Analysis of purely random forests

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Colloquium, Department of Statistics and Actuarial Science,
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References: arXiv:1407.3939 (v2 upcoming!)
arXiv:1604.01515

Outline

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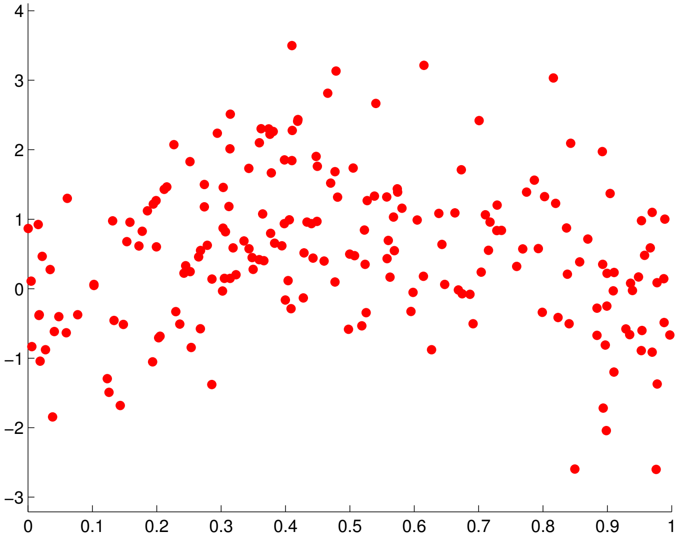
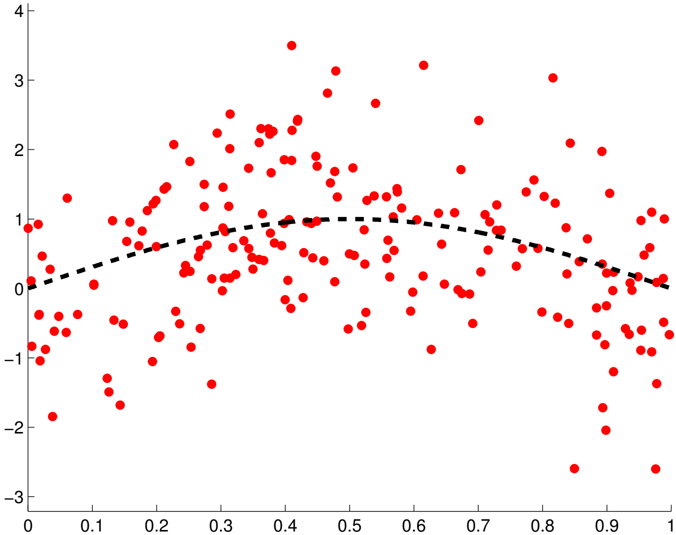
Regression: data $(X_1, Y_1), \ldots, (X_n, Y_n)$



Goal: find the signal (denoising)



Regression

- Data D_n : $(X_1, Y_1), \ldots, (X_n, Y_n) \in \mathbb{R}^p \times \mathbb{R}$ (i.i.d. $\sim P$)

$$Y_i = s^\star(X_i) + \varepsilon_i$$

with $s^\star(X) = \mathbb{E}[Y \mid X]$ (regression function).

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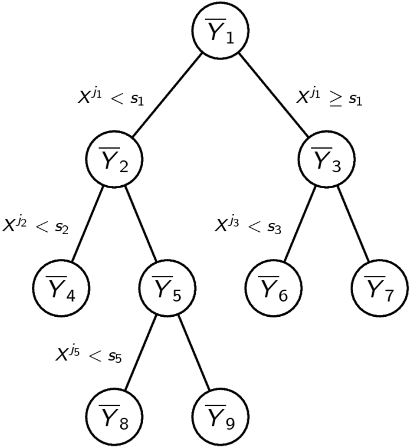
with $s^\star(X) = \mathbb{E}[Y \mid X]$ (regression function).

- Goal: learn f measurable function $\mathcal{X} \to \mathbb{R}$ s.t. the quadratic risk

$$\mathbb{E}_{(X,Y)\sim P}\left[\left(f(X) - s^\star(X)\right)^2\right]$$

is minimal.

Regression tree (Breiman et al, 1984)



Tree: piecewise-constant predictor, obtained by partitioning recursively $\mathbb{R}^p$.

Restriction: splits parallel to the axes.

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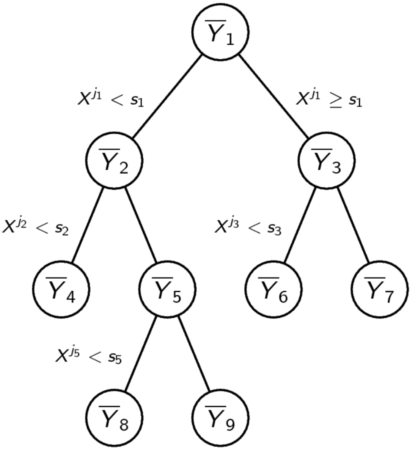
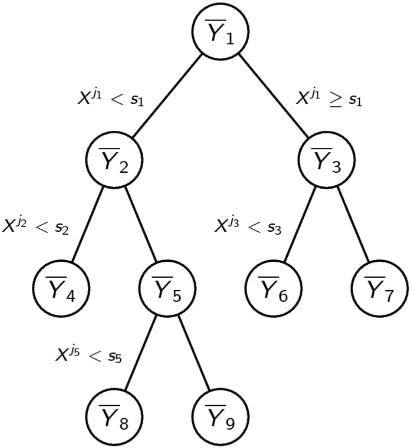


Tree: piecewise-constant predictor, obtained by partitioning recursively $\mathbb{R}^p$.
Restriction: splits parallel to the axes.

