Escaping the curse of dimensionality with a tree-based regressor

Samory Kpotufe

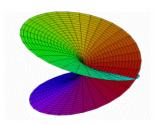
UCSD CSE

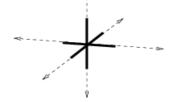
Curse of dimensionality

- **In general:** Computational and/or prediction performance deteriorate as the dimension *D* increases.
- For nonparametric regression: Worst case bounds on excess risk $||f_n f||^2$ are of the form $n^{-2/(2+D)}$.

Here $||f_n - f||^2 = \mathbb{E}_X ||f_n(X) - f(X)||^2$

Reasons for hope: data often has low intrinsic complexity



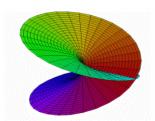


d-dimensional manifold

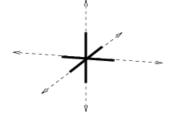
Curse of dimensionality

- **In general:** Computational and/or prediction performance deteriorate as the dimension *D* increases.
- For nonparametric regression: Worst case bounds on excess risk $||f_n f||^2$ are of the form $n^{-2/(2+D)}$. Here $||f_n - f||^2 = \mathbb{E}_X ||f_n(X) - f(X)||^2$.

Reasons for hope: data often has low intrinsic complexity



d-dimensional manifold

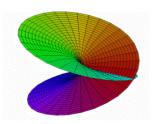


d-sparse data

Curse of dimensionality

- **In general:** Computational and/or prediction performance deteriorate as the dimension *D* increases.
- For nonparametric regression: Worst case bounds on excess risk $||f_n f||^2$ are of the form $n^{-2/(2+D)}$. Here $||f_n - f||^2 = \mathbb{E}_X ||f_n(X) - f(X)||^2$.

Reasons for hope: data often has low intrinsic complexity



d-dimensional manifold



d-sparse data

How do we take advantage of such situations?

- Manifold learning (e.g. LLE, Isomap): embed the data in a lower dimensional space where traditional learners might perform well.
- Adaptivity: can we design learners which run in \mathbb{R}^D but whose performance depend just on the intrinsic complexity of the data?

How do we take advantage of such situations?

- Manifold learning (e.g. LLE, Isomap): embed the data in a lower dimensional space where traditional learners might perform well.
- Adaptivity: can we design learners which run in \mathbb{R}^D but whose performance depend just on the intrinsic complexity of the data?

- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data.
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.

- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data.
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.

- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.

- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data.
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.

- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data.
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.

- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data.
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.



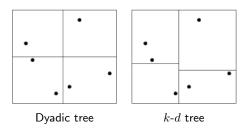
- Classification with dyadic trees (Scott and Nowak, 2006).
 Manifold data.
- Kernel regression (Bickel and Li, 2006).
 Manifold data.
- Vector Quantization with RPtree partitioning (Dasgupta and Freund, 2008).

Data with low Assouad dimension.

Tree-based regression

Build a hierarchy of nested partitions of \mathcal{X} , somehow pick a partition \mathbf{A} :

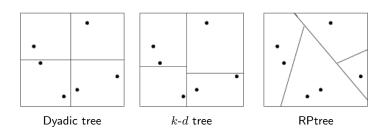
 $f_{n,\mathbf{A}}(x) \doteq \text{average } Y \text{ value in } \mathbf{A}(x), \text{ the cell of } \mathbf{A} \text{ in which } x \text{ falls.}$



Tree-based regression

Build a hierarchy of nested partitions of \mathcal{X} , somehow pick a partition \mathbf{A} :

 $f_{n,\mathbf{A}}(x) \doteq \text{average } Y \text{ value in } \mathbf{A}(x), \text{ the cell of } \mathbf{A} \text{ in which } x \text{ falls.}$



Random Partition tree (RPtree)

Recursively bisect the data near the median along a random direction.

