

Estimation and Inference in Modern Nonparametric Statistics

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Final Public Oral Examination | May 7th, 2024

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Some of my recent work consists of

- Inference and estimation with Mondrian random forests
- Uniform inference for dyadic kernel density estimators
- Yurinskii's coupling for martingales

Why do tree-based models still outperform deep learning on tabular data?

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- Ensemble methods for regression and classification, with good performance, flexibility, robustness and efficiency
- Many variants including the popular “Random Forest”
- Estimation theory has developed rapidly in recent years but applicability to statistical inference is less well understood
- In joint work with Matias D. Cattaneo and Jason M. Klusowski, I develop **valid feasible inference** procedures and **minimax optimal estimation** results for Mondrian random forests

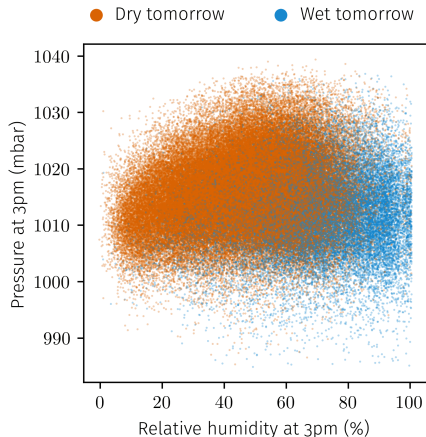
Nonparametric regression setting

- Data (X_i, Y_i) in $[0, 1]^d \times \mathbb{R}$ i.i.d. for $1 \leq i \leq n$
- $Y_i = \mu(X_i) + \varepsilon_i$ with $\mathbb{E}[\varepsilon_i \mid X_i] = 0$
- Aim is to estimate and perform inference on unknown $\mu(x)$

Random forest regression estimators

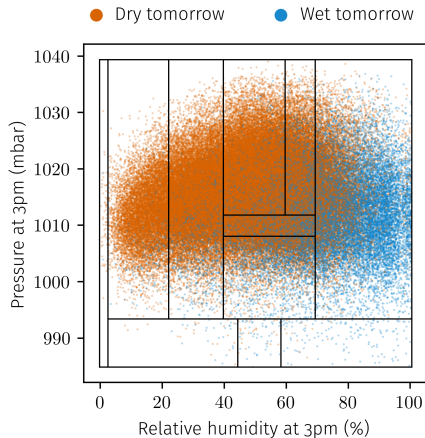
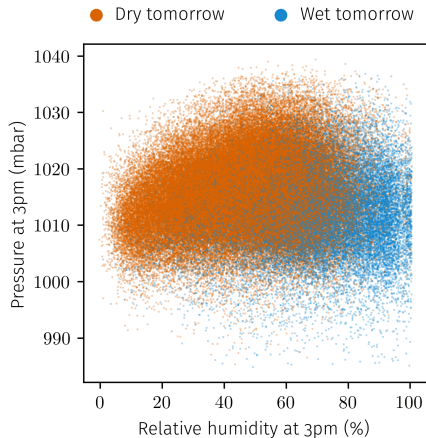
- 1) Form a **partition** of $[0, 1]^d$, usually using a tree structure
- 2) Fit constant estimates of μ on each cell in the partition
- 3) Repeat with different partitions and **average** the estimates

Motivating example: weather forecasting in Australia



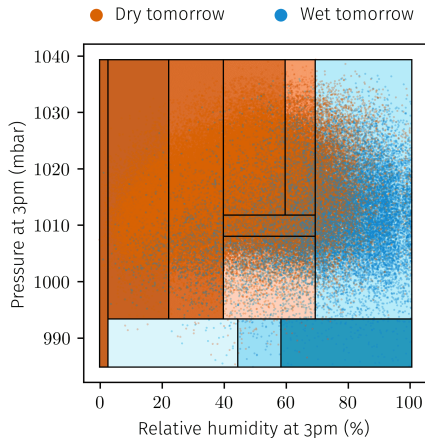
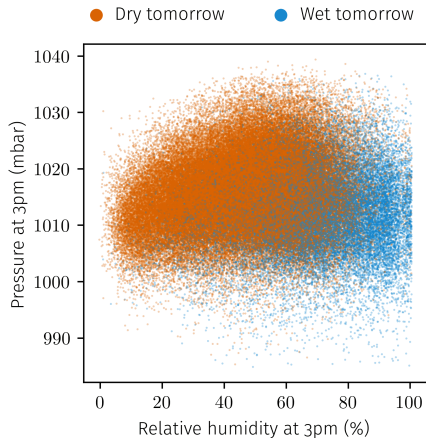
- Weather data from Australian Bureau of Meteorology
- Rainfall from 2007–2017 at 49 locations with 125 927 samples
- Predict **dry** or **wet** tomorrow with humidity and pressure today
- Random forest classification

Motivating example: weather forecasting in Australia



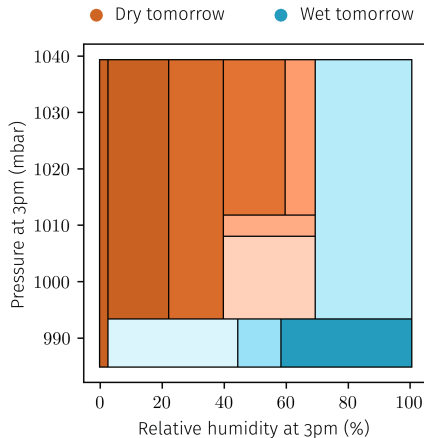
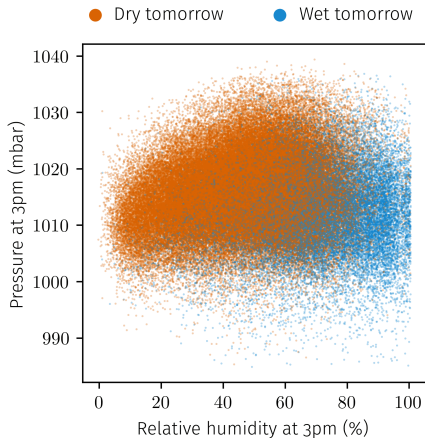
- First generate a partition of the predictor space