1. Choice of the partition $\mathbb{U}$ (tree structure)
   Usually, at each step, one looks for the best split of the data into two groups (minimize sum of within-group variances) D_n.

Regression tree (Breiman et al, 1984)



Tree: piecewise-constant predictor, obtained by partitioning recursively $\mathbb{R}^p$.
Restriction: splits parallel to the axes.

1. Choice of the partition $\mathbb{U}$ (tree structure)
2. For each $\lambda \in \mathbb{U}$ (tree leaf), choice of the estimation $\widehat{\beta}_\lambda$ of $s^\star(x)$ when $x \in \lambda$.
   Here, $\widehat{\beta}_\lambda = \overline{Y}_\lambda$ average of the $(Y_i)_{X_i \in \lambda}$.

Random forest (Breiman, 2001)

Definition (Random forest (Breiman, 2001))

$\left\{ \widehat{s}_{\Theta_j}, 1 \leqslant j \leqslant q \right\}$ collection of tree predictors, $(\Theta_j)_{1 \leqslant j \leqslant q}$ i.i.d. r.v. independent from D_n.

Random forest predictor $\widehat{s}$ obtained by aggregating the tree collection.

$$\widehat{s}(x) = \frac{1}{q} \sum_{j=1}^{q} \widehat{s}_{\Theta_j}(x)$$

- ensemble method (Dietterich, 1999, 2000)
- powerful statistical learning algorithm, for both classification and regression.

Bagging (“bootstrap aggregating”)

- Bootstrap (Efron, 1979): draw n i.i.d. r.v., uniform over $\{(X_i, Y_i) \,/\, i = 1, \ldots, n\}$ (sampling with replacement) $\Rightarrow$ resample D_n^b
- Bootstrapping a tree: $\widehat{s}^b_{\mathrm{tree}} = \widehat{s}_{\mathrm{tree}}(D_n^b)$
- Bagging: bootstrap (q independent resamples) then aggregation

$$\widehat{s}_{\mathrm{bagging}}(x) = \frac{1}{q} \sum_{j=1}^{q} \widehat{s}^{b,j}_{\mathrm{tree}}(x)$$

Random Forest-Random Inputs (Breiman, 2001)

Definition (RI tree)

In a RI tree, at each node, `mtry` variables are randomly chosen. Then, the best cut direction is chosen only among the chosen variables.

Definition (Random forest RI)

A random forest RI (RF-RI) is obtained by aggregating RI trees built on independent bootstrap resamples.

RF-RI $\Leftrightarrow$ bagging on RI trees

Random Forest-Random Inputs

$$
\begin{tikzcd}
 & & D_n \arrow[dll, "\text{Bootstrap}"'] \arrow[dl] \arrow[drr] & & \\
D_n^{b,1} \arrow[dd, "\text{RI tree}"'] & D_n^{b,2} \arrow[dd] & \ldots & \ldots & D_n^{b,q} \arrow[dd] \\
 & & \ldots & \ldots & \\
\widehat{s}_{\Theta_1} \arrow[drr, "\text{Aggregation}"'] & \widehat{s}_{\Theta_2} \arrow[dr] & \ldots & \ldots & \widehat{s}_{\Theta_q} \arrow[dll] \\
 & & \widehat{s}_{\mathrm{RF-RI}} & &
\end{tikzcd}
$$

Theoretical results on RF-RI

- Few theoretical results on Breiman's original RF-RI, despite their excellent numerical performance (eg, Fernández-Delgado et al, 2014)
- Most results:
  - focus on a specific part of the algorithm (resampling, split criterion),
  - modify the algorithm (eg, subsampling instead of resampling)
  - make strong assumptions on $s^\star$
- References (see survey paper by Biau and Scornet, 2016): Scornet, Biau & Vert (2015), Mentch & Hooker (2016), Wager & Athey (2018), Genuer & Poggi (2019), ...

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$\Rightarrow$ Here, we consider simplified RF models, for which a precise analysis is possible: purely random forests

Outline

Purely random forests

Definition (Purely random tree)

$$\widehat{s}_{\mathbb{U}}(x) = \sum_{\lambda \in \mathbb{U}} \overline{Y_\lambda}(D_n) \mathbb{1}_{x \in \lambda}$$

where $\overline{Y_\lambda}(D_n)$ is the average of $(Y_i)_{X_i \in \lambda \, , \, (X_i, Y_i) \in D_n}$ and the partition $\mathbb{U}$ is independent from D_n.

