

# Analysis of some purely random forests

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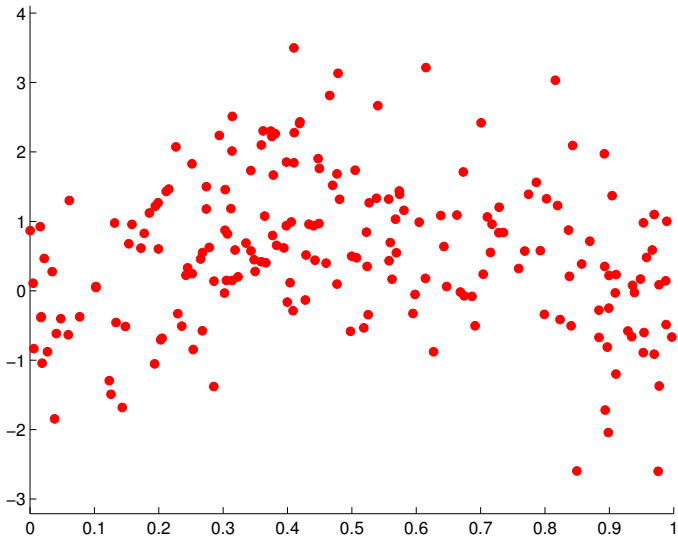
# Outline

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

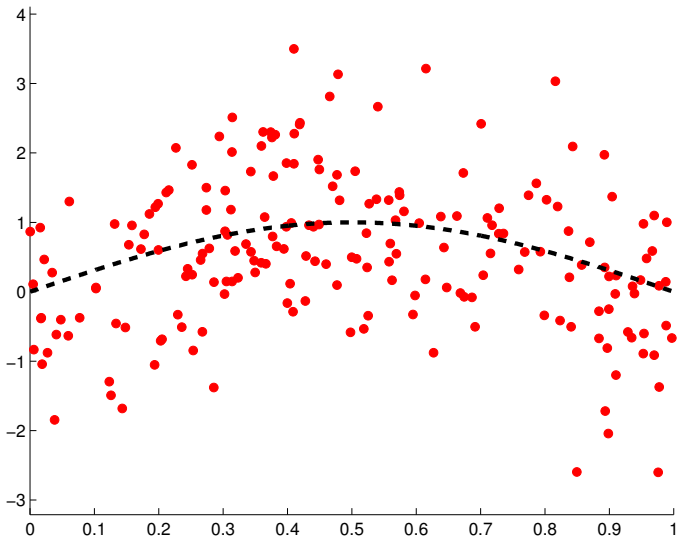
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# Regression: data $(X_1, Y_1), \dots, (X_n, Y_n)$



# 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).

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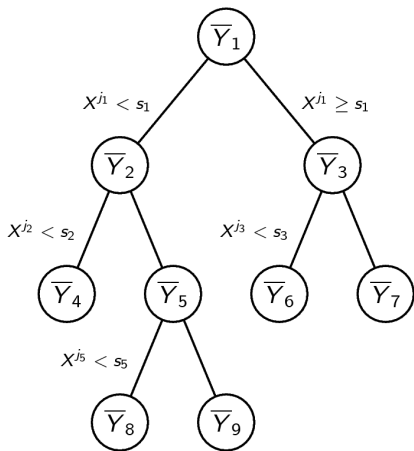
with  $s^*(X) = \mathbb{E}[Y | X]$  (regression function).

- **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)

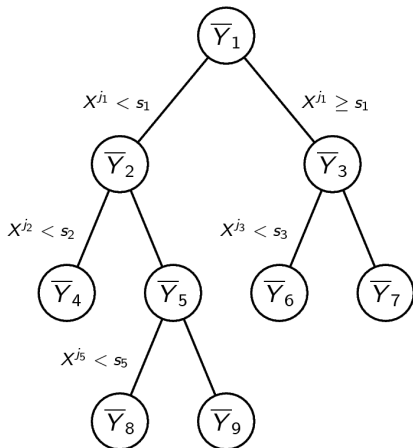


Tree: piecewise-constant predictor, obtained by partitioning recursively  $\mathbb{R}^d$ .

Restriction: splits parallel to the axes.



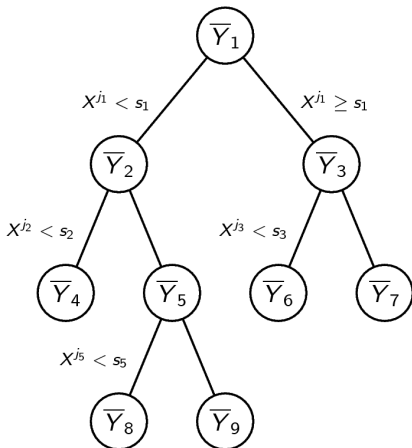
# Regression tree (Breiman et al, 1984)



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)  
⇒ **resample**  $D_n^b$

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 $\Rightarrow$  **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,  $m_{\text{try}}$  variables are randomly chosen. Then, the best cut direction is chosen only among the chosen variables.

