Apprentissage statistique

masedki.github.io

Univesité Paris-Saclay

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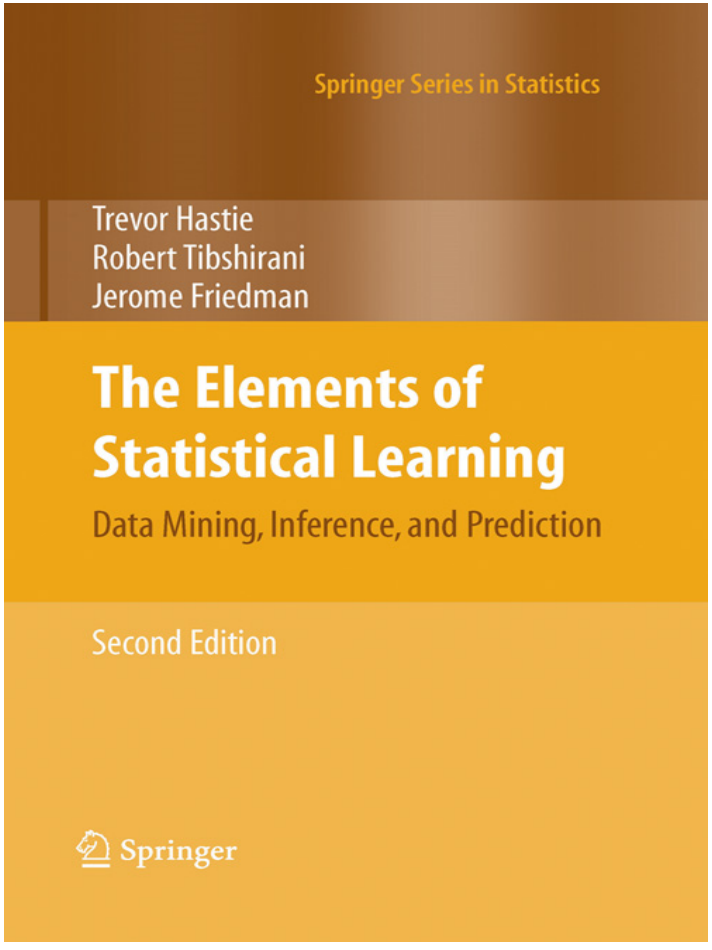
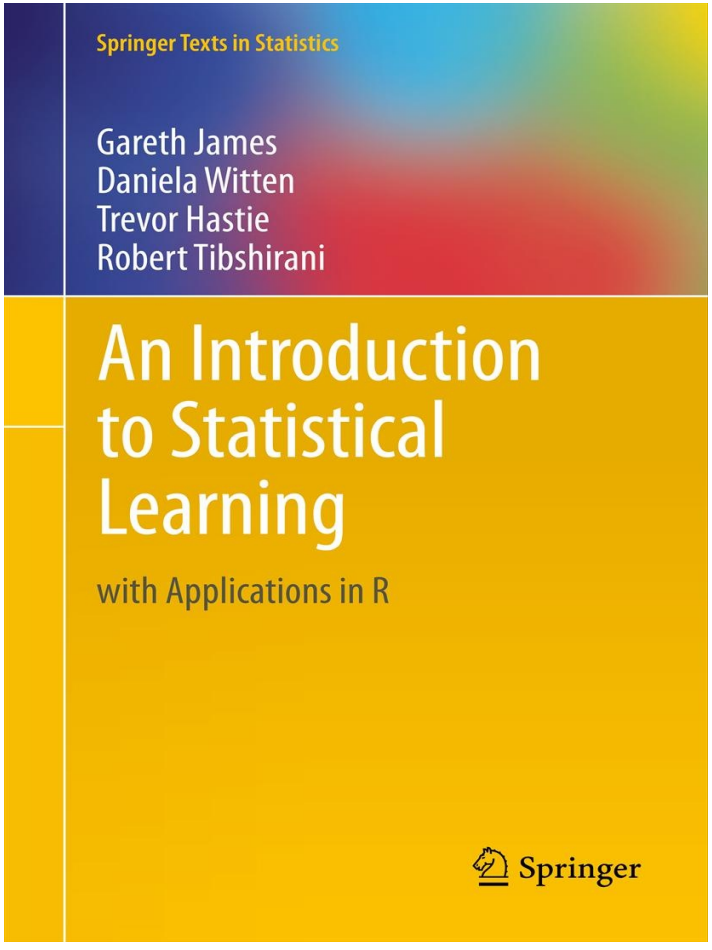
Références


Springer Series in Statistics
Trevor Hastie
Robert Tibshirani
Jerome Friedman
The Elements of Statistical Learning
Data Mining, Inference, and Prediction
Second Edition
Springer


Springer Texts in Statistics
Gareth James
Daniela Witten
Trevor Hastie
Robert Tibshirani
An Introduction to Statistical Learning
with Applications in R
Springer

Problèmes d'apprentissage statistique

- Identifier les facteurs de risque du cancer de la prostate
- Classifier des phonèmes à partir de périodogrammes
- Prédire si une personne est sujette aux crises cardiaques, à partir de mesures cliniques, son régime et des données démographiques
- Personnaliser un système de détection de spam email
- Lecture de codes postaux écrits à la main
- Classification d'échantillons de tissus dans différents types de cancer, en fonction de données d'expression de gènes
- Établir une relation entre salaires et variables démographiques
- Classifier les pixels d'une image satellite

Question

- Sur 4601 mails, on a pu identifier 1813 spams.
- On a également mesuré sur chacun de ces mails la présence ou absence de 57 mots.

Peut-on construire à partir de ces données une méthode de détection automatique de spam ?

Représentation du problème

La plupart de ces problèmes peuvent être appréhendés dans un contexte de régression : on cherche à expliquer une variable Y par d'autres variables dites explicatives $X_1, \ldots, X_p$:

Y	X
Chiffre	image
Mot	courbe
Spam ou pas	présence/absence d'un ensemble mots
Type de leucémie	expressions de gênes

- Lorsque la variable à expliquer est quantitative, on parle de régression.
- Lorsqu'elle est qualitative, on parle de discrimination ou classification supervisée.

Régression

- Un échantillon i.i.d d'apprentissage $(X_1, Y_1), \ldots, (X_n, Y_n)$ d'une loi conjointe $\mathbb{P}$ *inconnue* sur $\mathbb{R}^p \times \mathbb{R}$.
- Objectif : Prédire ou expliquer la variable Y à partir d'une nouvelle observation X.
- Méthode : construire une règle de prédiction (ou régression)

$$m : \mathbb{R}^p \mapsto \mathbb{R}.$$

- Soit $\ell : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}_+$ une fonction de perte (i.e, $\ell(y, y') = 0$ et $\ell(y, y') > 0$ pour $y \neq y'$), par exemple

$$\ell(y, y') = |y - y'|^q$$

(perte absolue si $q = 1$ et perte quadratique $q = 2$).

Risque ou erreur de généralisation

- Le risque ou erreur de généralisation d'une règle de décision (ou prédiction) m est défini par

$$R_{\mathbb{P}}(m) = \mathbb{E}_{(X,Y)}\Big[\ell\big(Y, m(X)\big)\Big].$$

La fonction de régression

- Un champion
$$m^*(x) = \mathbb{E}\big[Y|X = x\big]$$
appelé fonction de régression.
- Pour toute autre fonction m, on a
$$\mathbb{E}\left[\big(Y - m^*(X)\big)^2\right] \leq \mathbb{E}\left[\big(Y - m(X)\big)^2\right]$$
.