Definition (Purely random forest)

$$\widehat{s}(x) = \frac{1}{q} \sum_{j=1}^{q} \widehat{s}_{\mathbb{U}^j}(x)$$

with $\mathbb{U}^1, \ldots, \mathbb{U}^q$ i.i.d., independent from D_n.

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with $\mathbb{U}^1, \ldots, \mathbb{U}^q$ i.i.d., independent from D_n.

Example ("hold-out RF" model): use some extra data D_n' for building the trees: $\mathbb{U}^j = \mathbb{U}_{\mathrm{RI}}(D_n'^{\star j})$) (can be done by splitting the sample into two subsamples D_n and D_n').

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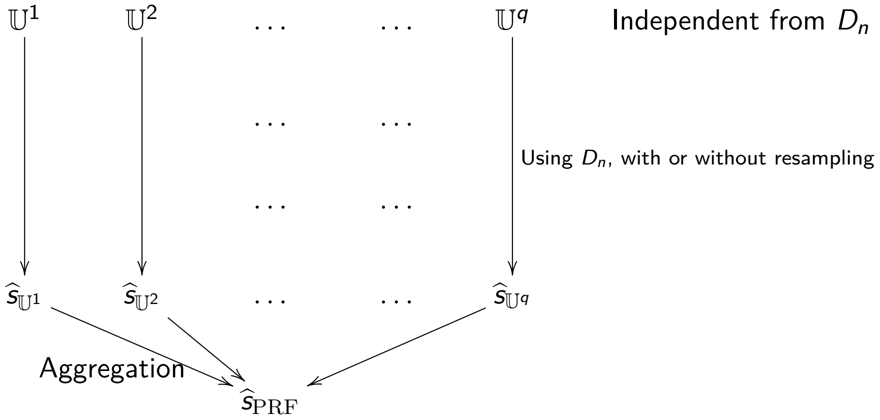
Example ("hold-out RF" model): use some extra data D'_n for building the trees: $\mathbb{U}^j = \mathbb{U}_{\mathrm{RI}}(D_n^{\prime\star j})$ (can be done by splitting the sample into two subsamples D_n and D'_n).

⚠ From now on, D_n is the sample used for computing $(\overline{Y_\lambda}(D_n))_{\lambda \in \mathbb{U}}$, and we assume its size is n.

Purely random forests



Purely random forests: theory

- Consistency: Biau, Devroye & Lugosi (2008), Scornet (2014)
- Rates of convergence: Breiman (2004), Biau (2012), Klusowski (2018), Duroux & Scornet (2018), Mourtada, Gaiffas & Scornet (2017 & 2020)
- Some adaptivity to dimension reduction (sparse framework): Biau (2012), Klusowski (2018)
- Forests decrease the estimation error (Biau, 2012; Genuer, 2012)

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$\Rightarrow$ What about approximation error?
Almost the same for a forest and a tree?

Risk of a single tree (regressogram)

Given the partition $\mathbb{U}$, regressogram estimator

$$\widehat{s}_{\mathbb{U}}(x) := \sum_{\lambda \in \mathbb{U}} \overline{Y_\lambda} \mathbb{1}_{x \in \lambda}$$

where $\overline{Y_\lambda}$ is the average of $(Y_i)_{X_i \in \lambda}$.

$$\widehat{s}_{\mathbb{U}} \in \operatorname*{argmin}_{f \in S_{\mathbb{U}}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \bigl(Y_i - f(X_i) \bigr)^2 \right\}$$

where $S_{\mathbb{U}}$ is the vector space of functions which are constant over each $\lambda \in \mathbb{U}$.

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Define:

$$\tilde{s}_{\mathbb{U}}(x) := \sum_{\lambda \in \mathbb{U}} \beta_\lambda \mathbb{1}_{x \in \lambda} \quad \text{where } \beta_\lambda := \mathbb{E}[s^\star(X) \,|\, X \in \lambda] \ .$$

$\Rightarrow \tilde{s}_{\mathbb{U}} \in \operatorname{argmin}_{f \in S_{\mathbb{U}}} \mathbb{E}\left[\bigl(f(X) - s^\star(X) \bigr)^2 \right]$ and $\tilde{s}_{\mathbb{U}}(x) = \mathbb{E}\left[\widehat{s}_{\mathbb{U}}(x) \,|\, \mathbb{U} \right]$

Risk decomposition: single tree

$$
\begin{aligned}
&\mathbb{E}\left[\left(s^\star(X) - \widehat{s}_{\mathbb{U}}(X)\right)^2\right] \\
&= \mathbb{E}\left[\left(s^\star(X) - \tilde{s}_{\mathbb{U}}(X)\right)^2\right] + \mathbb{E}\left[\left(\tilde{s}_{\mathbb{U}}(X) - \widehat{s}_{\mathbb{U}}(X)\right)^2\right] \\
&= \text{Approximation error} + \text{Estimation error}
\end{aligned}
$$

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If $s^\star$ is smooth, $X \sim \mathcal{U}([0,1]^p)$ and $\mathbb{U}$ regular partition into D pieces, then

$$\mathbb{E}\Big[\big(s^\star(X) - \tilde{s}_{\mathbb{U}}(X)\big)^2\Big] \propto \frac{1}{D^{2/p}}$$