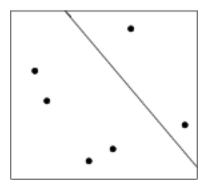


Figure: First level.

Random Partition tree (RPtree)

Recursively bisect the data near the median along a random direction.

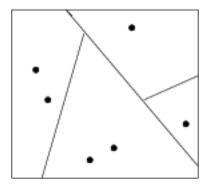


Figure: Second level.

Our results:

We show how to use the RPtree for regression and obtain rates that depend just on the intrinsic complexity of the data, namely its Assouad dimension.

This is the first such adaptivity result for tree-based regression

Our results:

We show how to use the RPtree for regression and obtain rates that depend just on the intrinsic complexity of the data, namely its Assouad dimension.

This is the first such adaptivity result for tree-based regression.

What we'll see next:

- Preliminaries: (1) Assouad dimension. (2) Algorithmic issues regarding the choice of a partition.
- How we choose an RPtree partition for regression.
- Analysis overview.

Assouad dimension.

Definition

The Assouad dimension (or doubling dimension) of $\mathcal X$ is the smallest d such that any ball $B\subset \mathcal X$ can be covered by 2^d balls of half its radius.

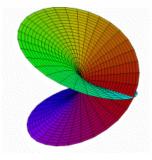


 2^2 balls

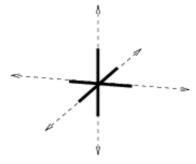


 2^3 balls

Examples of data with low Assouad dimension



d-dimensional manifold

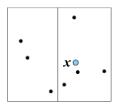


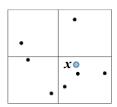
d-sparse data

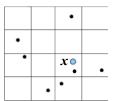
Partition A with small cell diameters?

Low bias: x is near all the data in $\mathbf{A}(x) \Longrightarrow \text{similar } Y$ values. High variance: fewer data in $\mathbf{A}(x) \Longrightarrow \text{unstable estimates}$.

So choose partition with mid-range cell diameters.



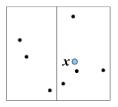


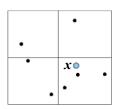


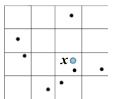
Partition A with small cell diameters?

Low bias: x is near all the data in $\mathbf{A}(x) \Longrightarrow \text{similar } Y$ values. High variance: fewer data in $\mathbf{A}(x) \Longrightarrow \text{unstable estimates}$.

So choose partition with mid-range cell diameters.



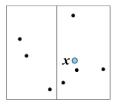


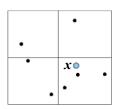


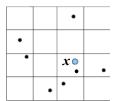
Partition A with small cell diameters?

Low bias: x is near all the data in $\mathbf{A}(x) \Longrightarrow$ similar Y values. High variance: fewer data in $\mathbf{A}(x) \Longrightarrow$ unstable estimates.

So choose partition with mid-range cell diameters



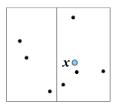


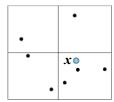


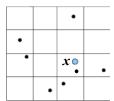
Partition A with small cell diameters?

Low bias: x is near all the data in $\mathbf{A}(x) \Longrightarrow$ similar Y values. High variance: fewer data in $\mathbf{A}(x) \Longrightarrow$ unstable estimates.

So choose partition with mid-range cell diameters.

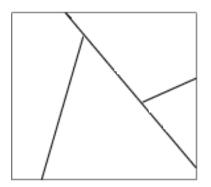






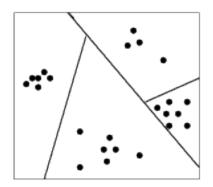
Problem with RPtree cells:

- Cell diameters are hard to assess.
- Cell diameters may not decrease at all.



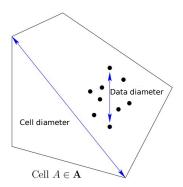
Problem with RPtree cells:

- Cell diameters are hard to assess.
- Cell diameters may not decrease at all.



