

Analysis of some purely random forests

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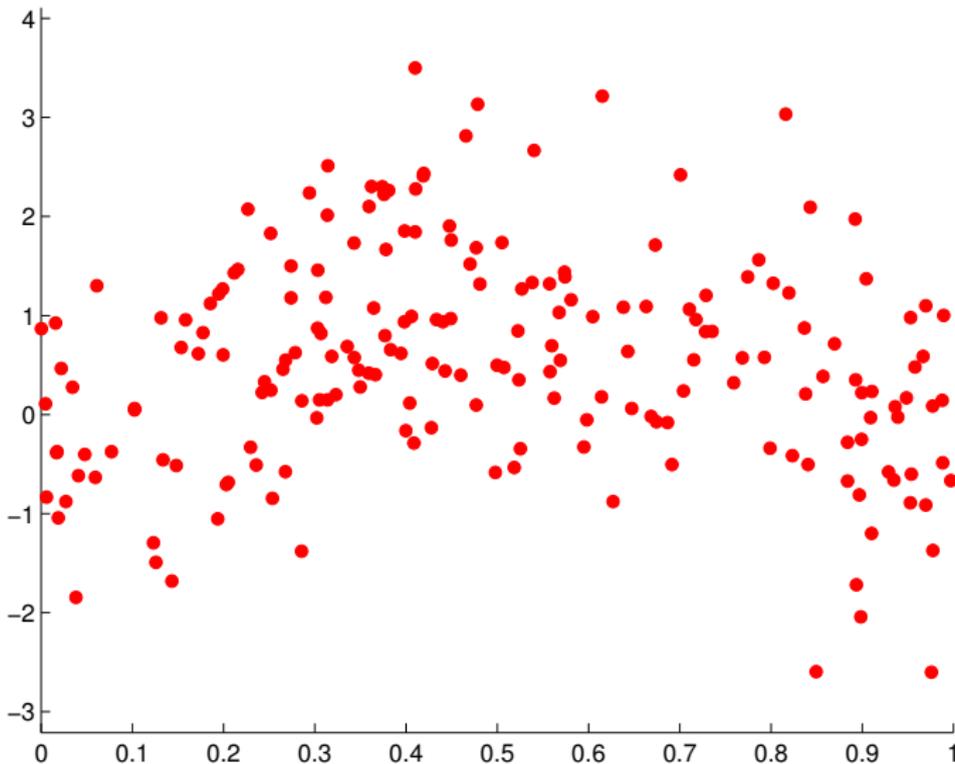
Outline

- 1 Random forests
- 2 Purely random forests
- 3 Toy forests in one dimension
- 4 Hold-out random forests

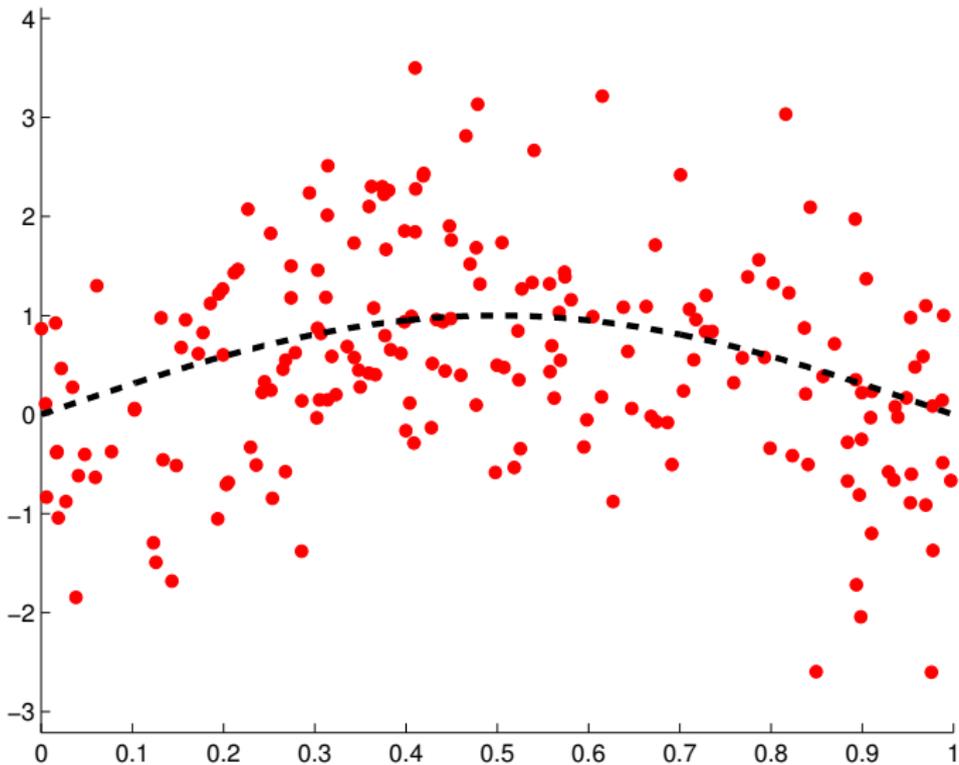
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Regression: data $(X_1, Y_1), \dots, (X_n, Y_n)$