La fonction de régression

Nous avons

$$\mathbb{E}_{X,Y}\Big[\Big(Y - m(X)\Big)^2\Big] = \mathbb{E}_X \mathbb{E}_{Y|X}\Big[\Big(Y - m(X)\Big)^2 \mid X\Big]$$

Donc il suffit de minimiser cette erreur ponctuellement en X

$$m(x) = \text{argmin}_c \mathbb{E}_{Y|X}\Big[\Big(Y - c\Big)^2 \mid X = x\Big].$$

La solution est donnée par

$$m^*(x) = \mathbb{E}\big[Y \mid X = x\big]$$

La classification binaire

- Un échantillon i.i.d d'apprentissage $(X_1, Y_1), \ldots, (X_n, Y_n)$ d'une loi conjointe $\mathbb{P}$ inconnue sur $\mathbb{R}^p \times \{0, 1\}$.
- Objectif : Prédire ou expliquer la variable Y à partir d'une nouvelle observation X.
- Méthode : construire une règle classification (ou décision)

$$g : \mathbb{R}^p \mapsto \{0, 1\}.$$

- La fonction de perte binaire $\ell(y, y') = 1_{y \neq y}$.
- Risque associé à g : taux de mauvais classement

$$R_{\mathbb{P}}(g) = \mathbb{E}\Big[\ell\big(g(X), Y\big)\Big] = \mathbb{P}\big(g(X) \neq Y\big).$$

La règle de Bayes

- Un champion appelé règle de Bayes

$$g^*(x) = \begin{cases} 1 & \text{si} \quad \eta(x) \geq \frac{1}{2} \\ 0 & \text{sinon,} \end{cases}$$

où $\eta(x) = \mathbb{P}(Y = 1 | X = x)$.

- Quelque soit la règle de décision g, nous avons

$$R_{\mathbb{P}}(g^*) = \mathbb{P}\big(g^*(X) \neq Y\big) \leq \mathbb{P}\big(g(X) \neq Y\big) = R_{\mathbb{P}}(g).$$

Règle de Bayes : un théorème

- Pour toute règle de classification $g : \mathcal{X} \mapsto \mathcal{Y}$, pour la fonction de perte binaire, nous avons

$$R(g) - R(g^*) = \mathbb{E}_X \left[1\Big\{ g(X) \neq g^*(X) \Big\} \Big| 2\eta(X) - 1 \Big| \right].$$

- Interpréter ce résultat lorsque

$$\eta(x) = \frac{1}{2}, \forall x \in \Big\{ x \in \mathcal{X} : g(x) \neq g^*(x) \Big\}$$

Début de preuve

On remarque que :

$$\begin{aligned}\mathbb{E}_{Y|X=x}\Big[1\big\{Y = g^*(x)\big\}\Big] &= \mathbb{P}_{Y|X}\big[Y = g^*(x)\big] \\ &= \begin{cases}\eta(x) & \text{si} \quad \eta(x) \geq \frac{1}{2} \\ 1-\eta(x) & \text{sinon}\end{cases} \\ &= \frac{1}{2} + \big|\eta(x) - \frac{1}{2}\big|.\end{aligned}$$

Rappel :

$$\mathbb{E}_{X,Y} h(X,Y) = \mathbb{E}_X \mathbb{E}_{Y|X} h(X,Y).$$

suite de la preuve : voir notes

Proposition

$$R^* = R(g^*) = \mathbb{E}_X \left[\min \left\{ \eta(X), 1 - \eta(X) \right\} \right]$$

Preuve : voir notes

Problème majeur !!

- Problème: m^* est inconnu en pratique. Il faut construire un régresseur $\widehat{m}_n$ à partir des données $(X_1, Y_1), \ldots, (X_n, Y_n)$, tel que

$$\widehat{m}_n(x) \approx m^*(x).$$

- Problème: g^* est inconnue en pratique. Il faut construire une règle $\widehat{g}_n$ à partir des données $(X_1, Y_1), \ldots, (X_n, Y_n)$, tel que

$$\widehat{g}_n(x) \approx g^*(x).$$

Un candidat naturel

À partir des expressions de m^* et g^*, proposer deux estimateurs intuitifs.

Décomposition de l'erreur

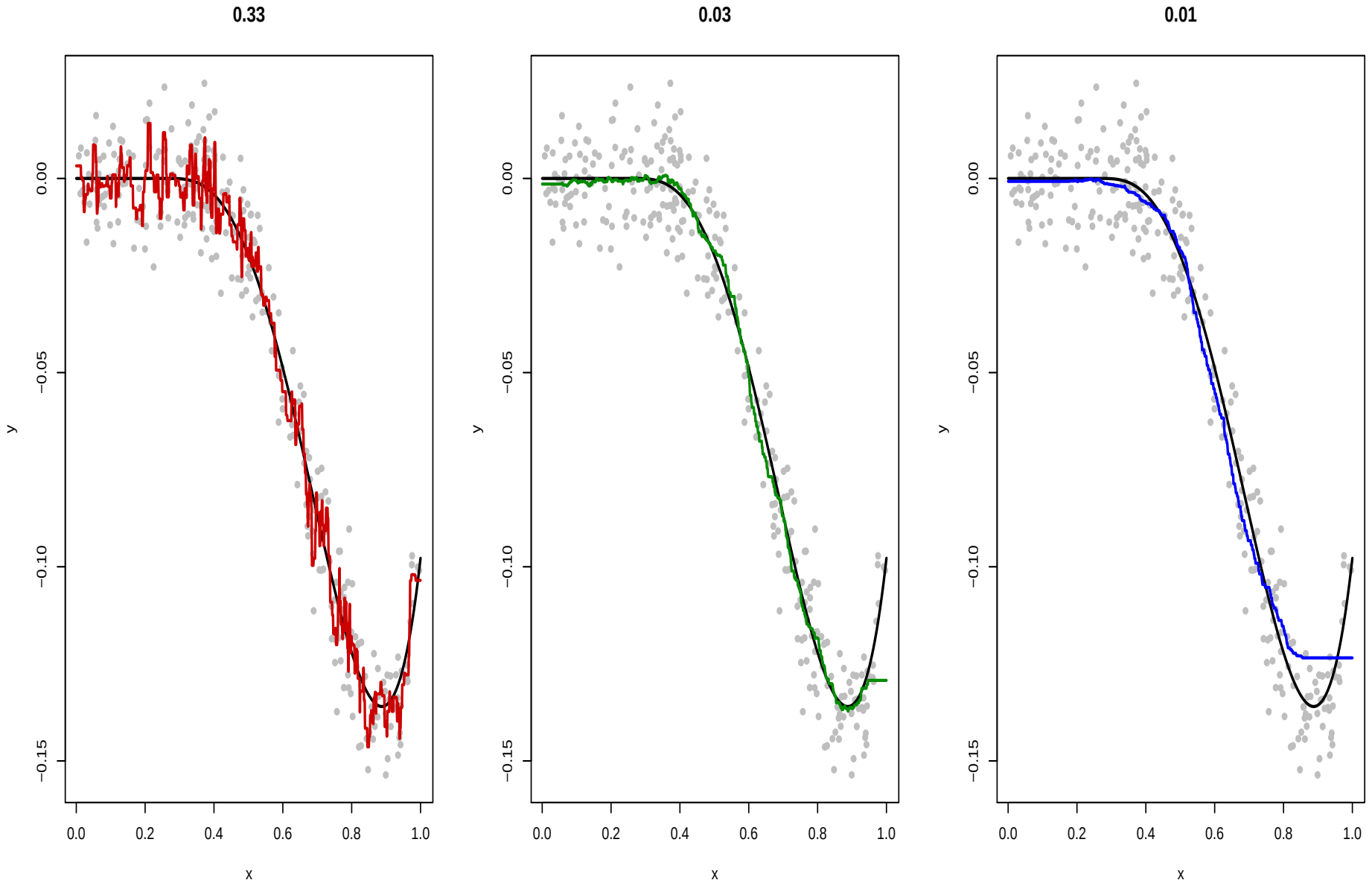
Pour tout estimateur $\widehat{m}_n(x)$ de $m^*(x)$ à x fixé, nous avons

$$\begin{aligned}
\mathbb{E}\Big[\Big(m^*(x) - \widehat{m}_n(x)\Big)^2\Big] &= \big[m^*(x)\big]^2 - 2m^*(x)\mathbb{E}\big[\widehat{m}_n(x)\big] \\
&\quad + \mathbb{E}\Big[\big(\widehat{m}_n(x)\big)^2\Big] \\
&= \Big[m^*(x) - \mathbb{E}\big(\widehat{m}_n(x)\big)\Big]^2 \\
&\quad + \mathbb{E}\Big[\big(\widehat{m}_n(x)\big)^2\Big] - \Big[\mathbb{E}\big(\widehat{m}_n(x)\big)\Big]^2 \\
&= \Big(\text{biais}\Big)^2 + \text{Var}\big[\widehat{m}_n(x)\big]
\end{aligned}$$

