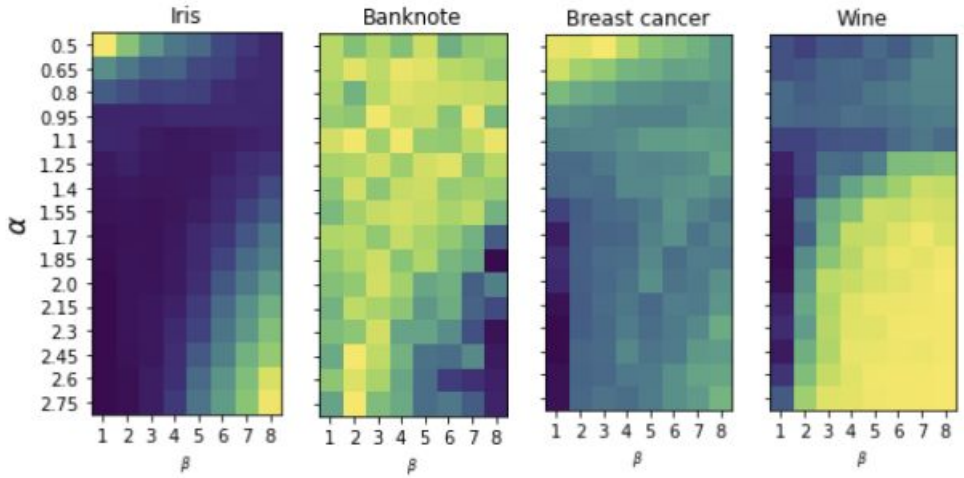
Gini impurity

$g_{\frac{1}{2},2}^{\text{TSALLIS}}(P)$

KM96

$\lim_{\alpha \to 1} g_{\alpha,1}^{\text{TSALLIS}}(P)$

Entropy

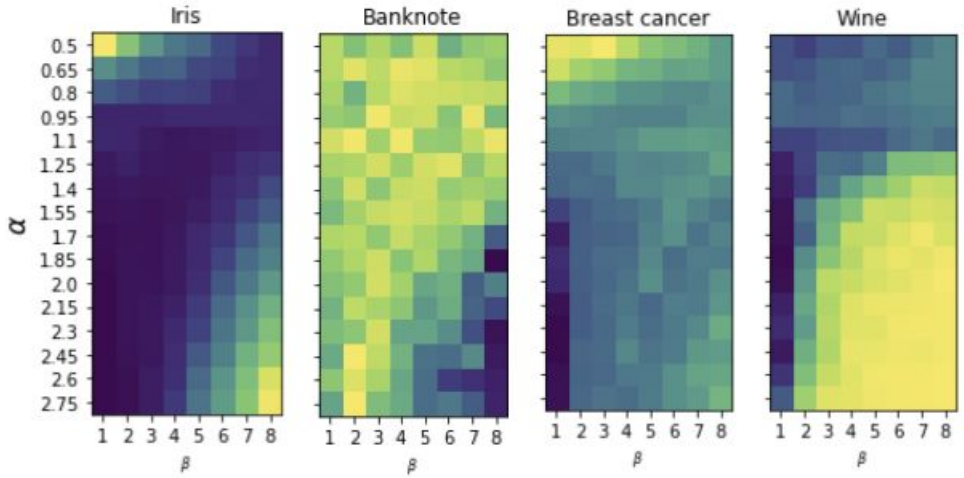


Splitting criterion

$g_{2,1}^{\text{TSALLIS}}(P)$ Gini impurity

$g_{\frac{1}{2},2}^{\text{TSALLIS}}(P)$ KM96

$\lim_{\alpha \to 1} g_{\alpha,1}^{\text{TSALLIS}}(P)$ Entropy



Theorem: We can learn to tune (α, β) using $O\left(\frac{t \log |\mathcal{F}| t}{\epsilon^2}\right)$ problem samples.