Goal: find the signal (denoising)



Regression

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

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

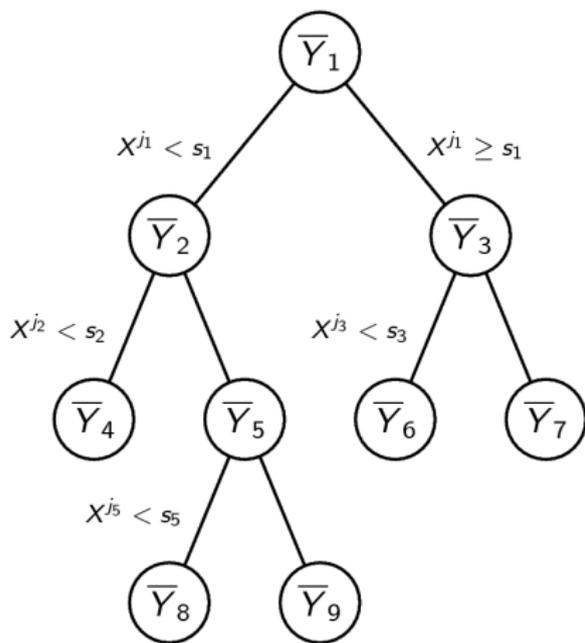
with $s^*(X) = \mathbb{E}[Y | X]$ (regression function).

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

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

is minimal.

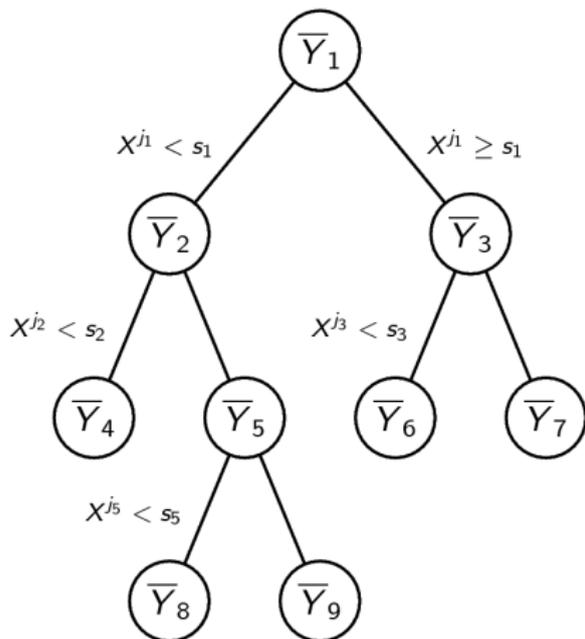
Regression tree (Breiman et al, 1984)



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

Restriction: splits parallel to the axes.