Motivating example: weather forecasting in Australia



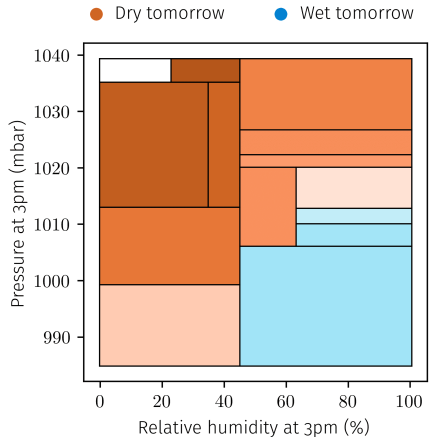
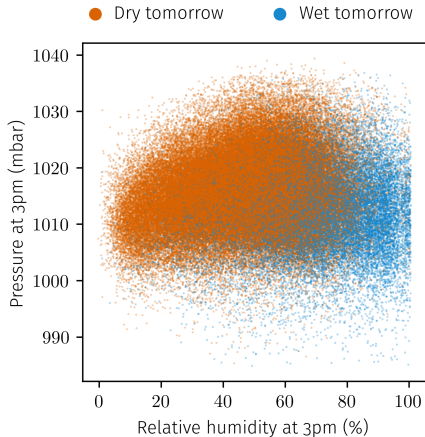
- Compute average response in each cell with $\text{dry} = 0$, $\text{wet} = 1$

Motivating example: weather forecasting in Australia



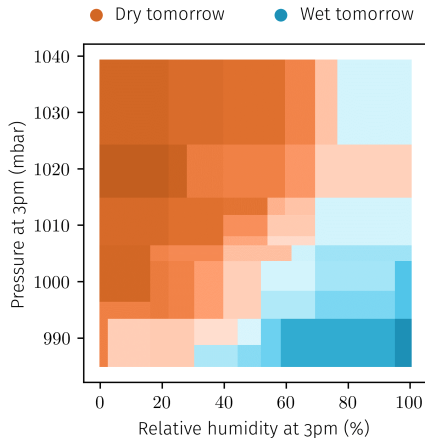
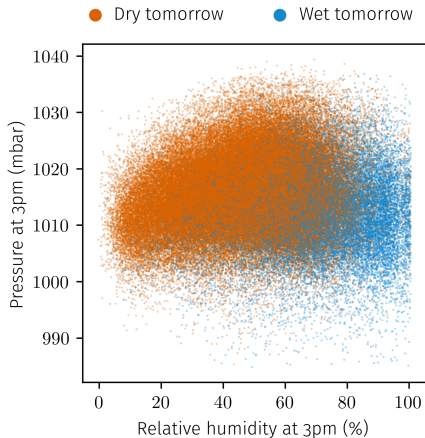
- This gives a single tree estimator of $\mu(x)$

Motivating example: weather forecasting in Australia



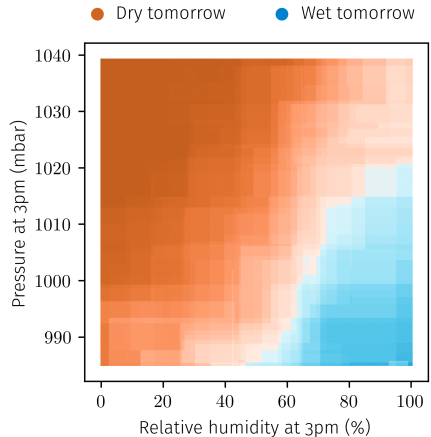
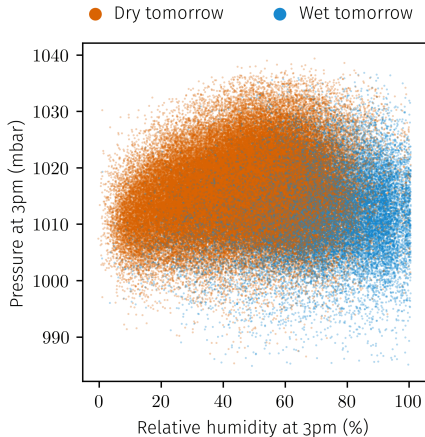
- Repeat with a different partition

Motivating example: weather forecasting in Australia



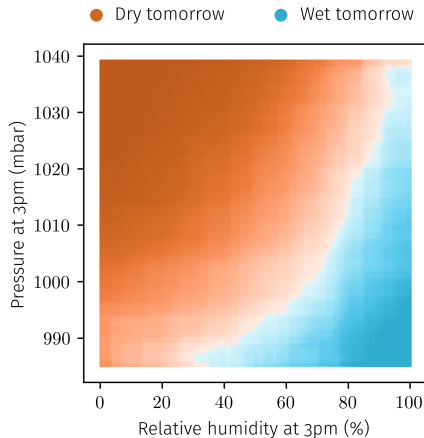
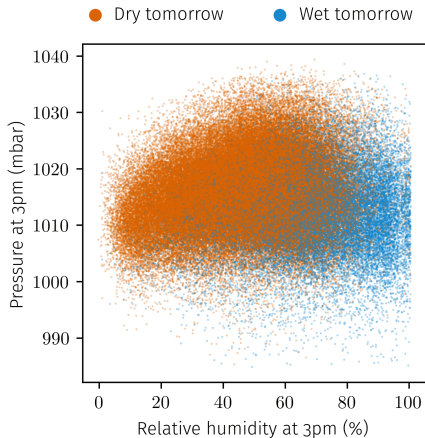
- Average predictions across 2 partitions