Risk decomposition: single tree

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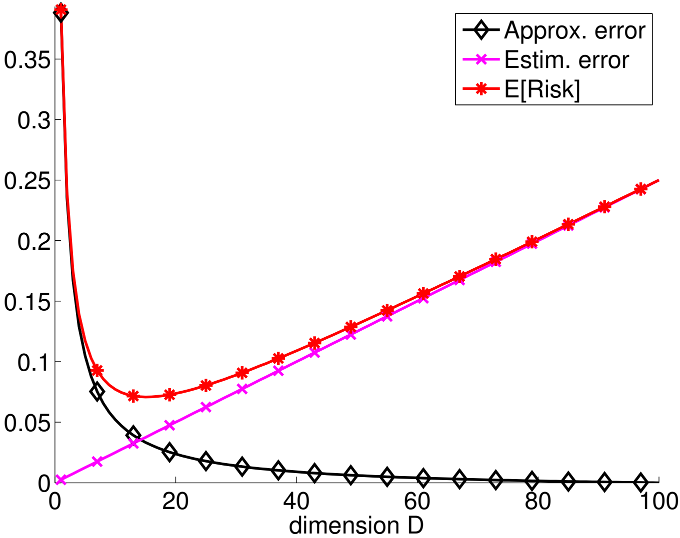
If $\operatorname{var}(Y \mid X) = \sigma^2$ does not depend on X, then

$$\mathbb{E}\Big[\big(\tilde{s}_{\mathbb{U}}(X) - \widehat{s}_{\mathbb{U}}(X)\big)^2\Big] \approx \frac{\sigma^2 D}{n}$$

Approximation and estimation errors, $p = 1$



Risk decomposition: purely random forest

$(\mathbb{U}^j)_{1 \leqslant j \leqslant q}$ finite partitions, i.i.d. $\sim \mathcal{U}$

Estimator (forest): $$\widehat{s}_{\mathbb{U}^{1 \cdots q}}(x) := \frac{1}{q} \sum_{j=1}^{q} \widehat{s}_{\mathbb{U}^j}(x)$$

Ideal forest: $$\tilde{s}_{\mathbb{U}^{1 \cdots q}}(x) := \frac{1}{q} \sum_{j=1}^{q} \tilde{s}_{\mathbb{U}^j}(x) = \mathbb{E}\left[\widehat{s}_{\mathbb{U}^{1 \cdots q}}(x) \,\middle|\, \mathbb{U}^{1 \cdots q}\right]$$

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Quadratic risk decomposition (given $X = x$)

$$\mathbb{E}\left[\left(s^\star(x) - \widehat{s}_{\mathbb{U}^{1 \cdots q}}(x)\right)^2\right] = \mathbb{E}\left[\left(s^\star(x) - \tilde{s}_{\mathbb{U}^{1 \cdots q}}(x)\right)^2\right] + \mathbb{E}\left[\left(\tilde{s}_{\mathbb{U}^{1 \cdots q}}(x) - \widehat{s}_{\mathbb{U}^{1 \cdots q}}(x)\right)^2\right] + \delta_{\mathbb{U}^{1 \cdots q}}(x)$$

Approximation error: $$\mathcal{B}_{\mathcal{U},q}(x) := \mathbb{E}\left[\left(s^\star(x) - \tilde{s}_{\mathbb{U}^{1 \cdots q}}(x)\right)^2\right]$$

Approximation error decomposition (given $X = x$)

$$\mathcal{B}_{\mathcal{U},q}(x) = \mathcal{B}_{\mathcal{U},\infty}(x) + \frac{\mathcal{V}_{\mathcal{U}}(x)}{q}$$

$$\text{where} \quad \mathcal{B}_{\mathcal{U},\infty}(x) := \Big(\mathbb{E}\big[s^{\star}(x) - \tilde{s}_{\mathbb{U}}(x)\big]\Big)^2$$

$$\text{and} \quad \mathcal{V}_{\mathcal{U}}(x) := \mathrm{var}\big(\tilde{s}_{\mathbb{U}}(x)\big)$$

$\mathcal{B}_{\mathcal{U},\infty}(x)$ is the approx. error of the infinite forest: $\tilde{s}_{\mathbb{U},\infty}(x) := \mathbb{E}\big[\tilde{s}_{\mathbb{U}}(x)\big]$

to be compared with the approximation error of a single tree

$$\mathcal{B}_{\mathcal{U},1}(x) = \mathcal{B}_{\mathcal{U},\infty}(x) + \mathcal{V}_{\mathcal{U}}(x)$$

Outline

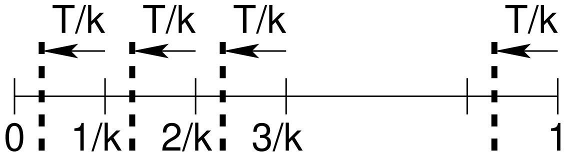
Toy forests

Assume: $\mathcal{X} = [0,1)^p$ and X uniform over $[0,1)^p$

If $p = 1$, $\mathbb{U} \sim \mathcal{U}_k^{\mathtt{toy}}$ defined by:

$$\mathbb{U} = \left\{ \left[0, \frac{1-T}{k}\right) , \left[\frac{1-T}{k}, \frac{2-T}{k}\right) , \ldots , \left[\frac{k-T}{k}, 1\right) \right\}$$

where T has uniform distribution over $[0,1]$.