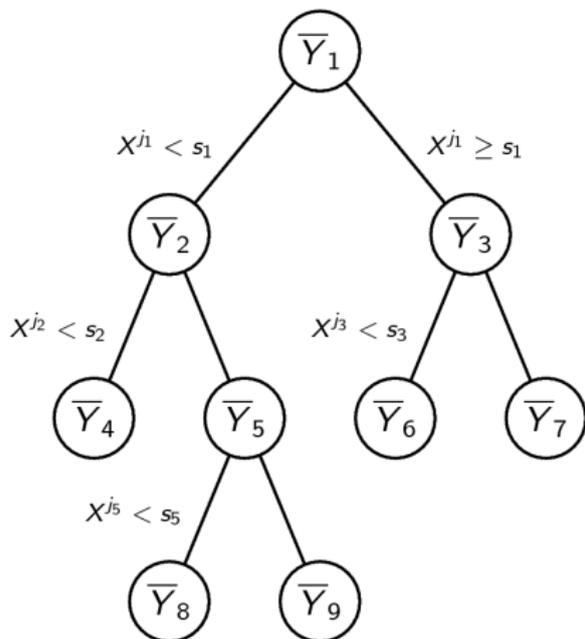
Regression tree (Breiman et al, 1984)



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

- 1 Choice of the partition \mathcal{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}^d .

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

Random forest (Breiman, 2001)

Definition (Random forest (Breiman, 2001))

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

Random forest predictor \hat{s} obtained by **aggregating the tree collection**.

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

- 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 $\{(X_i, Y_i) / i = 1, \dots, n\}$ (sampling with replacement)
 \Rightarrow **resample** D_n^b
- Bootstrapping a tree: $\hat{s}_{\text{tree}}^b = \hat{s}_{\text{tree}}(D_n^b)$
- **Bagging**: bootstrap (q independent resamples) then aggregation

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

Random Forest-Random Inputs (Breiman, 2001)

Definition (RI tree)

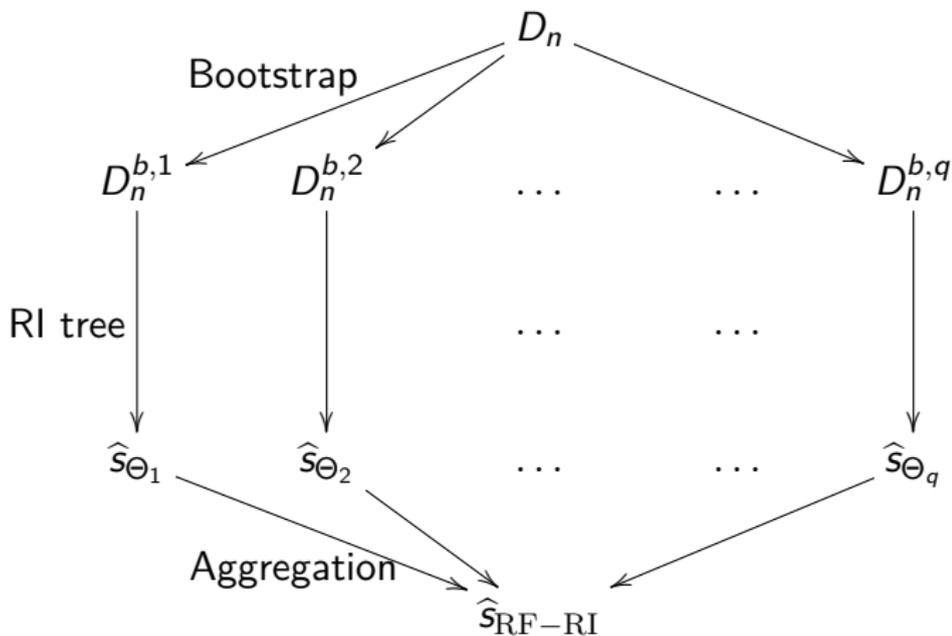
In a RI tree, at each node, **mtry** variables are randomly chosen. Then, the best cut direction is chosen only among the chosen variables.