Problem with RPtree cells:

- Cell diameters are hard to assess.
- Cell diameters may not decrease at all.



This is of general interest for algorithm design and risk analysis: many trees have misbehaved cell diameters like RPtree does.

Data diameters aren't stable \implies hard to generalize from.

RPtree quickly decreases data diameters from the root down: data diameters are halved every $d \log d$ levels [DF08].

This is of general interest for algorithm design and risk analysis: many trees have misbehaved cell diameters like RPtree does.

Data diameters aren't stable \implies hard to generalize from.

RPtree quickly decreases data diameters from the root down: data diameters are halved every $d \log d$ levels [DF08].

This is of general interest for algorithm design and risk analysis: many trees have misbehaved cell diameters like RPtree does.

Data diameters aren't stable \implies hard to generalize from.

RPtree quickly decreases data diameters from the root down data diameters are halved every $d \log d$ levels [DF08].

This is of general interest for algorithm design and risk analysis: many trees have misbehaved cell diameters like RPtree does.

Data diameters aren't stable \implies hard to generalize from.

RPtree quickly decreases data diameters from the root down: data diameters are halved every $d\log d$ levels [DF08].

This is of general interest for algorithm design and risk analysis: many trees have misbehaved cell diameters like RPtree does.

Data diameters aren't stable \implies hard to generalize from.

RPtree quickly decreases data diameters from the root down: data diameters are halved every $d\log d$ levels [DF08].

What we'll see next:

- Preliminaries: (1) Assouad dimension. (2) Algorithmic issues regarding the choice of a partition.
- How we choose an RPtree partition for regression.
- Analysis overview.

How we choose an RPtree partition for regression

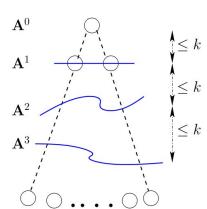
Identify candidate partitions A^i such that data diameters are halved from A^i to A^{i+1} .

Diameter decrease rate k: max levels between \mathbf{A}^i and \mathbf{A}^{i+1} .

Two stopping options:

I: Stop after $O(\log n)$ levels, and test all f_{n,\mathbf{A}^i} on new sample.

II: Stop when data diameters are small enough. **Requires no testing**.

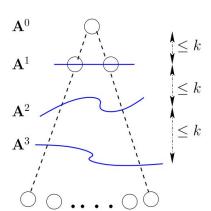


Identify candidate partitions A^i such that data diameters are halved from A^i to A^{i+1} .

Diameter decrease rate k: max levels between \mathbf{A}^i and \mathbf{A}^{i+1} .

Two stopping options:

I: Stop after $O(\log n)$ levels, and test all f_{n,\mathbf{A}^i} on new sample.

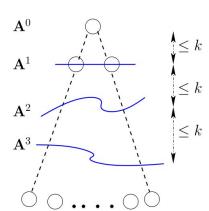


Identify candidate partitions A^i such that data diameters are halved from A^i to A^{i+1} .

Diameter decrease rate k: max levels between \mathbf{A}^i and \mathbf{A}^{i+1} .

Two stopping options:

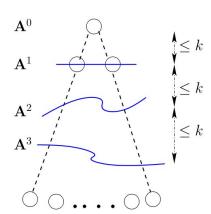
I: Stop after $O(\log n)$ levels, and test all f_{n,\mathbf{A}^i} on new sample.



Identify candidate partitions A^i such that data diameters are halved from A^i to A^{i+1} .

Diameter decrease rate k: max levels between \mathbf{A}^i and \mathbf{A}^{i+1} .

Two stopping options: I: Stop after $O(\log n)$ levels, and test all f_{n,\mathbf{A}^i} on new sample.

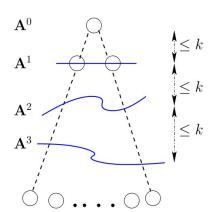


Identify candidate partitions A^i such that data diameters are halved from A^i to A^{i+1} .