Splitting criterion

Theorem: We can learn to tune (α, β) using $O\left(\frac{t \log |\mathcal{F}| t}{\epsilon^2}\right)$ problem samples.

Proof insights:

- Analyse accuracy as a function of (α, β) on a fixed instance (X, y)
- Induction over top-down rounds, bounding the number of distinct behaviors (which node is split and how) in each round
- Over t rounds, $\tilde{O}(|\mathcal{F}|^{2t} t^{2t})$ distinct behaviors, which implies pseudo-dimension is $O(t \log |\mathcal{F}| t)$.

Interpretability vs accuracy

$$\text{Modified objective, } R(T, D) = L(T, D) + \eta \, |\text{leaves}(T)|$$

Similar to cost-complexity pruning, but also modify **test loss**

- η controls the accuracy-interpretability trade-off
- we tune splitting/pruning hyperparameters simultaneously to maximize the modified objective

Gradient-boosted decision trees

Regularized objective over a collection of K trees (size at most t),

$L(\{T_i\}, D) = l(\{T_i\}, D) + \frac{1}{2} \lambda \sum_k ||\text{weights of leaves in } T_k||^2$

Splitting-criterion in XGBOOST [Chen and Guestrin (2016)]:

- Across all nodes of all trees in the ensemble, split the one that maximizes a score based on first and second order gradients $\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{G^2}{H + \lambda}$

State-of-the-art approach for tabular datasets!
[McElfresh et al. (NeurIPS 2023), Jayawardhana et al. (2025)]

We use a GJ framework based analysis.

Gradient-boosted decision trees

Regularized objective over a collection of K trees (size at most t),

$L(\{T_i\}, D) = l(\{T_i\}, D) + \frac{1}{2} \lambda \sum_k ||\text{weights of leaves in } T_k||^2$

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There are at most $tK|\mathcal{F}|$ different candidate splits, or at most $t^2K^2|\mathcal{F}|^2$ pairs
Also over the course of XGBOOST, we have at most tK splits.
⇒ Computable using a GJ algorithm with at most $(t^2K^2|\mathcal{F}|^2)^{tK}$ predicates (degree 6)
⇒ $\text{Pdim}(U) = O(tK \log(tK|\mathcal{F}|))$

Open questions and research directions

- Efficient implementations of learning algorithms
- Extensions to other interpretable techniques
- Lower bounds on sample efficiency
- Online learning
- Combining with other guarantees e.g. robustness

Roadmap

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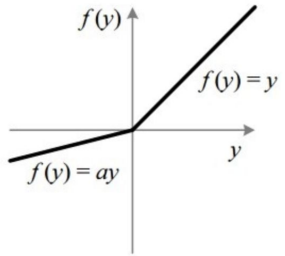
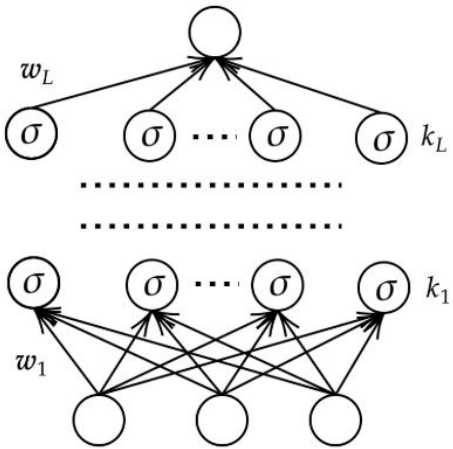
- Other aspects, ongoing and future research

Tuning deep networks: parameters and hyperparameters

- **Hyperparameter space** $A = [\alpha_{\min}, \alpha_{\max}] \subset \mathbb{R}$ (**hyperparameter** α) ← fixed during training
- **Model parameter space** $W \subset \mathbb{R}$ (**parameters/weights** w) ← updated during training
- Example (learning activation functions):
  - Consider a DNN $\tau_{\alpha,w}$ with model weights $w = (w_1, \ldots, w_L)$
  - Parametric ReLU activation function

$$\mathrm{PReLU}(x) = \begin{cases} x, & \text{if } x \geq 0 \\ ax, & \text{otherwise} \end{cases}$$