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



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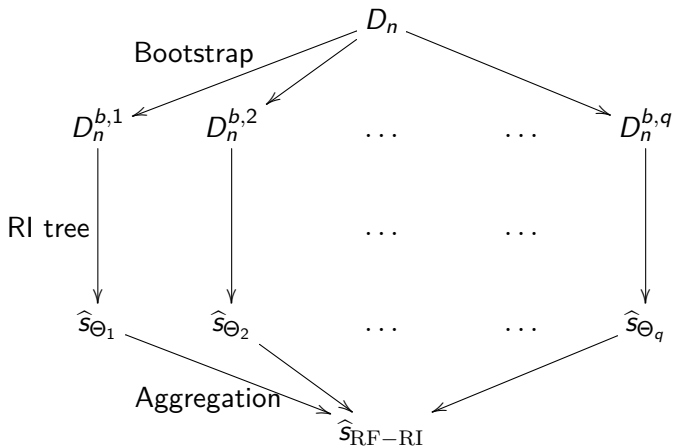
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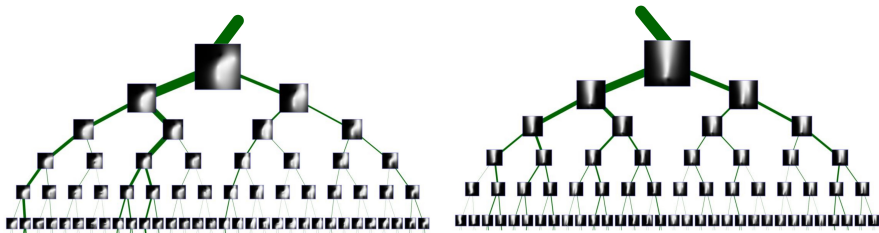
RF-RI  $\Leftrightarrow$  bagging on RI trees


# 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) 12/39

# 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),  
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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

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




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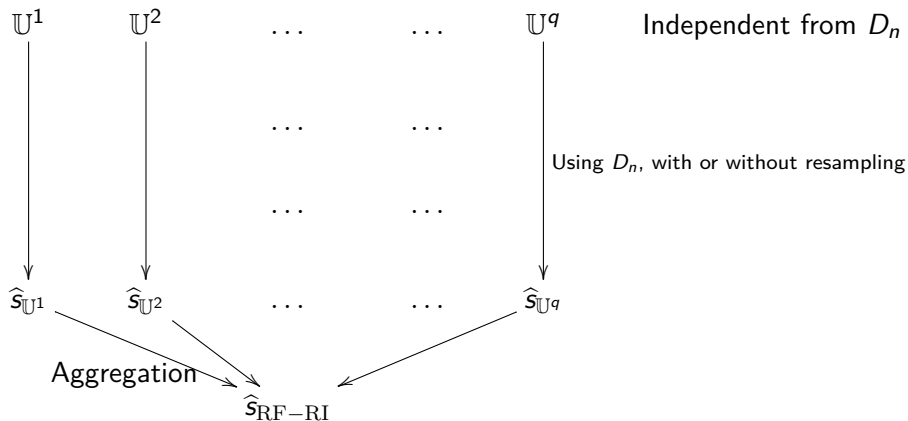
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 From now on,  $D_n$  is the sample used for computing the  $\overline{Y}_{\lambda}(D_n)$ , and we assume its size is  $n$ .

# 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)

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  - 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  $(Y_i)_{X_i \in \lambda}$ .

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

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Define:

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

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

# Risk decomposition: single tree

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

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

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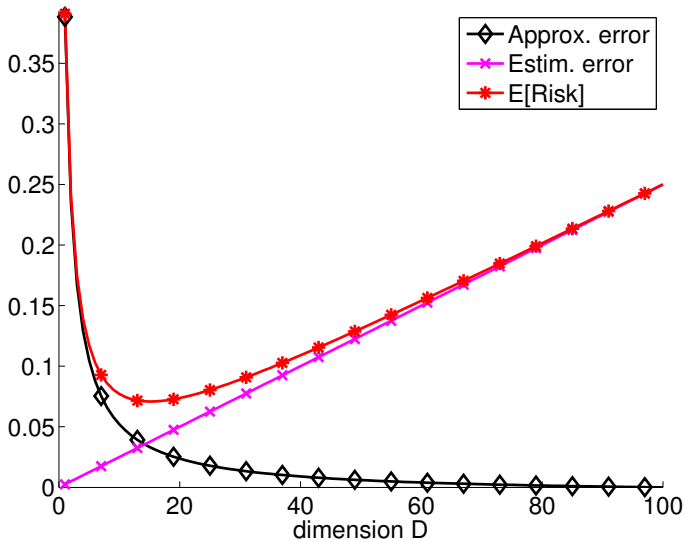
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If  $\text{var}(Y | X) = \sigma^2$  does not depend on  $X$ , then