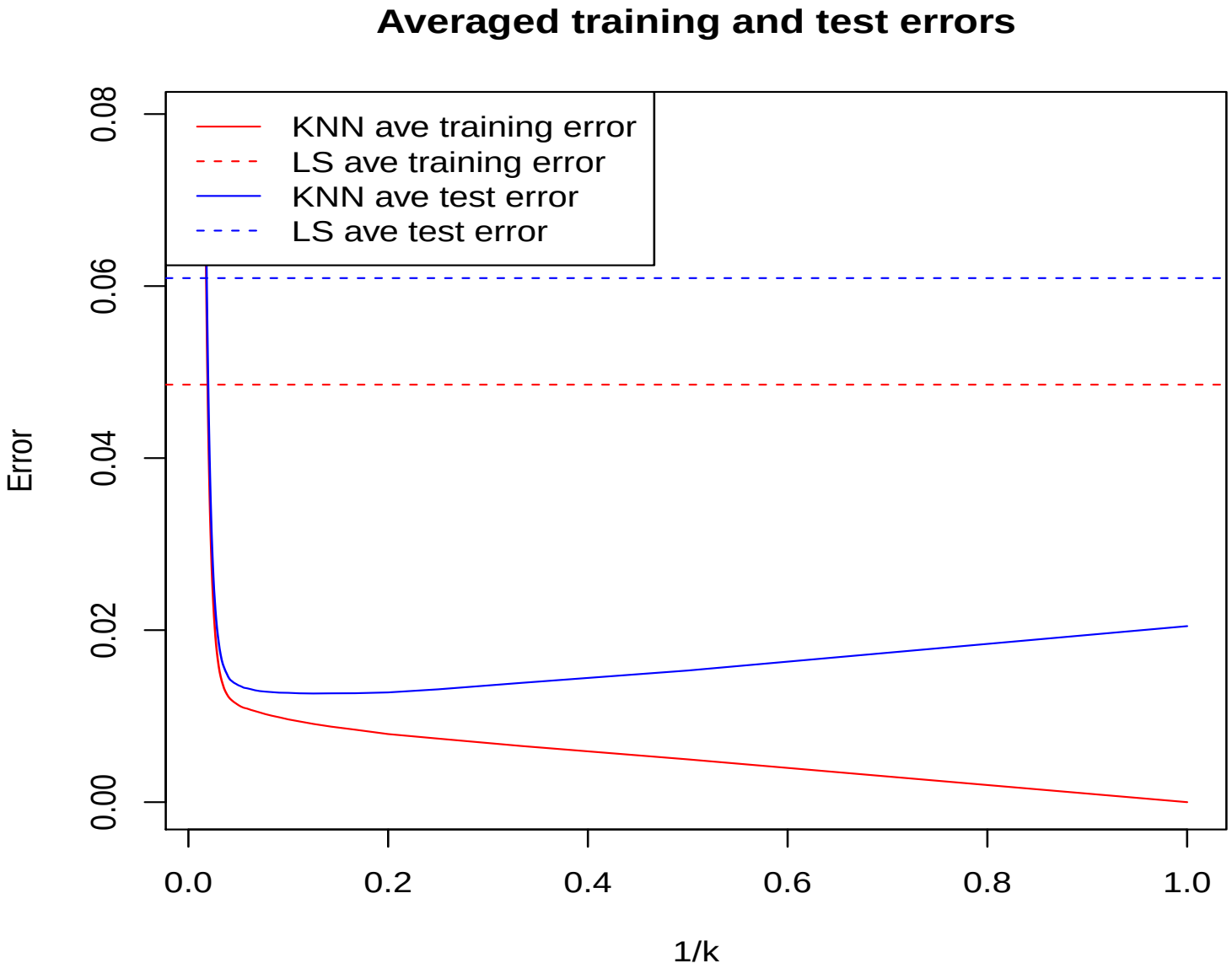
Notations

- On s'intéresse au cas où on cherche à expliquer une variable qualitative Y par p variables explicatives $X_1, \ldots, X_p$.
- Y est à valeurs dans un ensemble discret fini de modalités qui peuvent être numérotées par des les indices $\{1, 2, \ldots, K\}$ et les variables $X_1, \ldots, X_p$ peuvent être qualitatives et/ou quantitatives.
- Néanmoins, pour présenter les méthodes, on se restreint au cas où Y est à 2 modalités (0 et 1).

Complexité d'un modèle (compromis biais variance)



Évaluation de la précision : phénomène de sur-apprentissage



Évaluer la précision : premier pas

Supposons que l'on ajuste un modèle $\widehat{f}(x)$ sur des données d'apprentissage $\text{Tr} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$.

Performance de $\widehat{f}$?

Première idée : erreur moyenne de prédiction sur Tr :

$$\text{MSE}_{\mathbf{Tr}} = \text{Moyenne}_{i \in \mathbf{Tr}} \left(y_i - \widehat{f}(x_i) \right)^2$$

OPTIMISTE

(sur-apprentissage)

Meilleure idée : sur un jeu de données de *test*,
$\text{Te} = \{(x_{N+1}, y_{N+1}), \ldots, \}$,
indépendant de Tr :

$$\text{MSE}_{\mathbf{Te}} = \text{Moyenne}_{i \in \text{Te}} \left(y_i - \widehat{f}(x_i) \right)^2$$

Les Knn sont victimes du fléau de la dimension

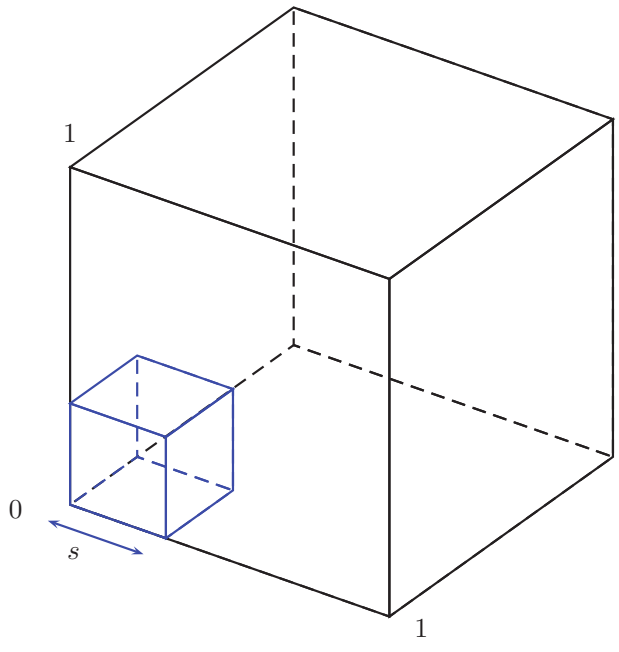
- Ces méthodes, basées sur des moyennes autour des voisins sont plutôt bonnes si
  - petite dimension $p \leq 4$
  - grand échantillon $n \gg p$
- des versions lissées, obtenues par
  - méthodes à noyaux
  - lissage par splines,
  - ...