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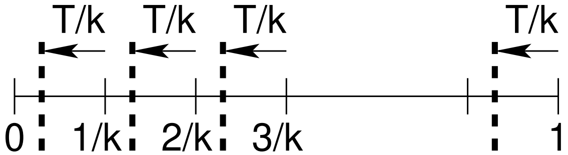
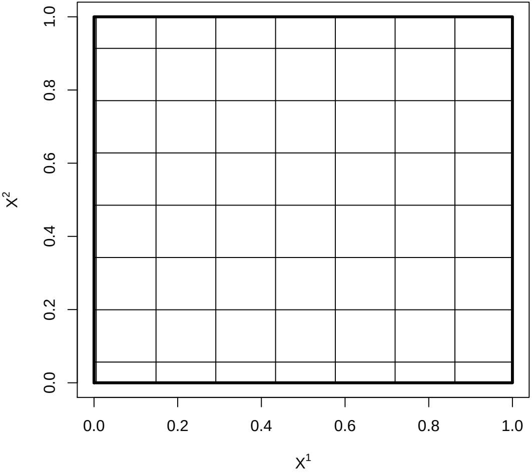


If $p > 1$, T_j for each coordinate $j = 1, \ldots, p$, independent

Toy forest, $p = 2$: example



Interpretation of the ideal infinite forest ($p = 1$)

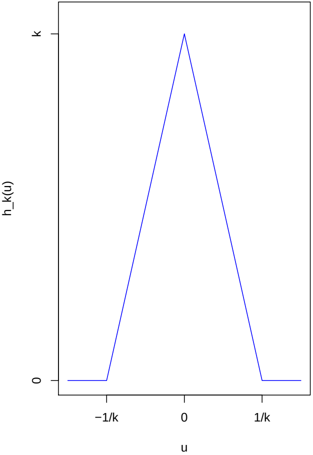
Proposition (A. & Genuer, 2014–2020)

For any $x \in \left[\frac{1}{k}, 1 - \frac{1}{k}\right]$, the ideal infinite forest at x satisfies:

$$\tilde{s}_{\mathbb{U},\infty}(x) = (s^\star * h_k)(x) = \int_0^1 s^\star(t) h_k(x - t) \, \mathrm{d}t$$

where

$$h_k(u) = \begin{cases} k(1 - ku) & \text{if } 0 \leqslant u \leqslant \frac{1}{k} \\ k(1 + ku) & \text{if } -\frac{1}{k} \leqslant u \leqslant 0 \\ 0 & \text{if } |u| \geqslant \frac{1}{k} \end{cases}$$



Interpretation of the ideal infinite forest ($p = 1$): proof

$I_{\mathbb{U}}(x) :=$ the interval of $\mathbb{U}$ to which x belongs

$$\tilde{s}_{\mathbb{U}}(x) = \frac{1}{|I_{\mathbb{U}}(x)|} \int_{I_{\mathbb{U}}(x)} s^{\star}(t) \, \mathrm{d}t$$

If $x \in \left[\frac{1}{k}, 1 - \frac{1}{k}\right]$, $\quad I_{\mathbb{U}}(x) = \left[x + \frac{V_x - 1}{k}, x + \frac{V_x}{k}\right)$

where V_x has uniform distribution over $[0, 1]$.

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where V_x has uniform distribution over $[0, 1]$.

$$\begin{aligned} \tilde{s}_{\mathbb{U},\infty}(x) &= \mathbb{E}_{\mathbb{U}}\left[\tilde{s}_{\mathbb{U}}(x)\right] \\ &= k \int_0^1 s^{\star}(t) \, \mathbb{P}\left(x + \frac{V_x - 1}{k} \leqslant t < x + \frac{V_x}{k}\right) \mathrm{d}t \\ &= k \int_0^1 s^{\star}(t) \underbrace{\mathbb{P}\left(k(t-x) < V_x \leqslant k(t-x) + 1\right)}_{= h_k(x-t) \text{ if } 1/k \leqslant x \leqslant 1 - 1/k} \mathrm{d}t \end{aligned}$$

Analysis of the approximation error, $p = 1$, $x \in \left[\frac{1}{k}, 1 - \frac{1}{k}\right]$

(H2) $s^\star$ twice differentiable over $(0,1)$ and $s^{\star\prime\prime}$ bounded

Taylor-Lagrange formula: for every $t \in (0,1)$, some $c_{t,x} \in (0,1)$ exists such that

$$s^\star(t) - s^\star(x) = s^{\star\prime}(x)(t-x) + \frac{1}{2} s^{\star\prime\prime}(c_{t,x})(t-x)^2$$

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Therefore,

$$\begin{aligned} \tilde{s}_{\mathbb{U}}(x) - s^\star(x) &= k \int_{x + \frac{V_x - 1}{k}}^{x + \frac{V_x}{k}} \left(s^\star(t) - s^\star(x)\right) \mathrm{d}t \\ &= k\, s^{\star\prime}(x) \int_{x + \frac{V_x - 1}{k}}^{x + \frac{V_x}{k}} (t - x)\, \mathrm{d}t + R_1(x) \\ &= \frac{s^{\star\prime}(x)}{k} \left(V_x - \frac{1}{2} \right) + R_1(x) \end{aligned}$$

where $R_1(x) = \frac{k}{2} \int_{x + \frac{V_x - 1}{k}}^{x + \frac{V_x}{k}} s^{\star\prime\prime}(c_{t,x})(t - x)^2 \, \mathrm{d}t$.