Motivating example: weather forecasting in Australia



- Average predictions across 10 partitions

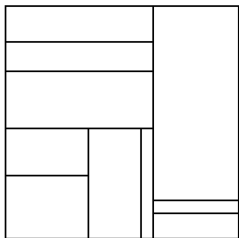
Motivating example: weather forecasting in Australia



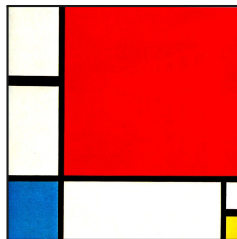
- Average across 30 partitions to get a random forest $\hat{\mu}(x)$

The Mondrian process

- Rectangular partitions sampled from a Mondrian process (Roy and Teh, 2008), write $T \sim \mathcal{MP}([0, 1]^d, \lambda)$
- Tree complexity is controlled by the **lifetime parameter** $\lambda > 0$
- The expected number of cells in T is $(1 + \lambda)^d$
- Mondrian random forests popular recently (Mourtada, Gaïffas and Scornet, NeurIPS 2017, AoS 2020, JRSSB 2021)

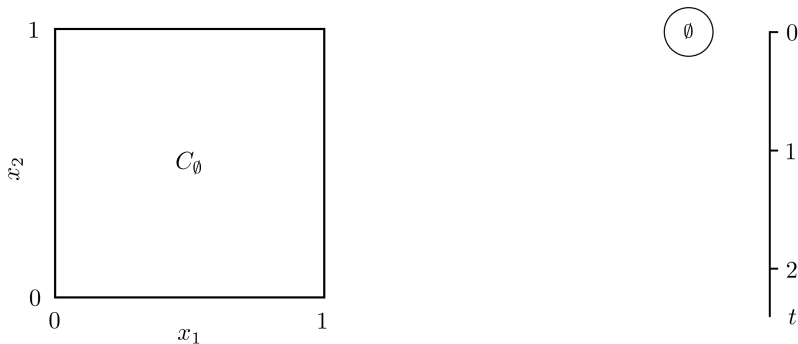


A typical two-dimensional
Mondrian partition with $\lambda = 4$



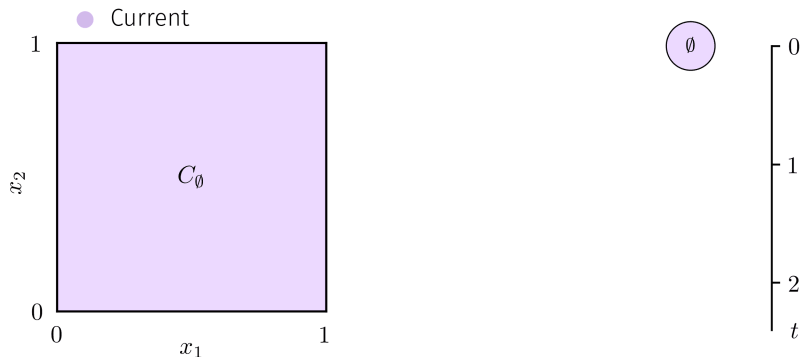
Composition II in Red, Blue,
and Yellow, Piet Mondrian, 1930

Sampling a partition from the Mondrian process



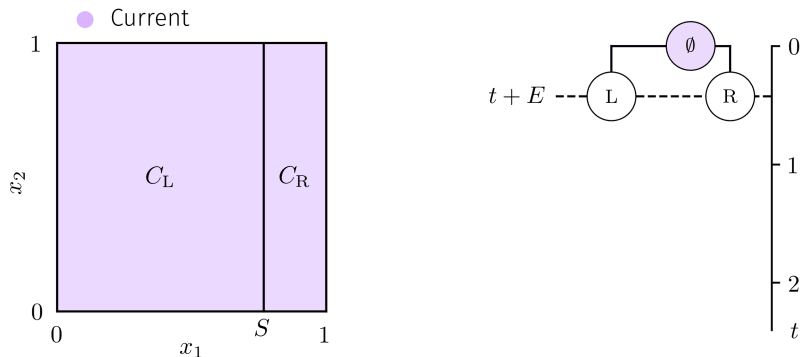
- Fix $\lambda = 2$ and set $t = 0$. The **root cell** is $C_\emptyset = [0, 1]^d$ with $d = 2$
- We make recursive axis-aligned splits to generate a partition
- The lifetime parameter λ determines when to stop splitting
- For any cell C , let $|C|_1 = \sum_{j=1}^d |C_j|$ be the half-perimeter

Sampling a partition from the Mondrian process



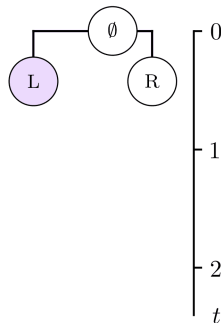
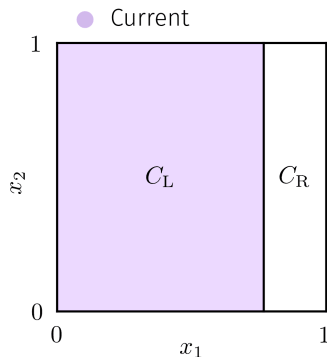
- Decide whether to split cell C_\emptyset
- Sample $E \sim \text{Exp}(|C_\emptyset|_1)$, so $\mathbb{E}[E] = 1/|C_\emptyset|$
- Get $t + E \leq \lambda$ so C_\emptyset is split