  - More generally, one can interpolate* any activation functions
    $\sigma(z) = \alpha\, o_1(z) + (1 - \alpha)\, o_2(z)$
    where o_1, o_2 are common activation functions, α is interpolation hyperparameter

*inspired by DARTS approach for Neural Architecture Search [Liu et al. ICLR'19]

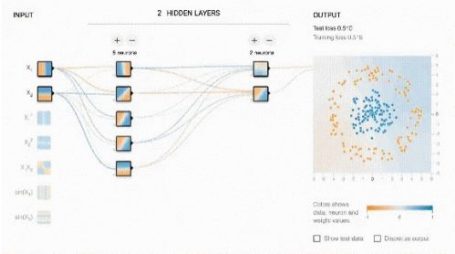
Model vs optimization hyperparameters

“model” or “architectural” hyperparameters:

- Are directly a part of the learned deep network $\tau_{\alpha,w}$
- Impact training, but stay fixed as we learn the weights w

e.g. activation function parameters,

kernel parameter in graph neural networks



“optimization” hyperparameters in the training procedure:

- They impact training too, but their effect on the learned network is fully captured by w

e.g. learning rate

Formalism: the utility function

- **Parameter-dependent utility function** $f(\boldsymbol{x}, \alpha, \boldsymbol{w})$
  the performance when using hyperparameter α and parameter $\boldsymbol{w}$, operating on problem instance $\boldsymbol{x}$

- **Utility function** $u_{\alpha}(\boldsymbol{x}) = \sup_{\boldsymbol{w}} f(\boldsymbol{x}, \alpha, \boldsymbol{w})$

  the performance of trained network using hyperparameter α, operating on problem instance $\boldsymbol{x}$

- Example
  - $f(\boldsymbol{x}, \alpha, \boldsymbol{w}) = H - ||\boldsymbol{y} - \tau_{\alpha,\boldsymbol{w}}(X)||_2^2$ is the parameter-dependent **utility** function

    (the loss is $||\boldsymbol{y} - \tau_{\alpha,\boldsymbol{w}}(X)||_2^2$)
  - $u_{\alpha}(\boldsymbol{x}) = \sup_{\boldsymbol{w}} f(\boldsymbol{x}, \alpha, \boldsymbol{w})$ is the utility function

Formalism: data-driven hyperparameter tuning

- Tuned hyperparameter $\hat{a}$ that has performance close to the optimal $\alpha^* = \max_\alpha \mathrm{E}_{x \sim D}[u_\alpha(x)]$

$$|\mathrm{E}_{x \sim D}[u_{\hat{a}}(x)] - \mathrm{E}_{x \sim D}[u_{\alpha^*}(x)]| < \varepsilon$$

  with probability at least $1 - \delta$, using problem instances $x_1, \ldots, x_m \sim D^m$

- **Question**: How many problem instances $m(\varepsilon, \delta)$ are enough?

Statistical learning theory: sample complexity and pseudo-dimension

Given $\varepsilon > 0$ and $0 < \delta < 1$, what is the sample complexity $m(\varepsilon, \delta)$?

- Standard PAC-Learning approach: bound the learning-theoretic complexity of U

$$U = \{u_\alpha : \boldsymbol{\mathcal{X}} \to [0, \mathrm{H}] \mid \alpha \in A\}$$

- Complexity measure: pseudo-dimension, Pdim(U)
  - The maximum size n such that U can "shatter" $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$, using thresholds $\boldsymbol{t}_1, \ldots, \boldsymbol{t}_n \in \mathbb{R}$
  - by "shattering", we mean $|\{\mathrm{sign}(u_\alpha(\boldsymbol{x}_1) - \boldsymbol{t}_1), \ldots, \mathrm{sign}(u_\alpha(\boldsymbol{x}_n) - \boldsymbol{t}_n) \mid u_\alpha \in U\}| = 2^n$