Raison. le *fléau de la dimension*. Les voisins les plus proches peuvent être éloignés en grande dimension

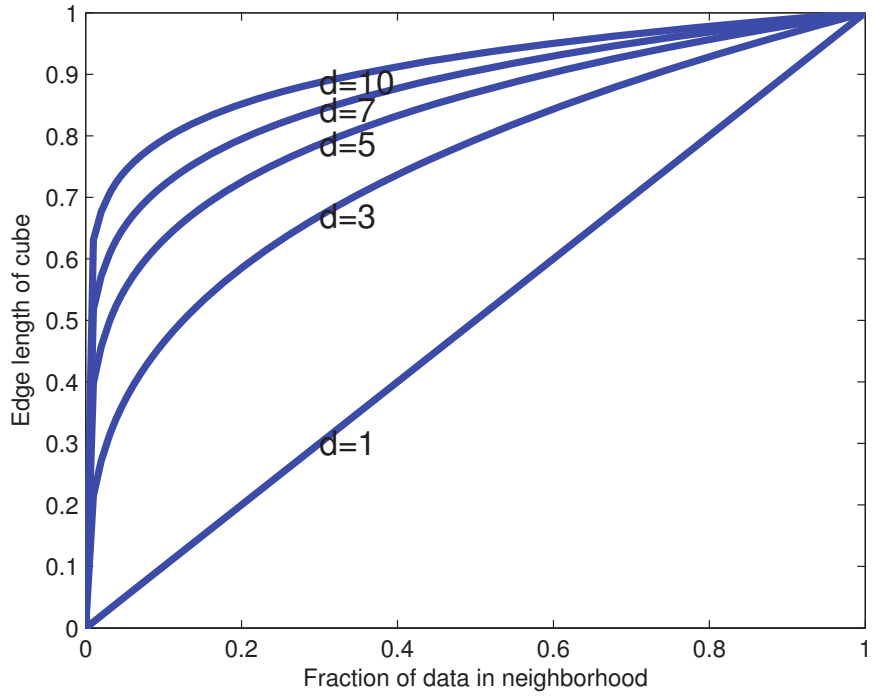
- Il faut une quantité raisonnable de valeurs de y_i à moyenner pour que $\widehat{f}(x)$ ait une faible variance
- En grande dimension, pour obtenir cette quantité d'observation, il faut s'éloigner beaucoup de x.

On perd l'idée de moyenne **locale** autre de $X = x$.

Le fléau de la dimension



(a)



(b)

Validation croisée

But

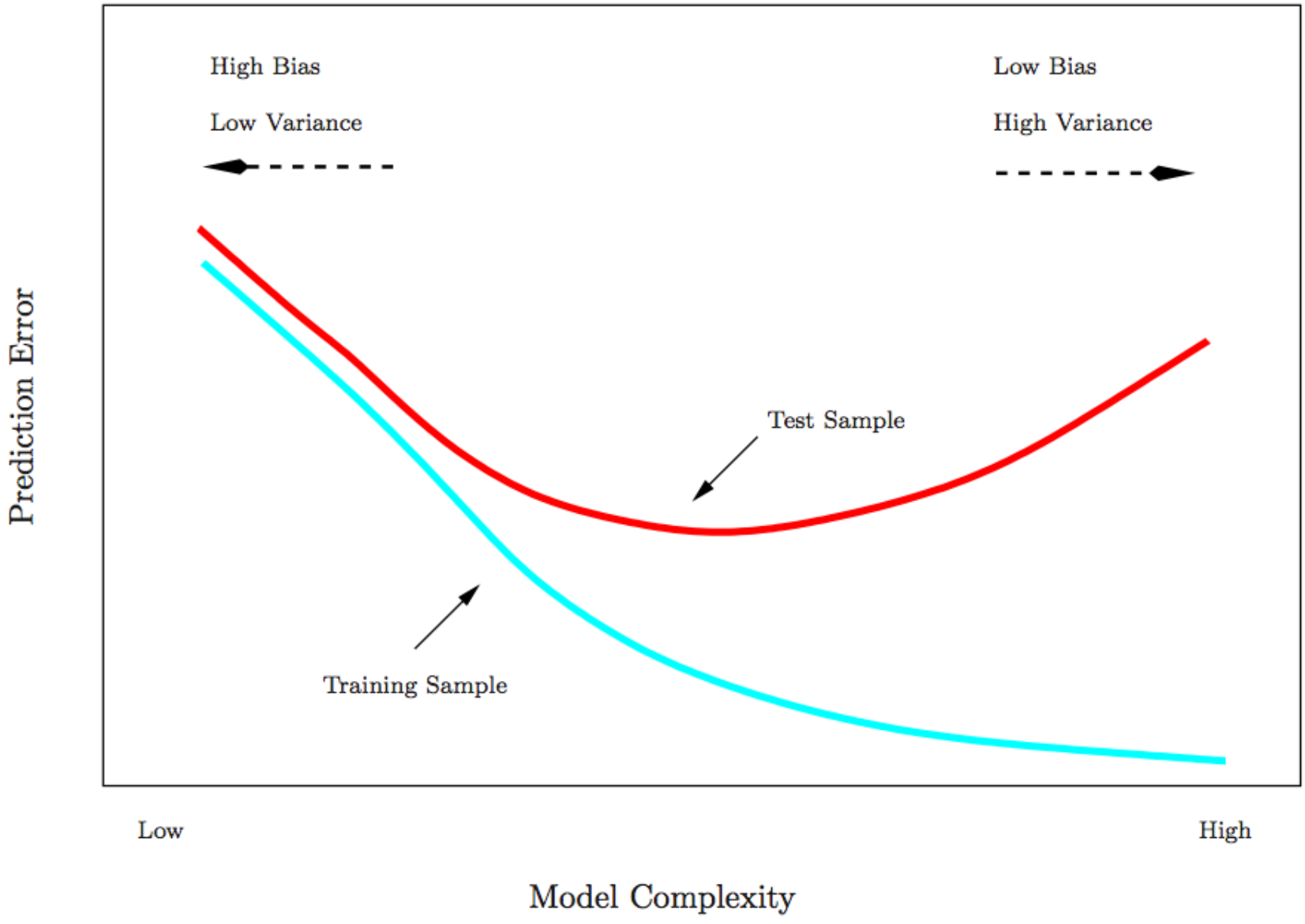
- Dans cette partie, nous allons discuter de deux méthodes de *ré-échantillonnage* : la validation croisée et le bootstrap
- Ces méthodes ré-ajustent le modèle que l'on souhaite sur des échantillons issus de l'échantillon d'apprentissage, dans le but d'obtenir des informations supplémentaires sur ce modèle
- Par exemples, ces méthodes fournissent des estimations de l'erreur sur des ensembles de test, le biais et la variance des estimations de paramètres...

Erreur d'entraînement et erreur de test

On rappelle la différence entre *erreur de test* et *erreur d'entraînement* :

- L'*erreur de test* est l'erreur moyenne commise par une méthode d'apprentissage statistique pour prédire une réponse sur une nouvelle observation, qui n'a pas été utilisée pour ajuster le modèle.
- En revanche, l'*erreur d'entraînement* peut être facilement calculée en appliquant la méthode d'apprentissage sur les données d'entraînement.
- Mais l'erreur d'entraînement est souvent bien différente de l'erreur de test, et en particulier, l'erreur d'entraînement sous-estime parfois grandement l'erreur de test — on parle d'erreur trop *optimiste*.

Erreur d'entraînement et erreur de test



Estimations de l'erreur de prédiction

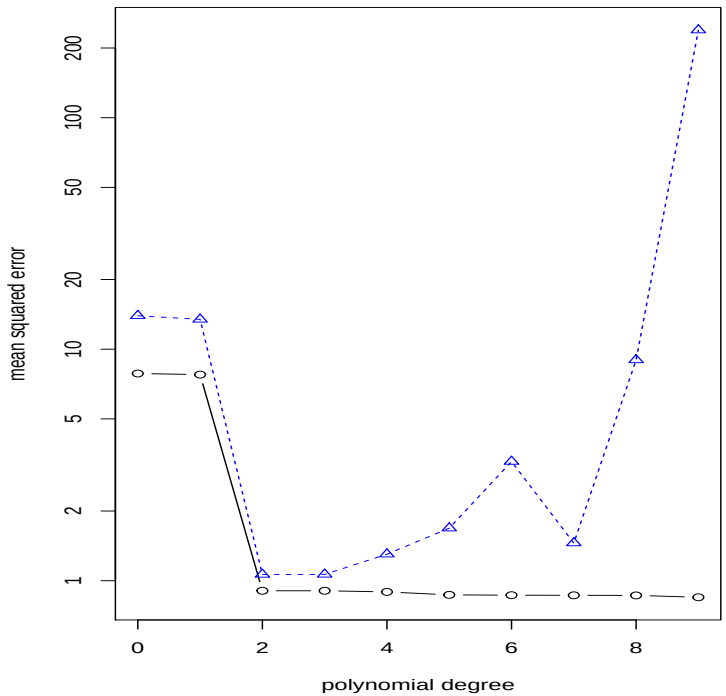
- La meilleure solution : un grand ensemble de test clairement désigné. Bien souvent, ce n'est pas disponible.
- Certaines méthodes permettent de corriger l'erreur d'entrainement pour estimer l'erreur de test, avec des arguments fondés mathématiquement.
  Cela inclut les C_p *de Mallows*, les critères AIC et BIC. Ils seront discutés plus tard.
- Ici, nous nous intéressons à une classe de méthodes qui estime l'erreur de test en mettant de côté un sous-ensemble des données d'entraînement disponibles pour ajuster les modèles, et en appliquant la méthodes ajustée sur ces données mises de côté.