Sampling a partition from the Mondrian process



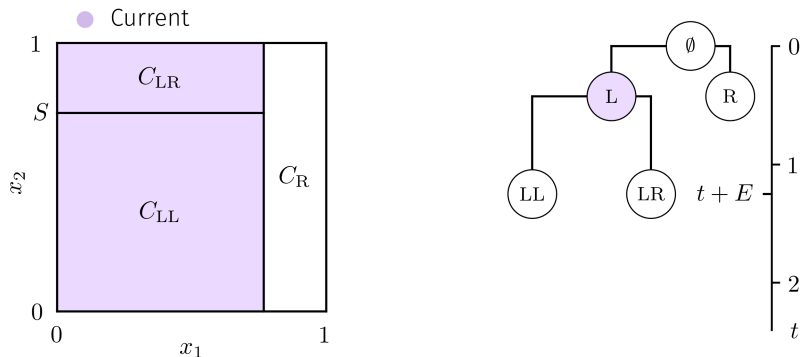
- Choose split axis by $\mathbb{P}(J = j) = \frac{|C_{\emptyset j}|}{|C_{\emptyset}|_1}$, get $J = 1$
- Select split location by $S \sim \text{Unif}(C_{\emptyset J})$
- Replace C_{\emptyset} by $C_L = \{x \in C : x_J \leq S\}$ and $C_R = C \setminus C_L$

Sampling a partition from the Mondrian process



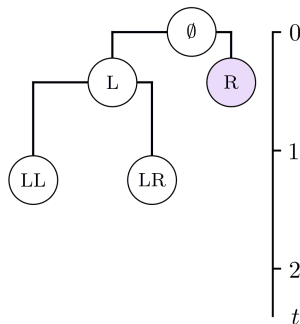
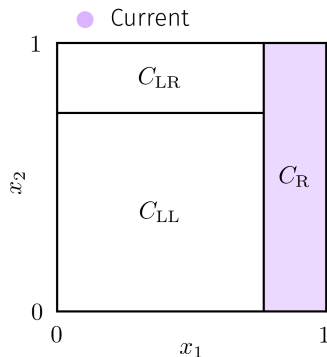
- Decide whether to split cell C_L
- Sample $E \sim \text{Exp}(|C_L|_1)$
- Get $t + E \leq \lambda$ so C_L is split

Sampling a partition from the Mondrian process



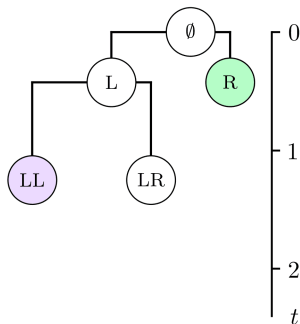
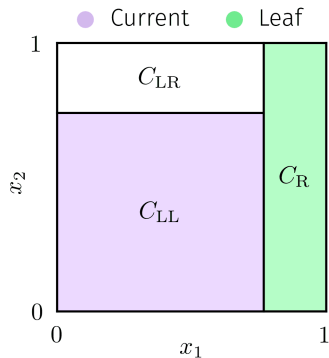
- Choose split axis by $\mathbb{P}(J = j) = \frac{|C_{Lj}|}{|C_L|_1}$, get $J = 2$
- Select split location by $S \sim \text{Unif}(C_{LJ})$
- Replace C_L by $C_{LL} = \{x \in C_L : x_J \leq S\}$ and $C_{LR} = C_L \setminus C_{LL}$

Sampling a partition from the Mondrian process



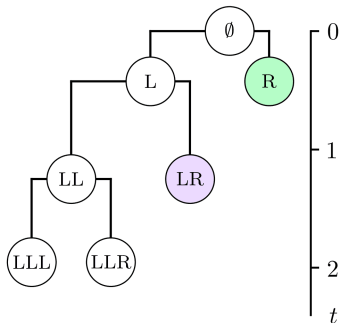
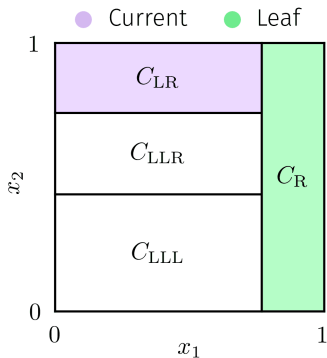
- Decide whether to split cell C_R
- Sample $E \sim \text{Exp}(|C_R|_1)$
- Get $t + E > \lambda$ so C_R is not split and becomes a leaf

Sampling a partition from the Mondrian process



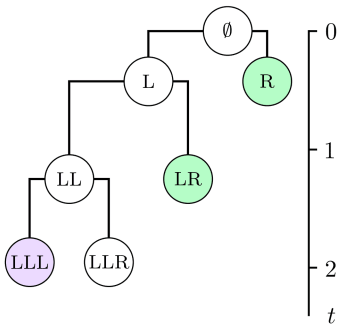
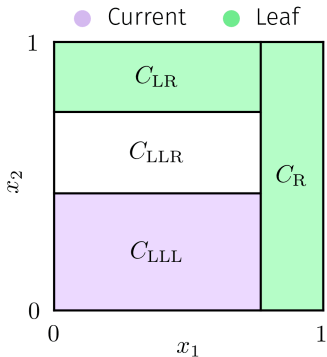
- We continue this process