- Classical learning theory: If Pdim(U) is finite, then $m(\varepsilon, \delta) = \mathrm{O}(\mathrm{H}^2/\varepsilon^2(\mathrm{Pdim}(U) + \log 1/\delta))$

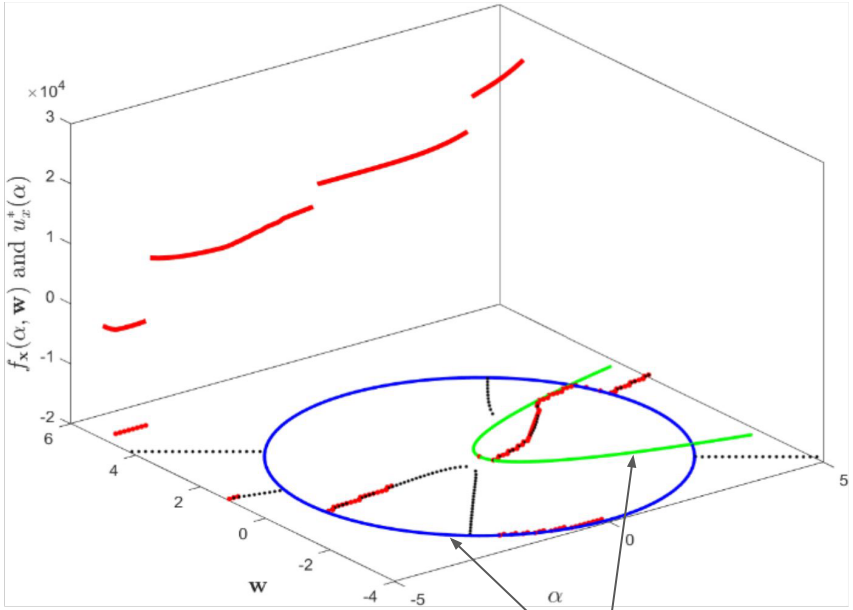
Piecewise polynomial parameter-dependent utility function [BNS Arxiv'25]

- Recall utility function: $u_\alpha(\boldsymbol{x}) = \sup_w f(\boldsymbol{x}, \alpha, w)$, where parameter-dependent utility: $f(\boldsymbol{x}, \alpha, w)$

- Motivated by classical work on NNs*, we assume: for any fixed problem instance $\boldsymbol{x}$, the **parameter-dependent dual** $f_{\boldsymbol{x}}(\alpha, w) := f(\boldsymbol{x}, \alpha, w)$ admits a **piecewise polynomial structure**:
  - There are polynomial **boundary functions** $h_{\boldsymbol{x},1}(\alpha, w), \ldots, h_{\boldsymbol{x},M}(\alpha, w)$ …
  - that partition the domain $A \times W$ of $f_{\boldsymbol{x}}(\alpha, w)$ into connected components "pieces" $R_{\boldsymbol{x},1}, \ldots, R_{\boldsymbol{x},N}$
  - $f_{\boldsymbol{x}}(\alpha, w)$ restricted on $R_{\boldsymbol{x},i}$ is polynomial $f_{\boldsymbol{x},i}(\alpha, w)$ (**piece function**)