Definition (Random forest RI)

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

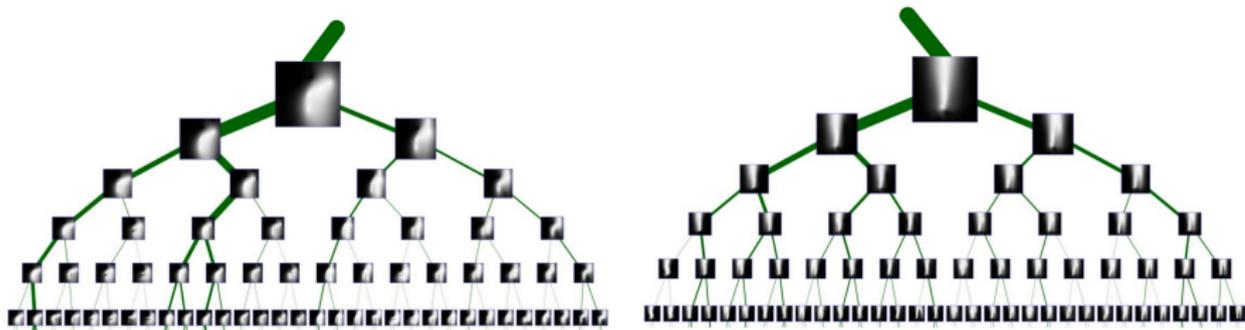
RF-RI \Leftrightarrow bagging on RI trees

Random Forest-Random Inputs



Example of application of random forests: Kinect

Depth image  ⇒ depth comparison features at each pixel



⇒ body part at each pixel  ⇒ body part positions  ⇒ ...

Figures from Shotton et al (2011) 12/38

Theoretical results on RF-RI

- Few theoretical results on Breiman's original RF-RI
- 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^*
- References (see **survey paper** by Biau and Scornet, 2016):
Mentch & Hooker (2014), Scornet, Biau & Vert (2015),
Wager & Athey (2015), ...

Theoretical results on RF-RI

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- ⇒ Here, we consider simplified RF models, for which a precise analysis is possible: **purely random forests**

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Purely random forests

Definition (Purely random tree)

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

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)

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

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

Purely random forests

Definition (Purely random forest)

$$\hat{s}(x) = \frac{1}{q} \sum_{j=1}^q \hat{s}_{\mathcal{U}^j}(x) = \frac{1}{q} \sum_{j=1}^q \sum_{\lambda \in \mathcal{U}^j} \overline{Y}_{\lambda}(D_n) \mathbb{1}_{x \in \lambda}$$

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

Example (“hold-out RF” model): (random) split of the sample into D_n (used for defining the labels \overline{Y}_{λ}) and D'_n (used for building the trees $\mathcal{U}^j = \mathcal{U}_{\text{RI}}(D_n'^j)$).