Approche par ensemble de validation

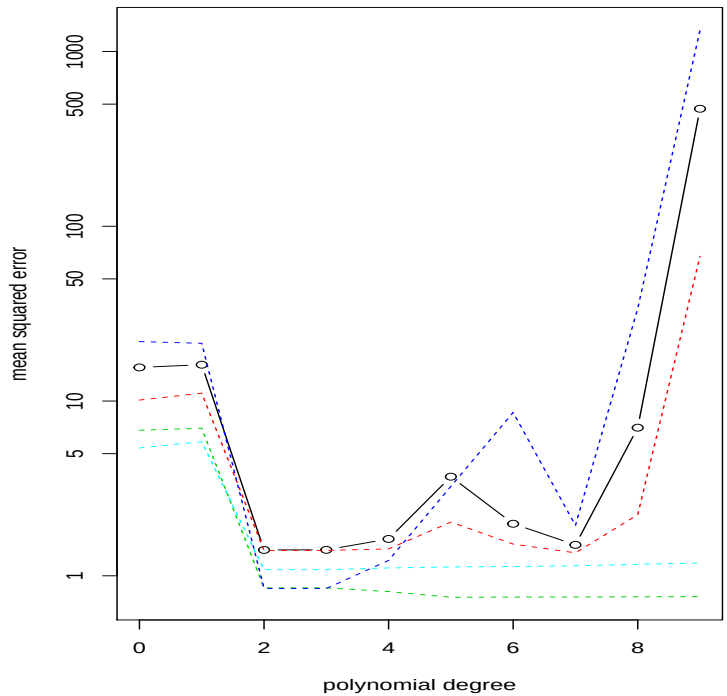
- Cette méthode propose de diviser l'échantillon d'apprentissage en deux : un ensemble d'entraînement et un ensemble de validation
- Le modèle est ajusté sur l'ensemble d'entraînement, et on l'utilise ensuite pour prédire les réponses sur l'échantillon de validation.
- L'erreur obtenue en comparant prédiction et observation sur cet échantillon de validation approche l'erreur de test. On utilise typiquement des moindres carrés (MSE) en régression et des taux de mauvaises classification si la réponse est qualitative (ou une fonction de coût d'erreur)

Exemple sur les données simulées (degré 2)

- On veut comparer la régression linéaires à des régressions polynomiales de différents degrés
- On divise en deux les 200 observations : 100 pour l'entrainement, 100 pour le test.



Sur une partition aléatoire



Variabilité d'une partition à l'autre

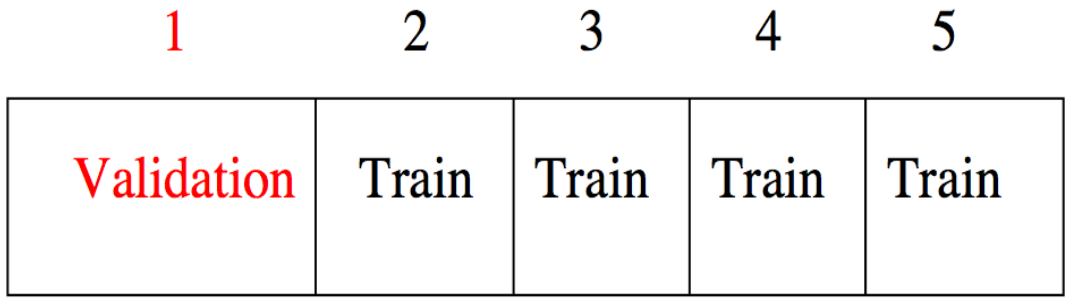
Inconvénients de l'approche par ensemble de validation

- L'estimation obtenue par cette méthode peut être très variable, et dépend de la chance ou malchance dans la construction du sous-échantillon de validation
- Dans cette approche, seule une moitié des observations est utilisée pour ajuster les modèles — celles qui sont dans l'ensemble d'entrainement.
- Cela suggère que l'erreur calculée peut surestimer l'erreur de test d'un modèle ajusté sur l'ensemble des données (moins de variabilité d'échantillonnage dans l'inférence des paramètres du modèle)

Déjà mieux : échanger les rôles entrainement-validation et faire la moyenne des deux erreurs obtenues. On *croise* les rôles.

Validation croisée à K groupes

- C'est la méthode la plus couramment utilisée pour estimer l'erreur de test
- L'estimation peut être utilisée pour choisir le meilleur modèle (la meilleure méthode d'apprentissage), ou approcher l'erreur de prédiction du modèle finalement choisi.
- L'idée est de diviser les données en K groupes de même taille. On laisse le k-ème bloc de côté, on ajuste le modèle, et on l'évalue sur le bloc laissé de côté.
- On répète l'opération en laissant de côté le bloc $k = 1$, puis $k = 2, \ldots$ jusqu'à $k = K$. Et on combine les résultats



Détails

- Pour chacune des observations, on obtient une prédiction $\widehat{y_i} = \widehat{f}(x_i)$ ou $\widehat{g}(x_i)$ au moment où i est dans le groupe mis de côté, et une seule prédiction.
- On compare alors ces prédictions aux observations comme pour l'erreur de test