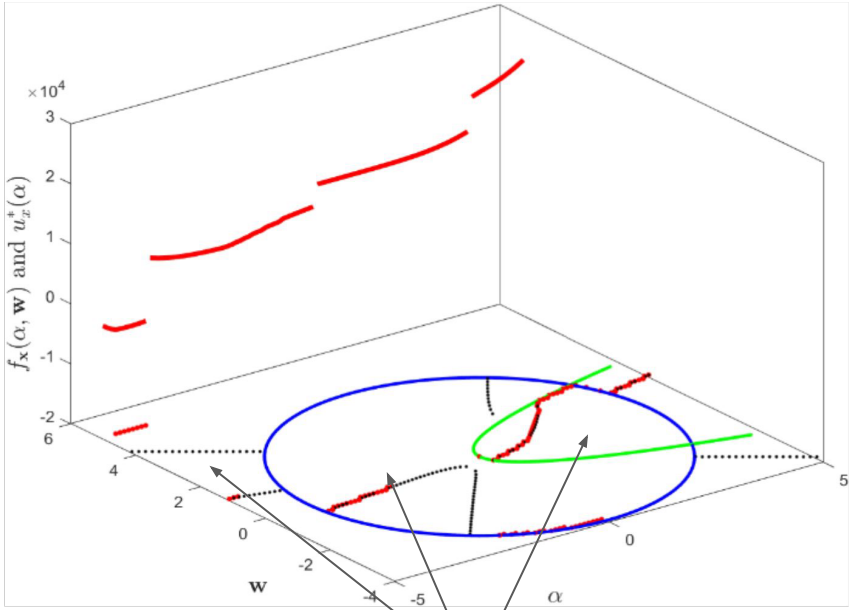
*[Bartlett et al. 1998, Bartlett et al. 2019]

Piecewise polynomial structure: an example



- Boundary functions $h_{x,1}$ and $h_{x,2}$

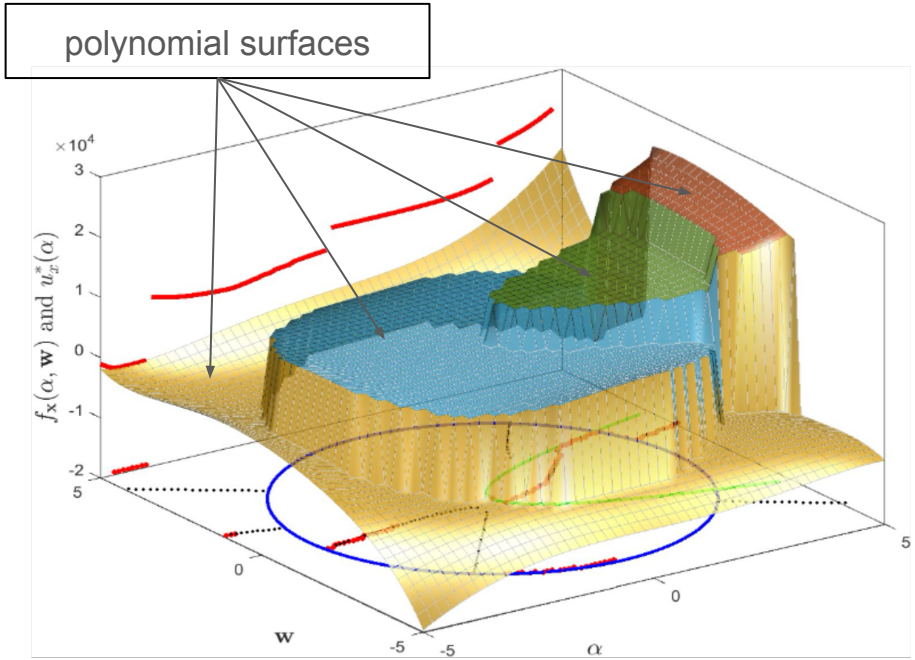
Piecewise polynomial structure: an example