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

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

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## Quadratic risk decomposition (given $X = x$ )

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

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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

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

# Interpretation of the ideal infinite forest: proof

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

$$\tilde{s}_{\mathbb{U}}(x) = \frac{1}{|I_{\mathbb{U}}(x)|} \int_{I_{\mathbb{U}}(x)} s^*(t) dt$$

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

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

$$\begin{aligned} \tilde{s}_{\mathbb{U}, \infty}(x) &= \mathbb{E}_{\mathbb{U}}[\tilde{s}_{\mathbb{U}}(x)] \\ &= k \int_0^1 s^*(t) \mathbb{P}\left(x + \frac{V_x - 1}{k} \leq t < x + \frac{V_x}{k}\right) dt \\ &= k \int_0^1 s^*(t) \mathbb{P}(k(t - x) < V_x \leq k(t - x) + 1) dt \end{aligned}$$

# 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

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

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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  $x \in \left[\frac{1}{k}, 1 - \frac{1}{k}\right]$ ,

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

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

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Rate  $k^{-4}$  is tight assuming:

(H3)  $s^*$  three times differentiable over  $(0, 1)$  and  $s^{*'''}$  bounded 28/39

# Estimation error

General fact (Jensen's inequality):

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



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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

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

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

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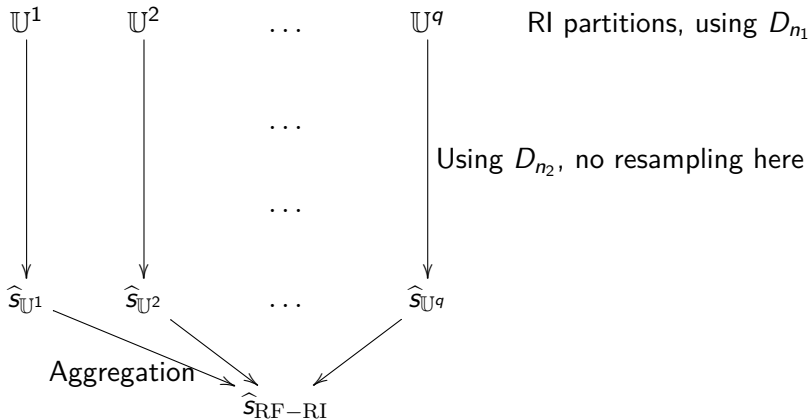
- $q \geq \square (k_n^*)^2$  is sufficient to get an “infinite” forest
- with subsampling  $a$  out of  $n$  for computing labels: estimation error of a single tree  $\frac{\sigma^2 k}{a}$  instead of  $\frac{\sigma^2 k}{n}$ ; no change for infinite forest

# Outline

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

# Definition (Biau, 2012)

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



⇒ purely random forest 33/39

# 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<br>mtry = $d$                       | $\frac{0.13}{k^{0.17}} + \frac{1.04\sigma^2 k}{n_2}$ |  | $\frac{0.13}{k^{0.17}} + \frac{1.04\sigma^2 k}{n_2}$ |  |
| <b>Bootstrap</b><br>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<br>mtry = $\lfloor d/3 \rfloor$     | $\frac{0.23}{k^{0.19}} + \frac{1.01\sigma^2 k}{n_2}$ |  | $\frac{0.06}{k^{0.31}} + \frac{0.06\sigma^2 k}{n_2}$ |  |
| <b>Bootstrap</b><br>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<br>mtry = $d$                       | $\frac{0.11}{k^{0.12}} + \frac{1.03\sigma^2 k}{n_2}$ | $\frac{0.11}{k^{0.12}} + \frac{1.03\sigma^2 k}{n_2}$ |
| <b>Bootstrap</b><br>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<br>mtry = $\lfloor d/3 \rfloor$     | $\frac{0.21}{k^{0.18}} + \frac{1.08\sigma^2 k}{n_2}$ | $\frac{0.08}{k^{0.25}} + \frac{0.04\sigma^2 k}{n_2}$ |
| <b>Bootstrap</b><br>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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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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- **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?