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$$\tilde{s}_{\mathbb{U}}(x) - s^\star(x) = \frac{s^{\star\prime}(x)}{k}\left(V_x - \frac{1}{2}\right) + R_1(x)$$

where $R_1(x) = \frac{k}{2}\int_{x+\frac{V_x-1}{k}}^{x+\frac{V_x}{k}} s^{\star\prime\prime}(c_{t,x})(t-x)^2 \,\mathrm{d}t$.

Hence,

$$\mathcal{B}_{\mathcal{U}_k^{\mathrm{toy}},\infty}(x) = \Bigl(\mathbb{E}_{\mathbb{U}}\left[s^\star(x) - \tilde{s}_{\mathbb{U}}(x)\right]\Bigr)^2 = \Bigl(\mathbb{E}_{\mathbb{U}}\left[R_1(x)\right]\Bigr)^2 \leqslant \frac{\square}{k^4}$$

and

$$\mathcal{V}_{\mathcal{U}_k^{\mathrm{toy}}}(x) = \operatorname{var}\left(\frac{s^{\star\prime}(x)}{k}\left(V_x - \frac{1}{2}\right) + R_1(x)\right) \underset{k\to+\infty}{\sim} \frac{s^{\star\prime}(x)^2 \operatorname{var}(V_x)}{k^2} .$$

Analysis of the approximation error, $p \geqslant 1$

(Hθ) $s^\star \in \mathcal{C}^{1,(\theta-1)}(\mathcal{X})$ Hölder space, $\theta \in [1,2]$

$$\mathcal{B}_{\mathcal{U}_k^{\mathtt{toy}},\infty}(x) = \Bigl(\mathbb{E}_{\mathbb{U}} \bigl[s^\star(x) - \tilde{s}_{\mathbb{U}}(x) \bigr] \Bigr)^2 \leqslant \frac{\square}{k^{2\theta/p}} \qquad \mathcal{V}_{\mathcal{U}_k^{\mathtt{toy}}}(x) \underset{k \to +\infty}{\sim} \frac{\square}{k^{2/p}}$$

Proposition (A. & Genuer, 2014–2020)

Assuming (Hθ), $\theta \in [1,2]$, $\forall x \in \bigl[\frac{1}{k}, 1-\frac{1}{k}\bigr]^p$,

$$\mathcal{B}_{\mathcal{U}_k^{\mathtt{toy}},1}(x) \underset{k \to +\infty}{\sim} \frac{\square}{k^{2/p}} \qquad \mathcal{B}_{\mathcal{U}_k^{\mathtt{toy}},\infty}(x) \leqslant \frac{\square}{k^{2\theta/p}}$$

$$\int_{[\frac{1}{k},1-\frac{1}{k}]^p} \mathcal{B}_{\mathcal{U}_k^{\mathtt{toy}},1}(x)\,\mathrm{d}x \underset{k \to +\infty}{\sim} \frac{\square}{k^{2/p}} \qquad \int_{[\frac{1}{k},1-\frac{1}{k}]^p} \mathcal{B}_{\mathcal{U}_k^{\mathtt{toy}},\infty}(x)\,\mathrm{d}x \leqslant \frac{\square}{k^{2\theta/p}}$$

Rate $k^{-4/p}$ is tight assuming θ-Hölder smoothness, $\theta > 2$.

Estimation error

General fact (Jensen's inequality):

$$\mathbb{E}\left[\left(\tilde{s}_{\mathbb{U},\infty}(X) - \widehat{s}_{\mathbb{U},\infty}(X)\right)^2\right] \leqslant \mathbb{E}\left[\left(\tilde{s}_{\mathbb{U}}(X) - \widehat{s}_{\mathbb{U}}(X)\right)^2\right]$$

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For the toy forest, without any resampling for computing labels and assuming that $\mathrm{var}(Y|X) = \sigma^2$:

$$\mathbb{E}\left[\left(\tilde{s}_{\mathbb{U}}(X) - \widehat{s}_{\mathbb{U}}(X)\right)^2\right] \approx \frac{\sigma^2 k}{n}$$

$$\mathbb{E}\left[\left(\tilde{s}_{\mathbb{U},\infty}(X) - \widehat{s}_{\mathbb{U},\infty}(X)\right)^2\right] \approx \frac{2}{3}\frac{\sigma^2 k}{n}$$

(A. & Genuer, 2016)

Summary: risk analysis

	Single tree	Infinite forest
	$(q=1)$	$(q=\infty)$

$$\mathbb{E}\left[\left(s^\star(x) - \widehat{s}_{\mathbb{U}^{1\cdots q}}(x)\right)^2\right] \approx \frac{c_1(s^\star, x)}{k^{2/p}} + \frac{\sigma^2 k}{n} \qquad \leqslant \frac{c'_\theta(s^\star, x)}{k^{2\theta/p}} + \frac{2\sigma^2 k}{3n}$$

where $\qquad c_1(s^\star, x) = \frac{s^{\star\prime}(x)^2}{12}$.