$$MSE_{(K)} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{f}(x_i))^2$$

ou

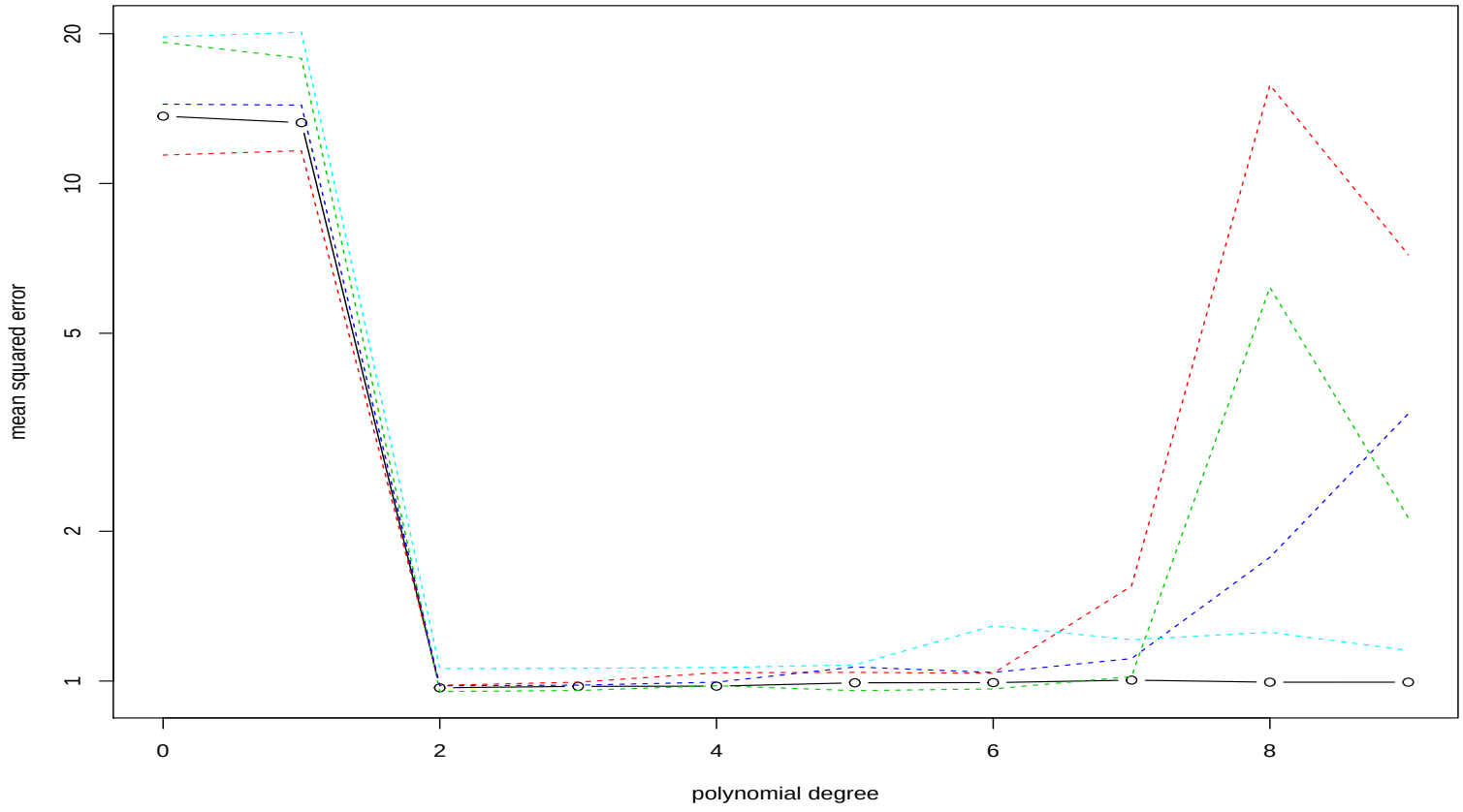
$$\tau_{(K)} = \frac{1}{n}\sum_{i=1}^{n} 1\{y_i \neq \widehat{g}(x_i)\}$$

- Lorsque $K = n$, on parle de *leave-one out cross-validation*(LOOCV)

Danger avec le leave-one out !

- On dit que LOOCV ne secoue pas assez les données. En effet, les classifiers $\widehat{C}$ ou les fonctions de régression inférées $\widehat{f}$ avec $(n-1)$ données sont très corrélés les uns aux autres.
- On ne voit plus l'erreur d'échantillonnage, autrement dit la variabilité de l'estimation de la fonction. C'était pourtant tout l'intérêt de la validation croisée. On choisit généralement $K = 5$ ou $K = 10$ blocs.

Retour au jeu de données simulé



En cas d'égalité, choisir le modèle le plus *parcimonieux* car il aura naturellement moins de variance d'estimation dans les coefficients du modèle.

Méthodes basées sur des arbres

- Nous décrivons ici des méthodes *basées sur des arbres* pour la classification et la régression.
- Cela implique de *stratifier* ou *segmenter* l'espace des prédicteurs en un certain nombre de régions simples.
- Comme les règles des partitionnement peuvent être résumées par un arbre, ce type d'approches sont connues comme des méthodes à *arbres de décision*.

Pours et contres

- Les méthodes basées sur des arbres sont simples et utiles pour l'interprétation.
- Cependant, elles ne sont pas capables de rivaliser avec les meilleures approches d'apprentissage supervisé en terme de qualité de prédiction.
- Nous discuterons donc aussi de *bagging*, *forêts aléatoires (random forests)*, et *boosting*. Ces méthodes développent de nombreux arbres de décision qui sont ensuite *combinés* pour produire une réponse consensus.

Decision trees

Can we collect data to automatically create a decision tree, without domain experts?

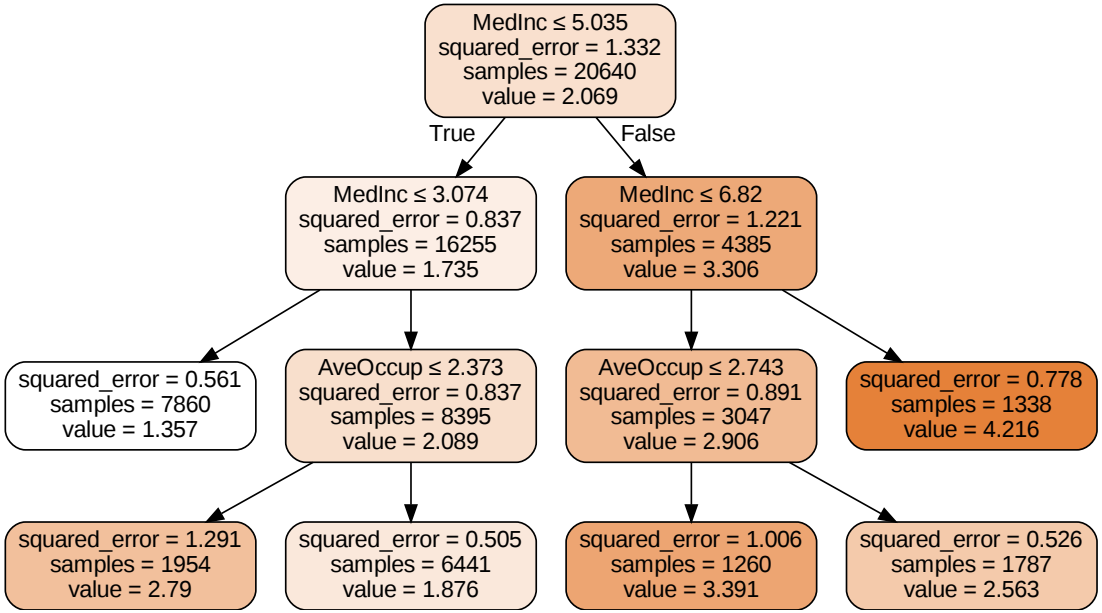
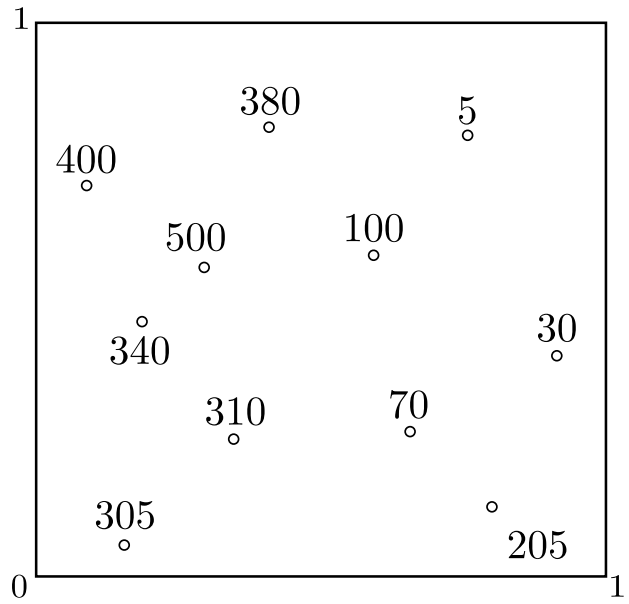


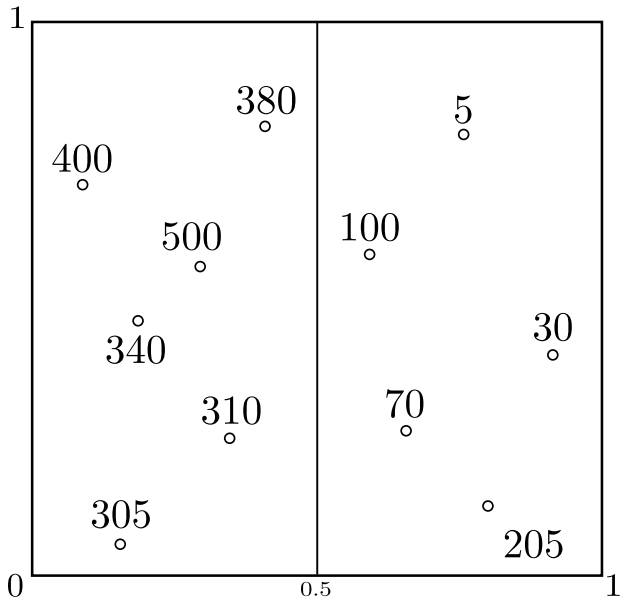
Figure: Output of a decision tree trained on a real-estate data set (1990 California housing data set).