Purely random forests

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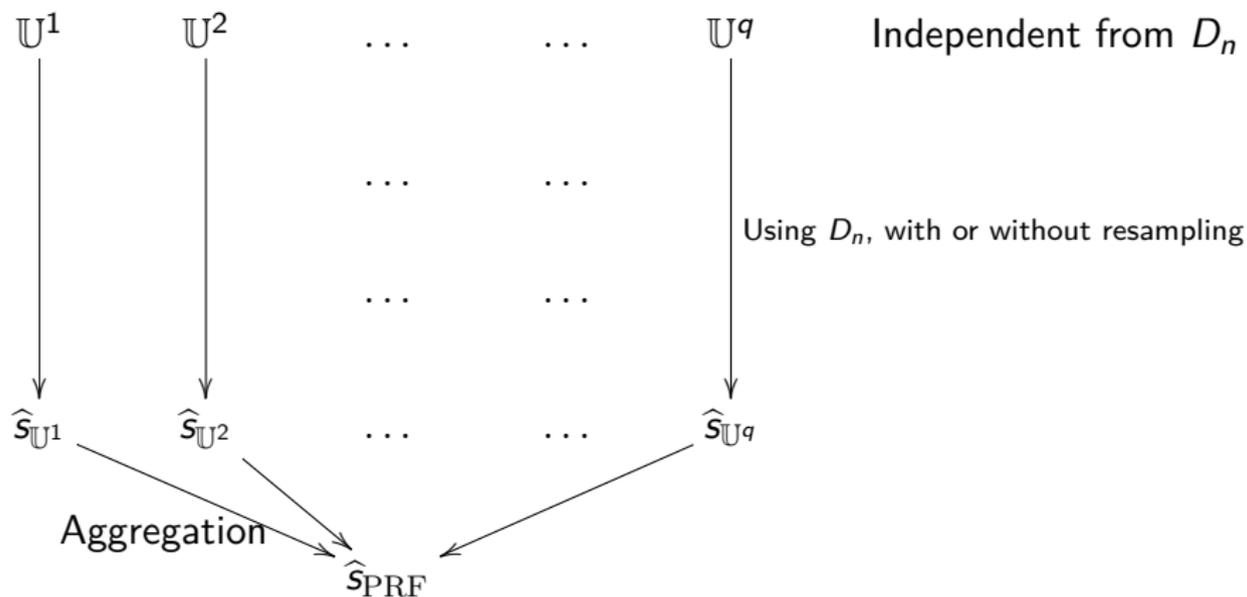
$$\hat{s}(x) = \frac{1}{q} \sum_{j=1}^q \hat{s}_{\mathbb{U}^j}(x) = \frac{1}{q} \sum_{j=1}^q \sum_{\lambda \in \mathbb{U}^j} \overline{Y}_{\lambda}(D_n) \mathbb{1}_{x \in \lambda}$$

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

Example (“hold-out RF” model): (random) split of the sample into D_n (used for defining the labels \overline{Y}_{λ}) and D'_n (used for building the trees $\mathbb{U}^j = \mathbb{U}_{\text{RI}}(D_n'^{*j})$).

 From now on, D_n is the sample used for computing the $\overline{Y}_{\lambda}(D_n)$, 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)
 - Some adaptivity to **dimension reduction** (sparse framework): Biau (2012)
 - Forests **decrease the estimation error** (Biau, 2012; Genuer, 2012)
- ⇒ 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

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

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

$$\hat{s}_{\mathbb{U}} \in \operatorname{argmin}_{f \in \mathcal{S}_{\mathbb{U}}} \left\{ \frac{1}{n} \sum_{i=1}^n (Y_i - f(X_i))^2 \right\}$$

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

Define:

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

$$\Rightarrow \tilde{s}_{\mathbb{U}} \in \operatorname{argmin}_{f \in \mathcal{S}_{\mathbb{U}}} \mathbb{E} \left[(f(X) - s^*(X))^2 \right] \quad \text{and} \quad \tilde{s}_{\mathbb{U}}(x) = \mathbb{E}[\hat{s}_{\mathbb{U}}(x) \mid \mathbb{U}]$$