Assumptions:

- $x \in (0,1)^p$ far from boundary
- (Hθ) $s^\star \in \mathcal{C}^{1,(\theta-1)}(\mathcal{X})$, $\theta \in [1,2]$
- X uniform over $[0,1)^p$
- $\operatorname{var}(Y|X) = \sigma^2$
- no resampling for computing labels

Rates of convergence

Corollary: risk convergence rates (far from boundaries, with $k = k_n^\star$ optimal), under (Hθ), $\theta \in [1, 2]$:

$$\text{Tree risk} \geqslant \square \, n^{-2/(2+p)} \qquad \text{if } s^\star \text{ not constant, } \theta > 1$$

$$\text{Infinite forest risk} \leqslant \square \, n^{-2\theta/(2\theta+p)} \qquad \Rightarrow \qquad \text{minimax } \mathcal{C}^\theta, \theta \in [1, 2]$$

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Remarks:

- $q \geqslant \square\, (k_n^\star)^2$ is sufficient to get an "infinite" forest
- with subsampling a out of n for computing labels: estimation error of a single tree $\frac{\sigma^2 k}{a}$ instead of $\frac{\sigma^2 k}{n}$; no change for infinite forest

Outline

Definition (Biau, 2012)

Split D_n into D_{n_1} and D_{n_2}

$\mathbb{U}^1$ $\quad$ $\mathbb{U}^2$ $\quad \ldots \quad$ $\mathbb{U}^q$ $\qquad$ RI partitions, using D_{n_1}

$\ldots$

$\ldots$ $\qquad$ Using D_{n_2}, no resampling here

$\ldots$

$\widehat{s}_{\mathbb{U}^1}$ $\quad$ $\widehat{s}_{\mathbb{U}^2}$ $\quad \ldots \quad$ $\widehat{s}_{\mathbb{U}^q}$

Aggregation

$\widehat{s}_{\mathrm{HO-RF}}$

$\Rightarrow$ purely random forest

closely related to double-sample trees (Wager & Athey, 2018)

Numerical experiments: framework

- Data generation:
  $X_i \sim \mathcal{U}([0,1]^p) \qquad Y_i = s^\star(X_i) + \varepsilon_i$
  $\varepsilon_i \sim \mathcal{N}(0, \sigma^2) \qquad \sigma^2 = 1/16$

$$s^\star : \mathbf{x} \in [0,1]^p \mapsto \frac{\mathbf{1}}{\mathbf{10}} \times \left[10 \sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10 x_4 + 5 x_5 \right] .$$

- Data split: $n_1 = 1\,280 \qquad n_2 = 25\,600$
- Forests definition:
  $\texttt{nodesize} = 1$
  $k \in \{2^5, 2^6, 2^7, 2^8, 2^9\}$
  "Large" forests are made of $q = k$ trees.
- Compute integrated approximation/estimation errors

Numerical experiments: results ($p = 5$)

	Single tree	Large forest
No bootstrap $\mathtt{mtry} = p$	$\frac{0.13}{k^{0.17}} + \frac{1.04\sigma^2 k}{n_2}$	$\frac{0.13}{k^{0.17}} + \frac{1.04\sigma^2 k}{n_2}$
Bootstrap $\mathtt{mtry} = p$	$\frac{0.14}{k^{0.17}} + \frac{1.06\sigma^2 k}{n_2}$	$\frac{0.15}{k^{0.29}} + \frac{0.08\sigma^2 k}{n_2}$
No bootstrap $\mathtt{mtry} = \lfloor p/3 \rfloor$	$\frac{0.23}{k^{0.19}} + \frac{1.01\sigma^2 k}{n_2}$	$\frac{0.06}{k^{0.31}} + \frac{0.06\sigma^2 k}{n_2}$
Bootstrap $\mathtt{mtry} = \lfloor p/3 \rfloor$	$\frac{0.25}{k^{0.20}} + \frac{1.02\sigma^2 k}{n_2}$	$\frac{0.06}{k^{0.34}} + \frac{0.05\sigma^2 k}{n_2}$

$$\frac{2}{2+p} \approx 0.286 \qquad \frac{4}{4+p} \approx 0.444$$

Numerical experiments: results ($p = 10$)