Construction of Decision trees - regression



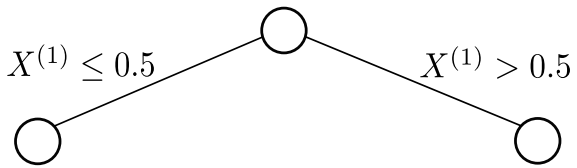
$k = 0$

Construction of Decision trees - regression

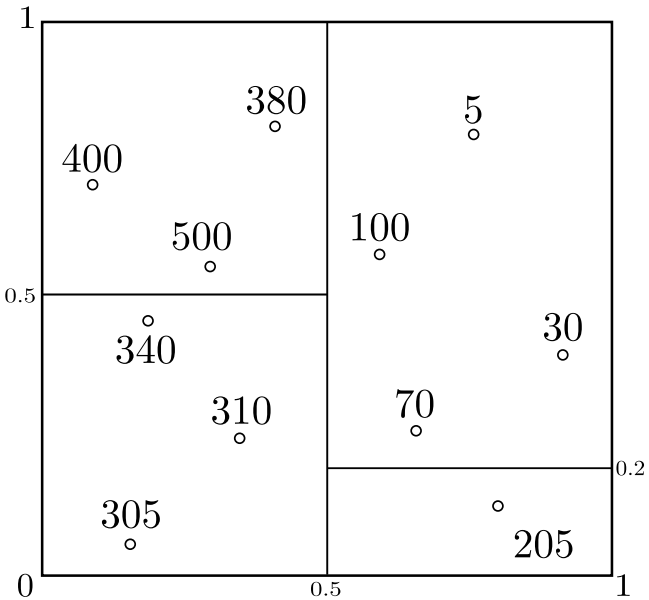


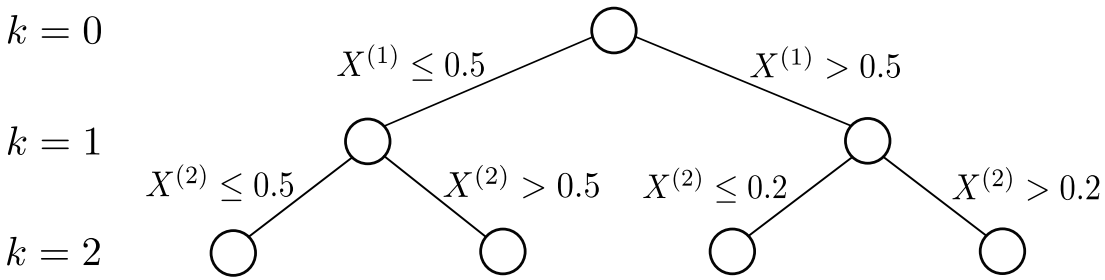
$k = 0$

$k = 1$

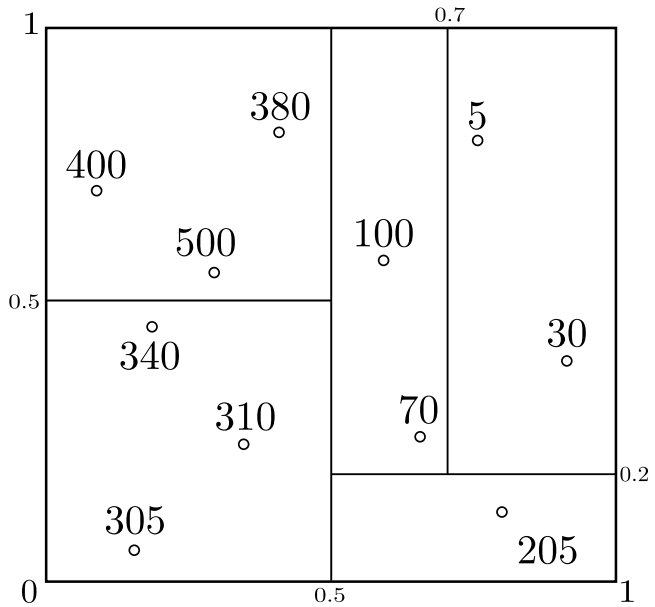


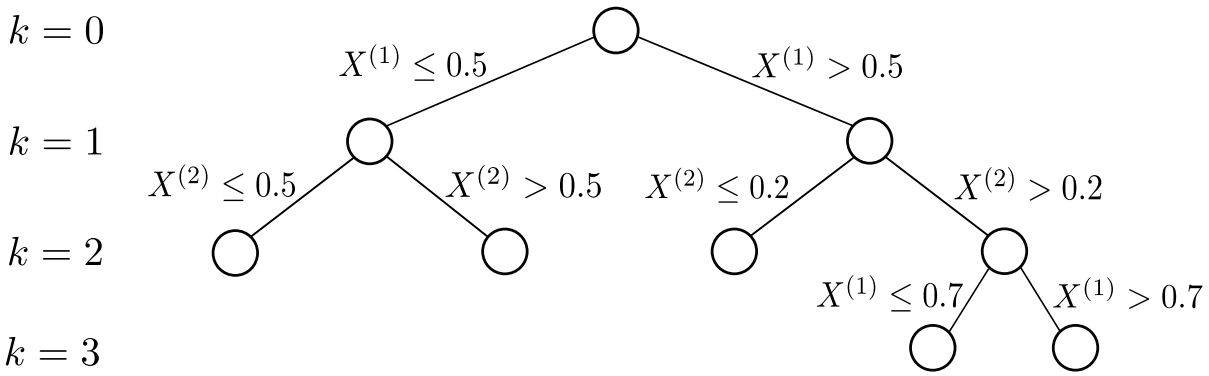
Construction of Decision trees - regression





Construction of Decision trees - regression





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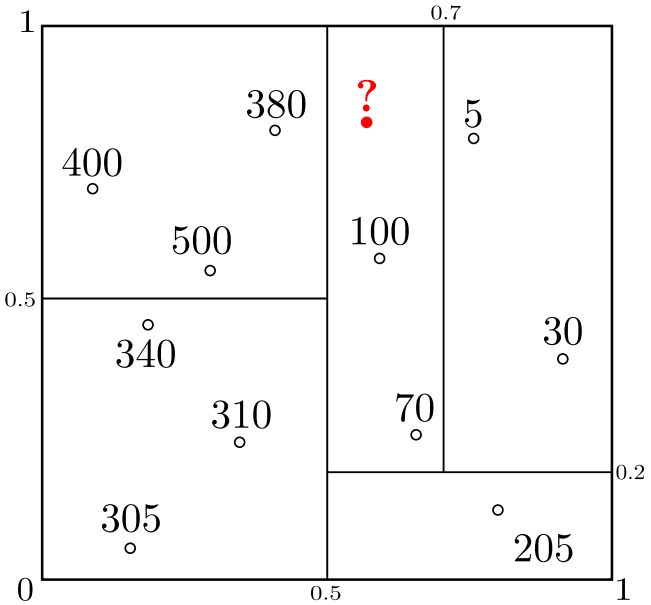