Sampling a partition from the Mondrian process



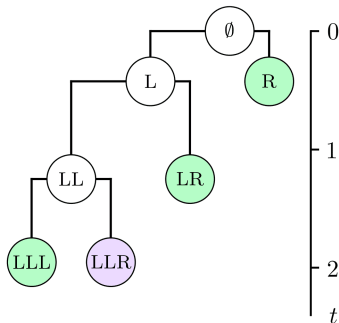
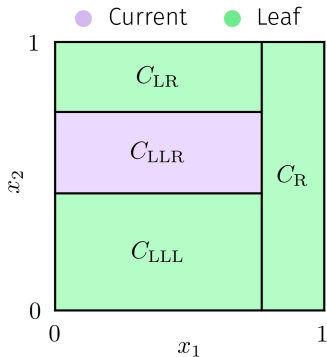
- C_{LR} is not split and becomes a leaf

Sampling a partition from the Mondrian process



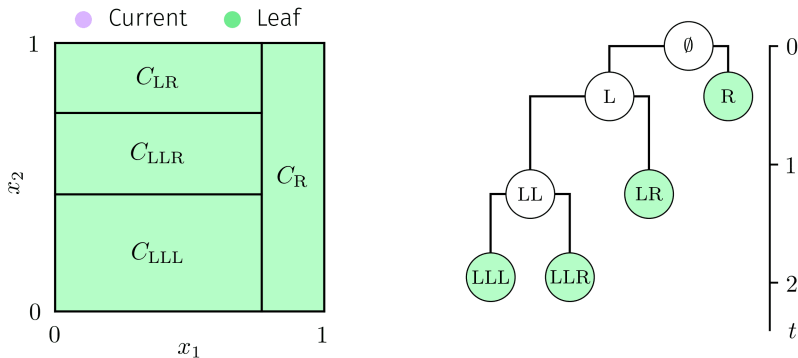
- C_{LLL} becomes a leaf

Sampling a partition from the Mondrian process



- C_{LLR} becomes a leaf

Sampling a partition from the Mondrian process



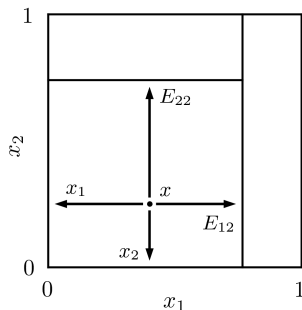
- All cells are now **leaves**, and the sampling is complete
- To increase λ we continue this process, allowing **online fitting**
- Australian weather data: rescaled to $[0, 1]^2$ and set $\lambda = 5$

Properties of the Mondrian process

Lemma (Cell shape distribution)

Let $T \sim \mathcal{MP}([0, 1]^d, \lambda)$, take $x \in [0, 1]^d$ and write $T(x)$ for the cell containing x . With E_{j1} and E_{j2} independent $\text{Exp}(\lambda)$,

$$T(x) = [0, 1]^d \cap \prod_{j=1}^d [x_j - E_{j1}, x_j + E_{j2}]$$



- Roy and Teh (NeurIPS 2008); Mourtada, Gaïffas and Scornet (NeurIPS 2017, AoS 2020, JRSSSB 2021)
- With $d = 1$, have a Poisson process on $[0, 1]$ with intensity λ
- The smallest cell is much smaller than the average cell

Mondrian random forests

- Let B be the desired number of trees in the forest
- Sample $T_1, \dots, T_B \sim \mathcal{MP}([0, 1]^d, \lambda)$ **independently**
- For each cell in T_b , compute the average Y_i value
- Finally average across all the trees
- Writing $N_b(x) = \sum_{i=1}^n \mathbb{I}\{X_i \in T_b(x)\}$ for the number of data points in the same cell as x , and with $0/0 = 0$, we have

Definition (Mondrian random forest estimator)

$$\hat{\mu}(x) = \underbrace{\frac{1}{B} \sum_{b=1}^B}_{\text{Forest}} \underbrace{\frac{1}{N_b(x)} \sum_{i=1}^n Y_i \mathbb{I}\{X_i \in T_b(x)\}}_{\text{Mean of } Y_i \text{ in cell containing } x}$$

Bias-variance decomposition

With $\mathbf{X} = (X_1, \dots, X_n)$ and $\mathbf{T} = (T_1, \dots, T_B)$,

$$\hat{\mu}(x) - \mu(x) = \underbrace{\hat{\mu}(x) - \mathbb{E}[\hat{\mu}(x) \mid \mathbf{X}, \mathbf{T}]}_{\text{Variance}} + \underbrace{\mathbb{E}[\hat{\mu}(x) \mid \mathbf{X}, \mathbf{T}] - \mu(x)}_{\text{Bias}}$$

- 1) Derive a central limit theorem for the **variance** term
- 2) Approximate the **bias** term in probability
- 3) Perform inference by ensuring the bias is negligible
- 4) Minimax optimal estimation with debiasing

Assumptions on data and estimator

- Recall (X_i, Y_i) in $[0, 1]^d \times \mathbb{R}$ i.i.d. with $Y_i = \mu(X_i) + \varepsilon_i$
- X_i has Lebesgue density f , bounded away from zero
- A version of $\sigma^2(X_i) = \mathbb{E} [\varepsilon_i^2 \mid X_i]$ is Lipschitz
- $\mathbb{E} [\varepsilon_i^4 \mid X_i]$ is bounded almost surely
- Both μ and f are β -Hölder continuous for some $\beta \geq 1$
- $x \in (0, 1)^d$ is an interior evaluation point
- $\frac{\lambda^d \log n}{n} \rightarrow 0$ and $\log \lambda \asymp \log B \asymp \log n$, so $\lambda \rightarrow \infty$ and $B \rightarrow \infty$

Definition (β -Hölder continuity)