	Single tree	Large forest
No bootstrap $\mathtt{mtry} = p$	$\frac{0.11}{k^{0.12}} + \frac{1.03\sigma^2 k}{n_2}$	$\frac{0.11}{k^{0.12}} + \frac{1.03\sigma^2 k}{n_2}$
Bootstrap $\mathtt{mtry} = p$	$\frac{0.11}{k^{0.11}} + \frac{1.05\sigma^2 k}{n_2}$	$\frac{0.10}{k^{0.19}} + \frac{0.04\sigma^2 k}{n_2}$
No bootstrap $\mathtt{mtry} = \lfloor p/3 \rfloor$	$\frac{0.21}{k^{0.18}} + \frac{1.08\sigma^2 k}{n_2}$	$\frac{0.08}{k^{0.25}} + \frac{0.04\sigma^2 k}{n_2}$
Bootstrap $\mathtt{mtry} = \lfloor p/3 \rfloor$	$\frac{0.20}{k^{0.16}} + \frac{1.05\sigma^2 k}{n_2}$	$\frac{0.07}{k^{0.26}} + \frac{0.03\sigma^2 k}{n_2}$

$$\frac{2}{2+p} \approx 0.167 \qquad \frac{4}{4+p} \approx 0.286$$

Conclusion

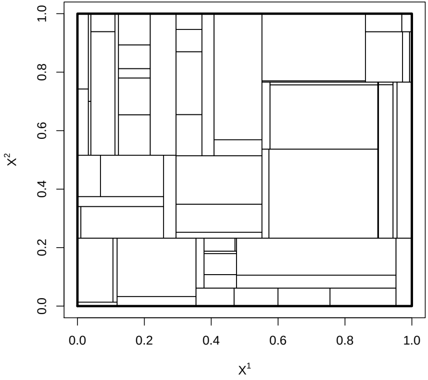
- Forests improve the order of magnitude of the approximation error, compared to a single tree
- Estimation error seems to change only by a constant factor (at least for toy forests);
  not contradictory with literature: here, we fix k; different picture if `nodesize` is fixed (+subsampling)

Conclusion

- Forests improve the order of magnitude of the approximation error, compared to a single tree
- Estimation error seems to change only by a constant factor (at least for toy forests);
  not contradictory with literature: here, we fix k; different picture if `nodesize` is fixed (+subsampling)
- Randomization:
  randomization of labels seems to have no impact;
  strong impact of randomization of partitions (hold-out RF: both bootstrap and `mtry`)

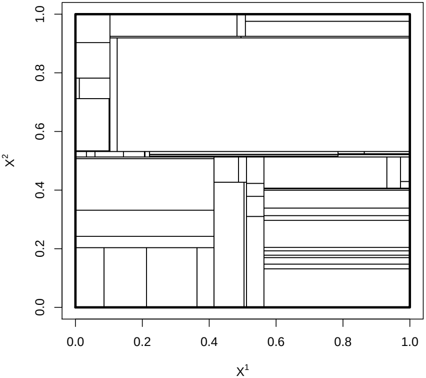
Approximation error: generalization: purf

Purely uniformly random forests:
split a random cell, chosen with probability equal to its volume
$\Rightarrow$ in dimension $p = 1$, rates similar to toy forests

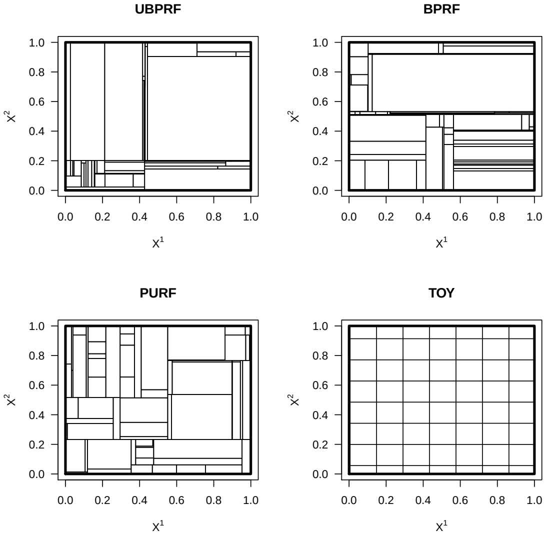


Approximation error: generalization: bprf

Balanced purely random forests in dimension p:
full binary tree, uniform splits $\Rightarrow k^{-\alpha}$ (tree) vs. $k^{-2\alpha}$ (forest)
where $\alpha = -\log_2\left(1 - \frac{1}{2p}\right) \Rightarrow$ not minimax rates!



Approximation error: 4 PRFs, different rates



Approximation error: generalization

- General result on the approximation error under (Hθ):
  e.g., roughly, if x is centered in its cell (on average over $\mathbb{U}$),

  tree approx. error $\propto \mathcal{M}_2$ infinite forest approx. error $\propto \mathcal{M}_2^2$

  where $\mathcal{M}_2 \approx$ average square distance from x to the boundary of its cell ($\propto k^{-2/p}$ for toy forests)

- other PRF studied in the literature: Mondrian forests (Mourtada, Gaïffas & Scornet 2017 & 2020), centered random forests (Biau, 2012; Klusowski, 2018), ...

Open problems / future work

- Theory on approximation error of hold-out RF?
  $\Rightarrow$ understand the typical shape of the cell that contains x, for a RI tree
  (x centered on average? square distance to boundary?)

- Theory on estimation error of other PRF (beyond toy and PURF), with lower bounds?
  of hold-out RF?

- Extensive numerical experiments? (other functions $s^\star$, ...)