Risk decomposition: single tree

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

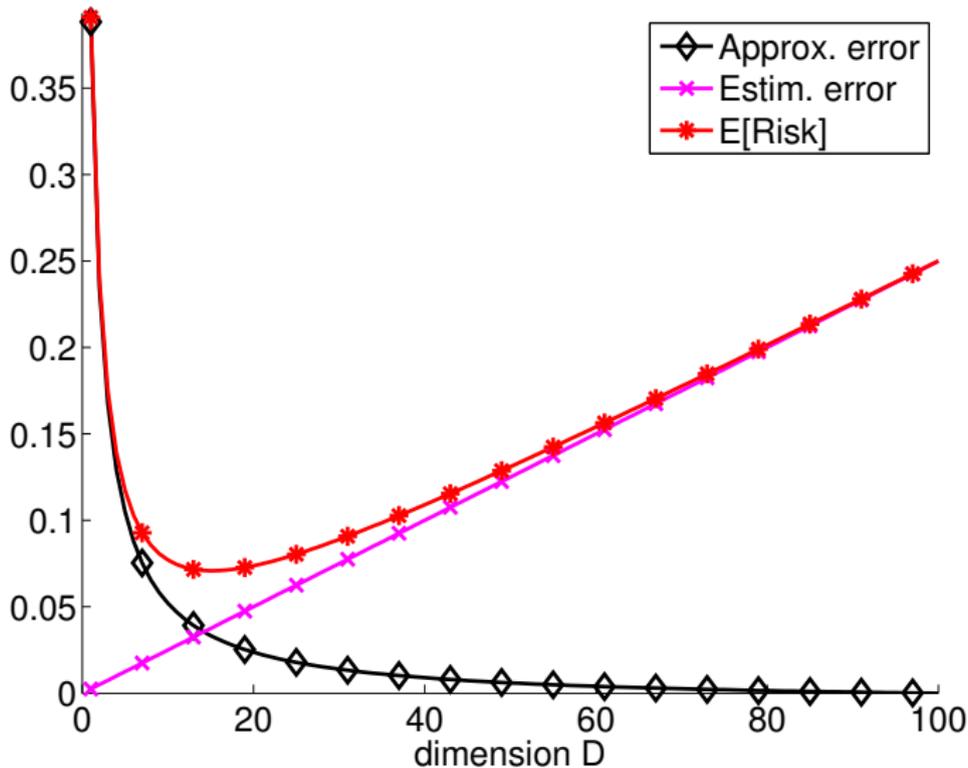
If s^* is smooth, $X \sim \mathcal{U}([0, 1])$ and \mathbb{U} regular partition into K pieces, then

$$\mathbb{E} \left[(\check{s}_{\mathbb{U}}(X) - s^*(X))^2 \right] \propto \frac{1}{K^2}$$

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

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

Approximation and estimation errors



Risk decomposition: purely random forest

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

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

Ideal forest: $\tilde{s}_{\mathbb{U}^{1 \dots q}}(x) := \frac{1}{q} \sum_{j=1}^q \tilde{s}_{\mathbb{U}^j}(x) = \mathbb{E}[\hat{s}_{\mathbb{U}^{1 \dots q}}(x) | \mathbb{U}^{1 \dots q}]$

Quadratic risk decomposition (given $X = x$)

$$\begin{aligned} \mathbb{E} \left[(\hat{s}_{\mathbb{U}^{1 \dots q}}(x) - s^*(x))^2 \right] &= \mathbb{E} \left[(\tilde{s}_{\mathbb{U}^{1 \dots q}}(x) - s^*(x))^2 \right] \\ &\quad + \mathbb{E} \left[(\hat{s}_{\mathbb{U}^{1 \dots q}}(x) - \tilde{s}_{\mathbb{U}^{1 \dots q}}(x))^2 \right] \end{aligned}$$

Bias term (approximation error):

$$B_{\mathcal{U},q}(x) := \mathbb{E} \left[(\tilde{s}_{\mathbb{U}^{1 \dots q}}(x) - s^*(x))^2 \right]$$

Bias decomposition (given $X = x$)

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

where $\mathcal{B}_{U,\infty}(x) := \left(\mathbb{E}[\tilde{s}_U(x)] - s^*(x) \right)^2$

and $\mathcal{V}_U(x) := \text{var}(\tilde{s}_U(x))$

$\mathcal{B}_{U,\infty}(x)$ is the **bias of the infinite forest**: $\tilde{s}_{U,\infty}(x) := \mathbb{E}[\tilde{s}_U(x)]$

to be compared with the **bias of a single tree**

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

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Toy forests in one dimension

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

$\mathbb{U} \sim \mathcal{U}_k^{\text{toy}}$ defined by:

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

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

Interpretation of the ideal infinite forest

Proposition (A. & Genuer, 2014)