With $\underline{\beta}$ the largest integer less than β , for all $x, x' \in [0, 1]^d$,

$$\max_{|\nu|=\underline{\beta}} |\partial^\nu g(x) - \partial^\nu g(x')| \lesssim \|x - x'\|_2^{\beta-\underline{\beta}}$$

Central limit theorem for Mondrian random forests

Theorem (Central limit theorem for Mondrian random forests)

$$\sqrt{\frac{n}{\lambda^d}} \left(\hat{\mu}(x) - \mathbb{E}[\hat{\mu}(x) \mid \mathbf{X}, \mathbf{T}] \right) \rightsquigarrow \mathcal{N}(0, \Sigma(x))$$

where

$$\Sigma(x) = \frac{\sigma^2(x)}{f(x)} \left(\frac{4 - 4 \log 2}{3} \right)^d$$

$$\hat{\mu}(x) - \mathbb{E}[\hat{\mu}(x) \mid \mathbf{X}, \mathbf{T}] = \frac{1}{B} \sum_{b=1}^B \frac{1}{N_b(x)} \sum_{i=1}^n \varepsilon_i \mathbb{I}\{X_i \in T_b(x)\}$$

- Essential that $B \rightarrow \infty$, or randomness persists in the limit
- No conditional independence as $N_b(x)$ depends on all X_i
- Replacing $N_b(x)$ by $nf(x)|T_b(x)|$ fails as $\mathbb{E} \left[\frac{1}{|T_b(x)|^2} \right] = \infty$
- Central limit theorems based on $2 + \delta$ moments inadequate

Central limit theorem for Mondrian random forests

$$\hat{\mu}(x) - \mathbb{E}[\hat{\mu}(x) \mid \mathbf{X}, \mathbf{T}] = \frac{1}{B} \sum_{b=1}^B \frac{1}{N_b(x)} \sum_{i=1}^n \varepsilon_i \mathbb{I}\{X_i \in T_b(x)\}$$

- Use a **martingale central limit theorem** (Hall and Heyde, 1980)
- Take the filtration $\mathcal{F}_{ni} = \sigma(\mathbf{X}, \mathbf{T}, \varepsilon_1, \dots, \varepsilon_i)$ and consider $\sum_{i=1}^n M_{ni}(x)$ with the martingale differences

$$M_{ni}(x) = \sqrt{\frac{n}{\lambda^d}} \frac{1}{B} \sum_{b=1}^B \frac{1}{N_b(x)} \varepsilon_i \mathbb{I}\{X_i \in T_b(x)\}$$

- Verify $\mathbb{E}[\max_{1 \leq i \leq n} M_{ni}(x)^2] \lesssim 1$ and $\sum_{i=1}^n M_{ni}(x)^2 \rightarrow_{\mathbb{P}} \Sigma(x)$
- Nonlinear structure handled by the Efron–Stein inequality

Bias of Mondrian random forests

Theorem (Bias of Mondrian random forests)

There exist $B_r(x)$ depending only on f and μ such that

$$\left| \mathbb{E}[\hat{\mu}(x) \mid \mathbf{X}, \mathbf{T}] - \mu(x) - \sum_{r=1}^{\lfloor \beta/2 \rfloor} \frac{B_r(x)}{\lambda^{2r}} \right| \lesssim_{\mathbb{P}} \frac{1}{\lambda^{\beta}} + \frac{1}{\lambda \sqrt{B}} + \frac{\log n}{\lambda} \sqrt{\frac{\lambda^d}{n}}$$

- We approximate the bias with a Taylor polynomial in $1/\lambda^2$
- If B does not diverge there is a **first-order bias** of size $1/\lambda$
- In large forests and with $\beta \geq 2$, leading bias is of size $1/\lambda^2$
- Setting $\lambda \asymp n^{\frac{1}{d+4}}$ and $B \gg n^{\frac{2}{d+4}}$ gives for $\beta \geq 2$

$$\left| \hat{\mu}(x) - \mu(x) \right| \lesssim_{\mathbb{P}} \underbrace{\sqrt{\frac{\lambda^d}{n}}}_{\text{Variance}} + \underbrace{\frac{1}{\lambda^2} + \frac{1}{\lambda \sqrt{B}}}_{\text{Bias}} \lesssim n^{-\frac{2}{d+4}}$$

Inference with Mondrian random forests

- Combine central limit theorem and bias bound for inference
- Bias is negligible if $\beta \geq 2$ and $\frac{1}{\lambda^2} + \frac{1}{\lambda\sqrt{B}} \ll \sqrt{\frac{\lambda^d}{n}}$
- We construct a variance estimator $\hat{\Sigma}(x) \rightarrow_{\mathbb{P}} \Sigma(x)$
- Let q_α be the $1 - \frac{\alpha}{2}$ quantile of $\mathcal{N}(0, 1)$

Theorem (Feasible confidence intervals)

With $\beta \geq 2$, if $\lambda \gg n^{\frac{1}{d+4}}$ and $B \gg n^{\frac{2}{d+4}}$ then

$$\mathbb{P} \left(\mu(x) \in \left[\hat{\mu}(x) \pm \sqrt{\frac{\lambda^d}{n}} \hat{\Sigma}(x)^{1/2} q_\alpha \right] \right) \rightarrow 1 - \alpha$$

Debiased Mondrian random forests

- Bias approximation with $\beta > 2$ for lifetimes λ and 2λ gives

$$\mathbb{E}[\hat{\mu}(x; \lambda) \mid \mathbf{X}, \mathbf{T}] \approx \mu(x) + \frac{B_1(x)}{\lambda^2} \quad (1)$$

$$\mathbb{E}[\hat{\mu}(x; 2\lambda) \mid \mathbf{X}, \mathbf{T}] \approx \mu(x) + \frac{B_1(x)}{4\lambda^2} \quad (2)$$