Connected components

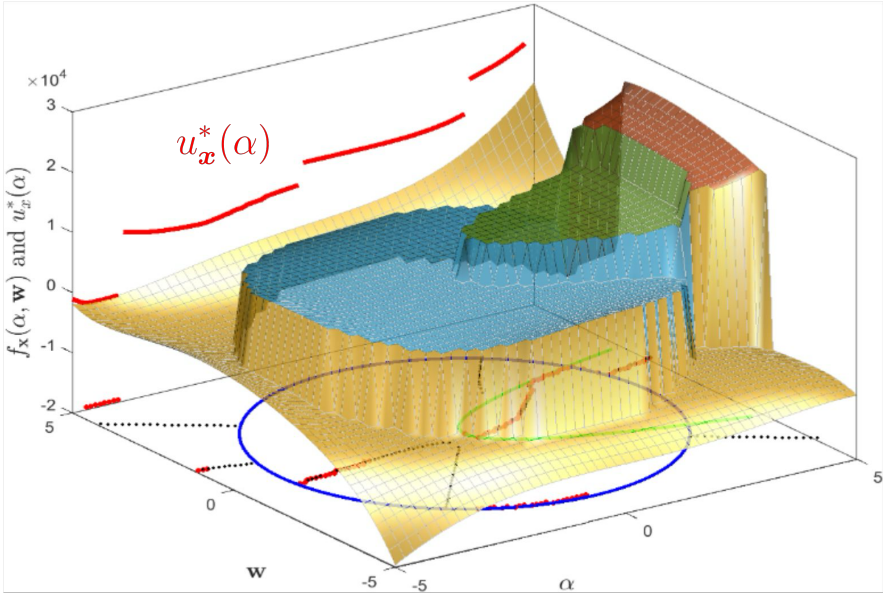
- Boundary functions $h_{x,1}$ and $h_{x,2}$
- partition domain into connected components $R_{x,1}$, …, $R_{x,N}$

Piecewise polynomial structure: an example



- Boundary functions $h_{x,1}$ and $h_{x,2}$
- partition domain into connected components $R_{x,1}$, …, $R_{x,N}$
- $f_x(\alpha, w)$ restricted on $R_{x,i}$ is poly. $f_{x,i}(\alpha, w)$

Piecewise polynomial structure: an example

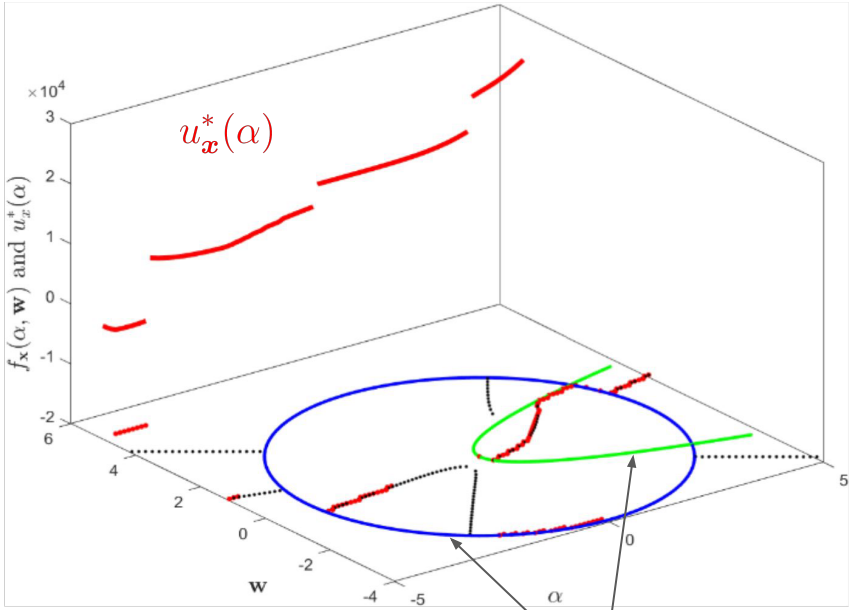


- Boundary functions $h_{x,1}$ and $h_{x,2}$
- partition domain into connected components $R_{x,1}, \ldots, R_{x,N}$
- $f_x(\alpha, w)$ restricted on $R_{x,i}$ is poly. $f_{x,i}(\alpha, w)$

To bound Pdim(U), we're interested in:

$$u^*_x(\alpha) := u_\alpha(x) = \sup_w f_x(\alpha, w)$$

Key mathematical question



- If $f_x(\alpha, w)$ is piecewise-polynomial, can we give a bound on the piecewise structure of

$$u^*_x(\alpha) := u_\alpha(x) = \sup_w f_x(\alpha, w)$$

- To bound Pdim(U), it is sufficient to bound the number of discontinuities and number of local maxima of $u^*_x(\alpha)$