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

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

where

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

Analysis of the approximation error

(H2) s^* twice differentiable over $(0, 1)$ and $s^{*''}$ bounded

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

$$s^*(t) - s^*(x) = s^{*'}(x)(t - x) + \frac{1}{2}s^{*''}(c_{t,x})(t - x)^2$$

Therefore,

$$\begin{aligned} \tilde{s}_{\cup}(x) - s^*(x) &= k \int_{x + \frac{V_x - 1}{k}}^{x + \frac{V_x}{k}} (s^*(t) - s^*(x)) dt \\ &= k s^{*'}(x) \int_{x + \frac{V_x - 1}{k}}^{x + \frac{V_x}{k}} (t - x) dt + R_1(x) \\ &= \frac{s^{*'}(x)}{k} \left(V_x - \frac{1}{2} \right) + R_1(x) \end{aligned}$$

where $R_1(x) = \frac{k}{2} \int_{x + \frac{V_x - 1}{k}}^{x + \frac{V_x}{k}} s^{*''}(c_{t,x})(t - x)^2 dt$

Analysis of the approximation error

$$\left(\mathbb{E}_{\mathcal{U}}[\tilde{s}_{\mathcal{U}}(x) - s^*(x)]\right)^2 \leq \frac{\square}{k^4} \quad \mathcal{V}_{\mathcal{U}}(x) \underset{k \rightarrow +\infty}{\sim} \frac{\square}{k^2}$$

Proposition (A. & Genuer, 2014)

Assuming (H2), for every $x \in \left[\frac{1}{k}, 1 - \frac{1}{k}\right]$,

$$\mathcal{B}_{\mathcal{U}_k^{\text{toy}},1}(x) \underset{k \rightarrow +\infty}{\sim} \frac{\square}{k^2} \quad \mathcal{B}_{\mathcal{U}_k^{\text{toy}},\infty}(x) \leq \frac{\square}{k^4}$$

$$\int_{\frac{1}{k}}^{1-\frac{1}{k}} \mathcal{B}_{\mathcal{U}_k^{\text{toy}},1}(x) dx \underset{k \rightarrow +\infty}{\sim} \frac{\square}{k^2} \quad \int_{\frac{1}{k}}^{1-\frac{1}{k}} \mathcal{B}_{\mathcal{U}_k^{\text{toy}},\infty}(x) dx \leq \frac{\square}{k^4}$$

Rate k^{-4} is tight assuming:

(H3) s^* three times differentiable over $(0, 1)$ and $s^{*'''}$ bounded 27/38

Estimation error

General fact (Jensen's inequality):

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

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General fact (Jensen's inequality):

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

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

(A. & Genuer, 2016)

Summary: risk analysis

$$\mathbb{E} \left[\left(\widehat{S}_{\cup 1 \dots q}(x) - s^*(x) \right)^2 \right] \approx \begin{array}{cc} \text{Single tree} & \text{Infinite forest} \\ (q = 1) & (q = \infty) \\ \frac{c_1(s^*, x)}{k^2} + \frac{\sigma^2 k}{n} & \frac{c_2(s^*, x)}{k^4} + \frac{2\sigma^2 k}{3n} \end{array}$$

$$\text{where } c_1(s^*, x) = \frac{s^{*'}(x)^2}{12} \quad \text{and} \quad c_2(s^*, x) = \frac{s^{*''}(x)^2}{144} .$$

Assumptions:

- $x \in (0, 1)$ far from boundary
- (H3) s^* three times differentiable over $(0, 1)$ and $s^{*'''}$ bounded
- \mathcal{X} uniform over $[0, 1]$
- $\text{var}(Y|X) = \sigma^2$
- no resampling for computing labels

Rates of convergence

Corollary: risk convergence rates (far from boundaries, with $k = k_n^*$ optimal):

$$\begin{aligned} \text{Tree} &\geq \square n^{-2/3} \\ \text{Infinite forest} &\leq \square n^{-4/5} \quad \Rightarrow \quad \text{minimax } \mathcal{C}^2 \end{aligned}$$