- Take a linear combination to annihilate the leading bias

$$\mathbb{E}\left[-\frac{1}{3}\hat{\mu}(x; \lambda) + \frac{4}{3}\hat{\mu}(x; 2\lambda) \mid \mathbf{X}, \mathbf{T}\right] \approx \mu(x) + 0$$

- Cancel all $J = \lfloor \beta/2 \rfloor$ bias terms to get the debiased estimator

$$\hat{\mu}_d(x) = \sum_{s=0}^J \omega_s \hat{\mu}(x; a_s \lambda)$$

- Here a_s are fixed, and ω_s solve the linear equations

$$\sum_{s=0}^J \omega_s = 1 \text{ and } \sum_{s=0}^J \omega_s a_s^{-2r} = 0 \text{ for } 1 \leq r \leq J$$

Results for debiased Mondrian random forests

Theorem (Improved bias bound)

$$|\mathbb{E}[\hat{\mu}_d(x) \mid \mathbf{X}, \mathbf{T}] - \mu(x)| \lesssim_{\mathbb{P}} \frac{1}{\lambda^\beta} + \frac{1}{\lambda\sqrt{B}} + \frac{\log n}{\lambda} \sqrt{\frac{\lambda^d}{n}}$$

Theorem (Central limit theorem with debiasing)

$$\sqrt{\frac{n}{\lambda^d}} \left(\hat{\mu}_d(x) - \mathbb{E}[\hat{\mu}_d(x) \mid \mathbf{X}, \mathbf{T}] \right) \rightsquigarrow \mathcal{N}(0, \Sigma_d(x))$$

Theorem (Feasible confidence intervals with debiasing)

If $\lambda \gg n^{\frac{1}{d+2\beta}}$ and $B \gg n^{\frac{2\beta-2}{d+2\beta}}$, with $\hat{\Sigma}_d(x)$ a variance estimator,

$$\mathbb{P} \left(\mu(x) \in \left[\hat{\mu}_d(x) \pm \sqrt{\frac{\lambda^d}{n}} \hat{\Sigma}_d(x)^{1/2} q_\alpha \right] \right) \rightarrow 1 - \alpha$$

Minimax optimality

Theorem (Minimaxity of debiased Mondrian random forests)

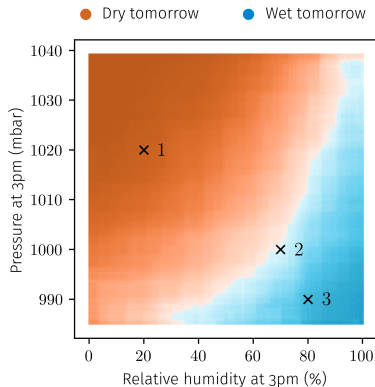
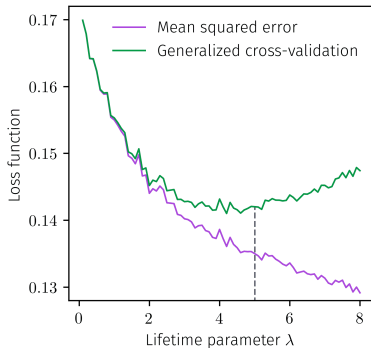
If $\lambda \asymp n^{\frac{1}{d+2\beta}}$ and $B \gtrsim n^{\frac{2\beta-2}{d+2\beta}}$, then

$$\mathbb{E} \left[(\hat{\mu}_d(x) - \mu(x))^2 \right]^{1/2} \lesssim \underbrace{\sqrt{\frac{\lambda^d}{n}}}_{\text{Variance}} + \underbrace{\frac{1}{\lambda^\beta} + \frac{1}{\lambda\sqrt{B}}}_{\text{Bias}} \lesssim n^{-\frac{\beta}{d+2\beta}}$$

| Estimator | Minimax condition |
|---------------------------------|-------------------------|
| Mondrian tree* | $\beta \in (0, 1]$ |
| Mondrian random forest* | $\beta \in (0, 2]$ |
| Debiased Mondrian random forest | $\beta \in (0, \infty)$ |

*Established by Mourtada et al. (2020)

Example: weather forecasting in Australia



| Point | Humidity | Pressure | Chance of rain | 95% confidence interval |
|-------|----------|-----------|----------------|-------------------------|
| 1 | 20% | 1020 mbar | 4.3% | 4.1% – 4.6% |
| 2 | 70% | 1000 mbar | 53.0% | 52.0% – 54.0% |
| 3 | 80% | 990 mbar | 77.5% | 74.4% – 80.6% |

Conclusion and ongoing work

Contributions to studying the Mondrian random forest estimator

- Provided a novel **central limit theorem** allowing fully feasible **statistical inference** via variance estimation
- Presented a new **debiasing procedure** allowing for inference under milder conditions
- Demonstrated **minimax optimality** for arbitrary dimension and smoothness, the first result for any forest estimator

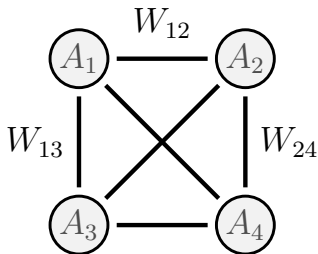
Ongoing and future work

- Heterogeneous and data-dependent lifetimes $\hat{\lambda}_j$ or $\hat{\lambda}(x)$
- Improved estimation with additive models or local regression
- Uniform inference via strong approximation