Diameter decrease rate k: max levels between \mathbf{A}^i and \mathbf{A}^{i+1} .

Two stopping options:

I: Stop after $O(\log n)$ levels, and test all f_{n,\mathbf{A}^i} on new sample.



Theorem

With probability at least $1 - \delta$, under either stopping option,

$$||f_n - f||^2 \le C \left(\frac{\log^2 n + \log 1/\delta}{n}\right)^{2/(2+k)},$$

where $k \leq C' d \log d$ is the observed diameter decrease rate.

Assumptions:

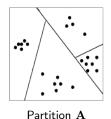
Regression function $f(x)=\mathbb{E}\left[Y|X=x\right]$ is Lipschitz, X and Y are bounded. No distributional assumption.

What we'll see next:

- Preliminaries: (1) Assouad dimension. (2) Algorithmic issues regarding the choice of a partition.
- How we choose an RPtree partition for regression.
- · Analysis overview.

Remember: Data diameters don't generalize well to distribution.

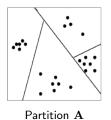
Solution: $orall \mathbf{A} \in \{\mathbf{A}^i\}$, replace \mathbf{A} with alternate partition \mathbf{A}' .



 Dense cells of A' have manageable diameters: cell diameters approximate data diameters.

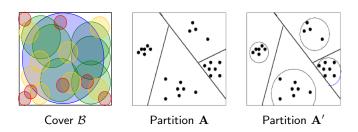
• $\operatorname{Risk}(f_{n,\mathbf{A}'}) \approx \operatorname{Risk}(f_{n,\mathbf{A}})$

Remember: Data diameters don't generalize well to distribution. Solution: $\forall \mathbf{A} \in \{\mathbf{A}^i\}$, replace \mathbf{A} with alternate partition \mathbf{A}' .



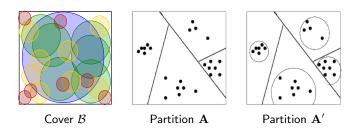
- Dense cells of A' have manageable diameters: cell diameters approximate data diameters.
- $\operatorname{Risk}(f_{n,\mathbf{A}'}) \approx \operatorname{Risk}(f_{n,\mathbf{A}})$

Remember: Data diameters don't generalize well to distribution. Solution: $\forall \mathbf{A} \in \{\mathbf{A}^i\}$, replace \mathbf{A} with alternate partition \mathbf{A}' .



- Dense cells of A' have manageable diameters: cell diameters approximate data diameters.
- $\operatorname{Risk}(f_{n,\mathbf{A}'}) \approx \operatorname{Risk}(f_{n,\mathbf{A}})$

Remember: Data diameters don't generalize well to distribution. Solution: $\forall \mathbf{A} \in \{\mathbf{A}^i\}$, replace \mathbf{A} with alternate partition \mathbf{A}' .



- Dense cells of A' have manageable diameters: cell diameters approximate data diameters.
- $\operatorname{Risk}(f_{n,\mathbf{A}'}) \approx \operatorname{Risk}(f_{n,\mathbf{A}}).$

So we can just analyze the risk of $f_{n,\mathbf{A}'}$, for every $\mathbf{A} \in \{\mathbf{A}^i\}$

Handle the empty cells and the dense cells separately.

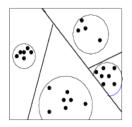


Figure: Partition A'.

So we can just analyze the risk of $f_{n,\mathbf{A}'}$, for every $\mathbf{A} \in \{\mathbf{A}^i\}$ Handle the empty cells and the dense cells separately.



Figure: Partition A'.

- $\mu_n(A') \approx 0 \implies \mu(A') \lesssim \frac{1}{n}$: empty cells don't affect risk.
- $\mu_n(A') \gg 0 \implies \mu_n(A') \approx \mu(A')$: dense cells will be stable.