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Remarks:

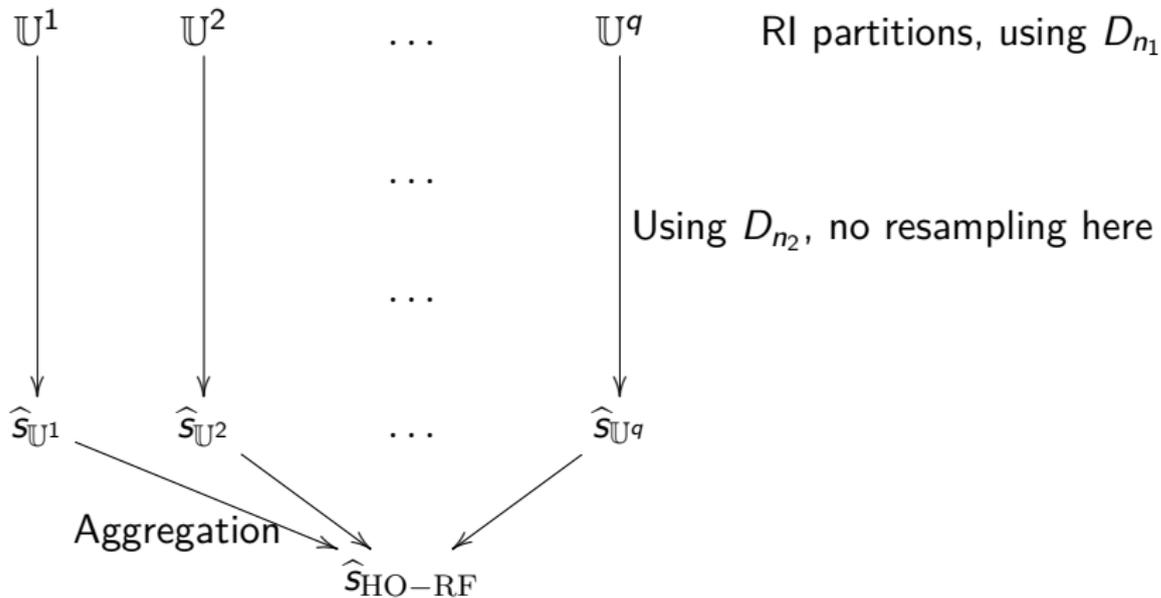
- $q \geq \square (k_n^*)^2$ is sufficient to get an “infinite” forest
- with subsampling a out of n for computing labels: estimation error of a single tree $\frac{\sigma^2 k}{a}$ instead of $\frac{\sigma^2 k}{n}$; no change for infinite forest

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Definition (Biau, 2012)

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



\Rightarrow purely random forest

Numerical experiments: framework

- Data generation:

$$\begin{aligned} X_i &\sim \mathcal{U}([0, 1]^d) & Y_i &= s^*(X_i) + \varepsilon_i \\ \varepsilon_i &\sim \mathcal{N}(0, \sigma^2) & \sigma^2 &= 1/16 \end{aligned}$$

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

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

Numerical experiments: results ($d = 5$)

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

Numerical experiments: results ($d = 10$)

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

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)

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- **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

- General result on the **approximation error** under (H2)/(H3):
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**
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rates similar to toy forests
- **balanced purely random forests** (full binary tree, uniform
splits) in dimension d : $k^{-\alpha}$ (tree) vs. $k^{-2\alpha}$ (forest) where
 $\alpha = -\log_2\left(1 - \frac{1}{2d}\right) \Rightarrow$ not minimax rates!

Open problems / future work

- Extensive numerical experiments? (other functions s^* , ...)
- Theory on **approximation error of hold-out RF**?
⇒ understand the typical shape of a cell of a RI tree
(x centered on average? square distance to boundary?)
- Theory on **estimation error** of other models (beyond toy)?
of hold-out RF?