Uniform Inference for Kernel Density Estimators with Dyadic Data

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Dyadic data



Example of dyadic data

- A_i is GDP of country i
- W_{ij} is value of trade $i \leftrightarrow j$

- W_{ij} random variables associated with edges of a network
- Write $W_{ij} = W(A_i, A_j, V_{ij})$ by Aldous–Hoover with A_i latent node variables and V_{ij} latent idiosyncratic shocks
- Unknown Lebesgue density $f(w)$ estimated by $\hat{f}(w)$ on \mathcal{W}
- We provide the **minimax-optimal estimation** rate for $\hat{f}(w)$
- **Uniform inference** on $f(w)$ by strong approximation

Dyadic kernel density estimation

Dyadic kernel density estimator

$$\hat{f}(w) = \frac{2}{n(n-1)} \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{1}{h} K\left(\frac{W_{ij} - w}{h}\right)$$

- Bandwidth h controls bias-variance tradeoff
- Higher-order boundary kernels K improve bias properties
- We analyze the U-statistic Hoeffding-type decomposition

$$\hat{f}(w) - f(w) = \underbrace{B(w)}_{\text{smoothing bias}} + \underbrace{L(w)}_{\text{i.i.d. average}} + \underbrace{E(w)}_{\text{conditional i.n.i.d. average}} + \underbrace{Q(w)}_{\text{U-statistic}}$$

- $L(w)$, $E(w)$ and $Q(w)$ are mean-zero and orthogonal

Minimax-optimal uniform dyadic estimation

- Using an order p boundary kernel, if f is β -Hölder then

$$\begin{aligned} \sup_{w \in \mathcal{W}} |B(w)| &\lesssim h^{p \wedge \beta} & \mathbb{E} \left[\sup_{w \in \mathcal{W}} |L(w)| \right] &\lesssim \frac{D}{\sqrt{n}} \\ \mathbb{E} \left[\sup_{w \in \mathcal{W}} |E(w)| \right] &\lesssim \sqrt{\frac{\log n}{n^2 h}} & \mathbb{E} \left[\sup_{w \in \mathcal{W}} |Q(w)| \right] &\lesssim \frac{1}{n} \end{aligned}$$

- Optimize the bound with $p \geq \beta$ and $h \asymp \left(\frac{\log n}{n^2} \right)^{\frac{1}{2\beta+1}}$
- Then we attain the minimax dyadic estimation rate

Theorem (Minimax-optimal uniform dyadic estimation)

$$\sup_{w \in \mathcal{W}} |\hat{f}(w) - f(w)| \lesssim_{\mathbb{P}} \underbrace{h^{p \wedge \beta}}_{B(w)} + \underbrace{\frac{D}{\sqrt{n}}}_{L(w)} + \underbrace{\sqrt{\frac{\log n}{n^2 h}}}_{E(w)} \lesssim \frac{D}{\sqrt{n}} + \left(\frac{\log n}{n^2} \right)^{\frac{\beta}{2\beta+1}}$$

Dyadic strong approximation construction

- Need distributional approximations for both $L(w)$ and $E(w)$
- No uniform central limit theorem as $E(w)$ is not tight
- For the i.i.d. sum $L(w)$, use KMT coupling (Komlós et al., 1975)

$$\sup_{w \in \mathcal{W}} \left| \sqrt{n} L(w) - Z_L(w) \right| \lesssim_{\mathbb{P}} \frac{D \log n}{\sqrt{n}}$$

- $E(w)$ is a sum of $\binom{n}{2}$ conditionally independent but not i.i.d. terms so use a version of Yurinskii's coupling (Yurinskii, 1978)

$$\sup_{w \in \mathcal{W}} \left| \sqrt{n^2 h} E(w) - Z_E(w) \right| \lesssim_{\mathbb{P}} \frac{(\log n)^{3/8}}{n^{1/4} h^{3/8}}$$

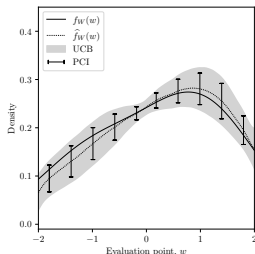
- Combine these with the uniform bounds on $B(w)$ and $Q(w)$

Dyadic uniform inference via strong approximation

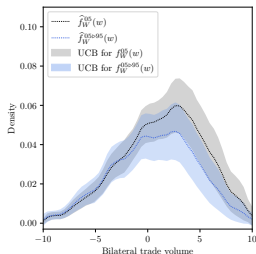
Theorem (Strong approximation and uniform confidence bands)

$$\sup_{w \in \mathcal{W}} \left| \frac{\hat{f}(w) - f(w)}{\sqrt{\text{Var}[\hat{f}(w)]}} - Z(w) \right| \rightarrow_{\mathbb{P}} 0, \quad Z(w) \text{ Gaussian process}$$

$$\mathbb{P} \left(f(w) \in \left[\hat{f}(w) \pm \hat{q}_{1-\alpha} \sqrt{\widehat{\text{Var}}[\hat{f}(w)]} \right] \forall w \in \mathcal{W} \right) \rightarrow 1 - \alpha$$

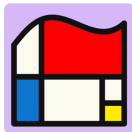


(a) Synthetic data with degeneracy



(b) Counterfactual trade analysis

Questions



Cattaneo, M. D., Klusowski, J. M., and Underwood, W. G. (2023)
Inference with Mondrian random forests

`arXiv:2310.09702`

`github.com/wgunderwood/MondrianForests.jl`



Cattaneo, M. D., Feng, Y., and Underwood, W. G. (2024).
Uniform inference for kernel density estimators with dyadic data

`arXiv:2201.05967`

`github.com/wgunderwood/DyadicKDE.jl`

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