Main result [Balcan, Nguyen, Sharma, Arxiv'25]

Theorem (informal): $\mathrm{Pdim}(U) = \mathrm{O}(\log N + d \log(\Delta M))$, where

N is the number of connected components

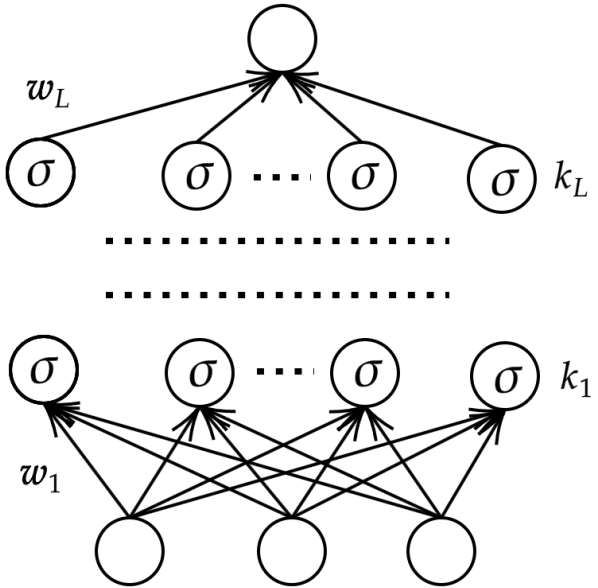
M is the number of boundaries

d is the dimension of $\boldsymbol{w}$

Δ is the maximum polynomial degree

Learning the interpolated activation function

- DNN $\tau_{\alpha,w}$ with L layers
- Layer i: W_i params (total W), k_i nodes (total k)
- $\sigma(z) = \alpha\, o_1(z) + (1-\alpha)\, o_2(z)$, where o_1, o_2 piecewise poly. with max degree Δ, p breakpoints
- T samples (not assumed iid) in each problem instance



Learning the interpolated activation function

Theorem (informal): $\mathrm{Pdim}(U) = \mathrm{O}(\log N + d \log(\Delta M))$, where

N is the number of connected components

M is the number of boundaries

d is the dimension of $\boldsymbol{w}$

Δ is the maximum polynomial degree

Application: For the activation function interpolation:
$\mathrm{Pdim}(U) = \mathrm{O}(L^2 W \log \Delta + LW \log(Tpk))$

Beyond model parameters: gradient descent

Gradient descent algorithm

Inputs: initial point x, iterations H, threshold θ. Hyperparameter: η

1: **Initialize** $x_1 \leftarrow x$
2: **for** $i = 1, \ldots, H$ **do**
3: **if** $||\nabla f(x_i)|| < \theta$ **then**
4: **Return** x_i
5: $x_{i+1} = x_i - \eta \nabla f(x_i)$

Output: x_i

Prior work by Gupta and Roughgarden (2016):

Assumes: f is convex and smooth

Sample complexity of tuning learning rate is $O(H^3/\varepsilon^2)$

We get $O(H^3/\varepsilon^2)$ sample complexity even for non-convex non-smooth functions!

Roadmap

- Algorithm design for machine learning (aka HP tuning)
- Current approaches in practice
  - Bayesian Optimization, Gradient-based and Bandit-based methods
- Machine learning for algorithm design
  - Learning-theoretic foundations
  - GJ algorithm framework
- Tuning core ML algorithms
  - Decision Trees
  - Neural networks
- **Ongoing and future research**

Open questions and research directions

- Other applications to tuning important hyperparameters and algorithms
- Focus on statistical complexity ⟶ computationally efficient methods?
- Making currently used approaches in practice more structure-aware
- Beyond the worst-case complexity: distribution-dependent bounds

  e.g. [Balcan, Goyal, Sharma (2025)]
- More challenging high-dimensional and distributed settings
- Connecting theory with practice!
  [NeurIPS 2025 tutorial with Colin White (Meta) and Nina Balcan (CMU)]

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