- Cells A' have random shapes.
- Define a VC class $C \supset \mathbf{A}'$ by conditioning on the randomness in the algorithm and n.

- $\mu_n(A') \approx 0 \implies \mu(A') \lesssim \frac{1}{n}$: empty cells don't affect risk.
- $\mu_n(A') \gg 0 \implies \mu_n(A') \approx \mu(A')$: dense cells will be stable.

- Cells A' have random shapes.
- Define a VC class $C \supset A'$ by conditioning on the randomness in the algorithm and n.

- $\mu_n(A') \approx 0 \implies \mu(A') \lesssim \frac{1}{n}$: empty cells don't affect risk.
- $\mu_n(A') \gg 0 \implies \mu_n(A') \approx \mu(A')$: dense cells will be stable.

- Cells A' have random shapes.
- Define a VC class $C \supset A'$ by conditioning on the randomness in the algorithm and n.

- $\mu_n(A') \approx 0 \implies \mu(A') \lesssim \frac{1}{n}$: empty cells don't affect risk.
- $\mu_n(A') \gg 0 \implies \mu_n(A') \approx \mu(A')$: dense cells will be stable.

- Cells A' have random shapes.
- Define a VC class $C \supset A'$ by conditioning on the randomness in the algorithm and n.

Risk bound for $f_{n,\mathbf{A}'}$, $\forall \mathbf{A} \in \{\mathbf{A}^i\}$:

$$\left\|f_{n,\mathbf{A}'} - f\right\|^2 \lesssim \frac{|\mathbf{A}'|}{n} + \operatorname{diam}_n^2\left(\mathbf{A}'\right).$$

Bound is minimized when:

$$\operatorname{diam}_{n}^{2}\left(\mathbf{A}'\right) \approx \frac{|\mathbf{A}'|}{n}$$
, in which case $\left\|f_{n,\mathbf{A}'} - f\right\|^{2} \lesssim n^{-2/(2+k)}$.

Show that we can find $\mathbf{A} \in \left\{\mathbf{A}^i\right\}$ s.t. \mathbf{A}' minimizes the bound, and conclude.

Risk bound for $f_{n,\mathbf{A}'}$, $\forall \mathbf{A} \in \{\mathbf{A}^i\}$:

$$\left\|f_{n,\mathbf{A}'} - f\right\|^2 \lesssim \frac{|\mathbf{A}'|}{n} + \operatorname{diam}_n^2\left(\mathbf{A}'\right).$$

Bound is minimized when:

$$\dim_n^2(\mathbf{A}') pprox rac{|\mathbf{A}'|}{n}$$
, in which case $\left\|f_{n,\mathbf{A}'} - f\right\|^2 \lesssim n^{-2/(2+k)}$.

Show that we can find $\mathbf{A} \in \left\{\mathbf{A}^i\right\}$ s.t. \mathbf{A}' minimizes the bound, and conclude.

Risk bound for $f_{n,\mathbf{A}'}$, $\forall \mathbf{A} \in \{\mathbf{A}^i\}$:

$$\left\|f_{n,\mathbf{A}'} - f\right\|^2 \lesssim \frac{|\mathbf{A}'|}{n} + \operatorname{diam}_n^2\left(\mathbf{A}'\right).$$

Bound is minimized when:

$$\operatorname{diam}_n^2\left(\mathbf{A}'\right) pprox rac{|\mathbf{A}'|}{n}$$
, in which case $\left\|f_{n,\mathbf{A}'} - f\right\|^2 \lesssim n^{-2/(2+k)}$.

Show that we can find $\mathbf{A} \in \left\{\mathbf{A}^i\right\}$ s.t. \mathbf{A}' minimizes the bound, and conclude.



Recap:

If the data space has low Assouad dimension d, the excess risk of an RPtree regressor depends just on d.

Extending to a more general setting

What if the data has high Assouad dimension overall, but the intrinsic dimension is low in smaller regions?