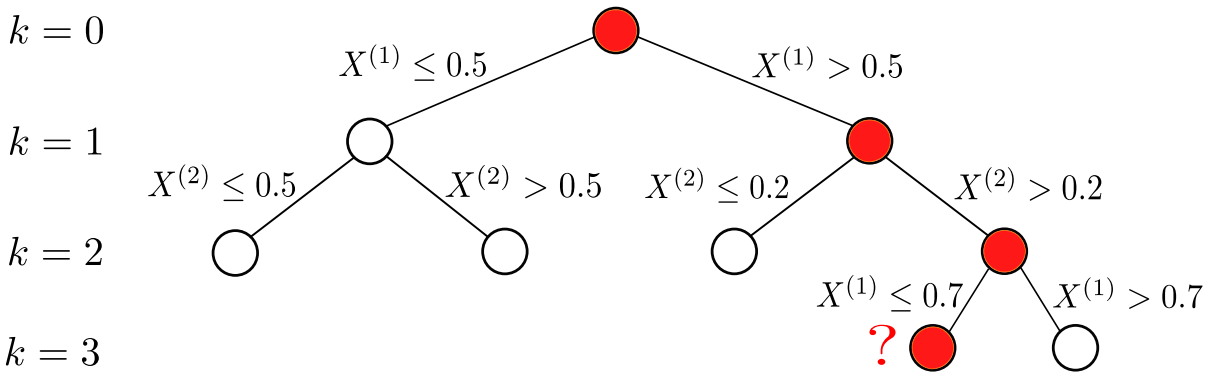

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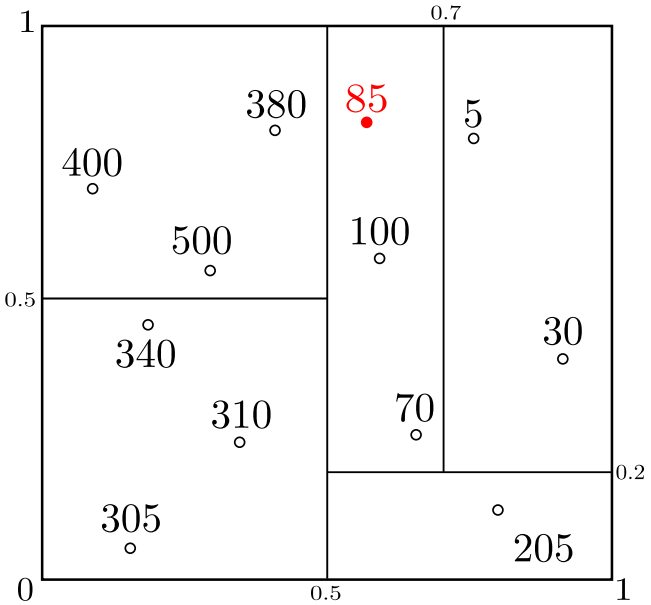

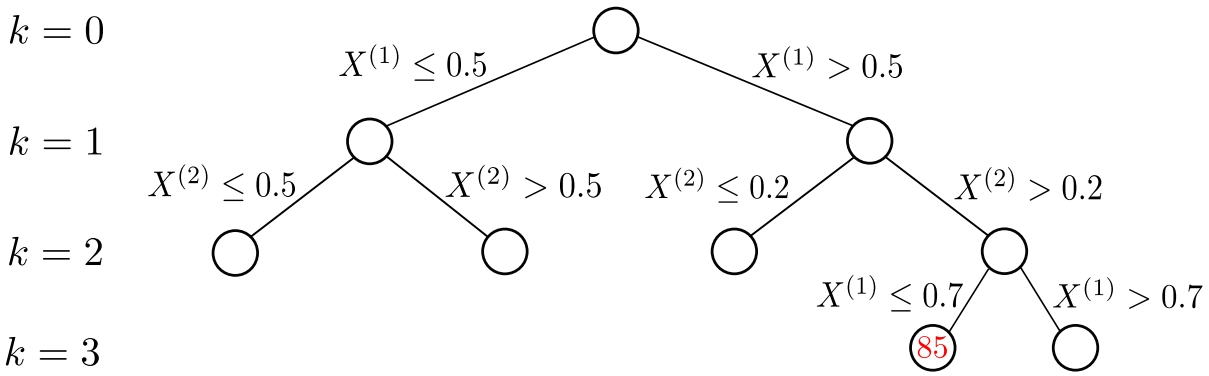

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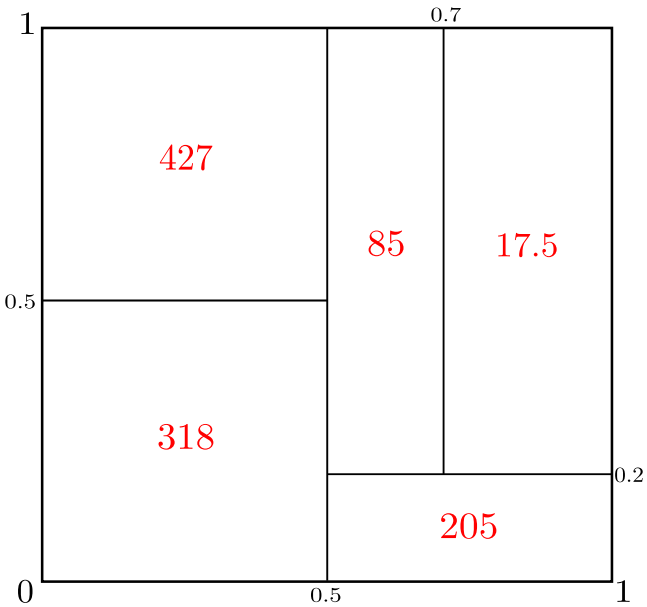

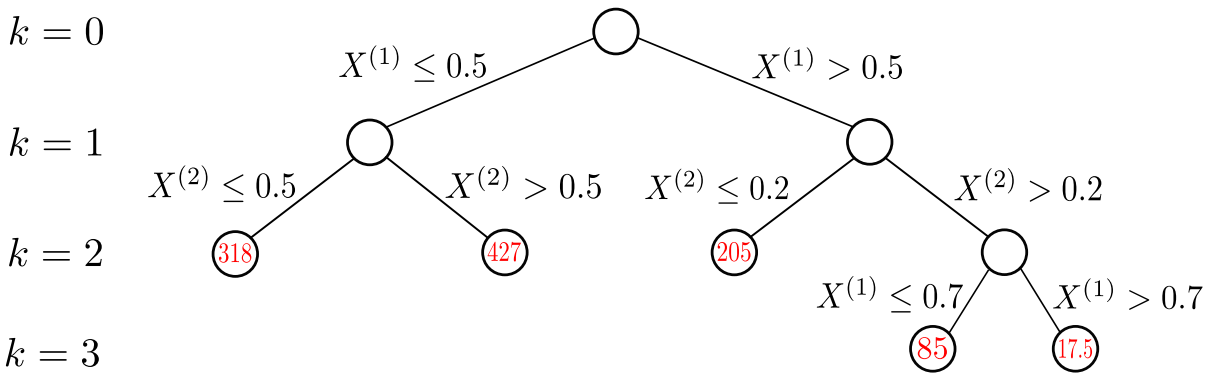

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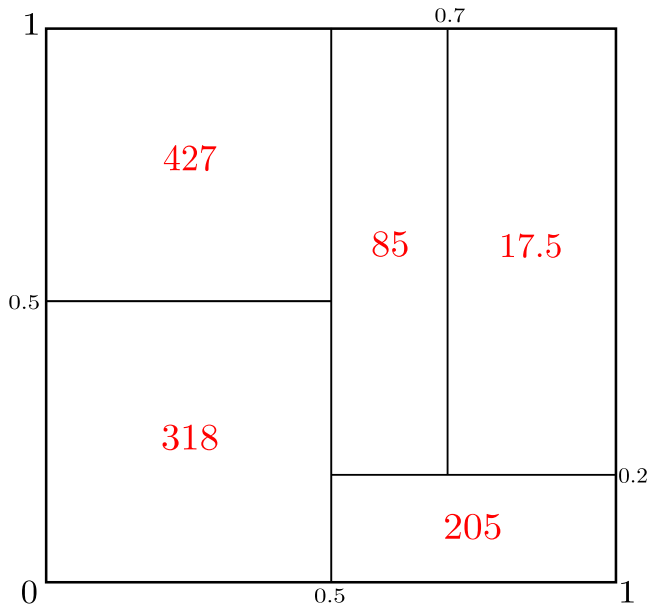
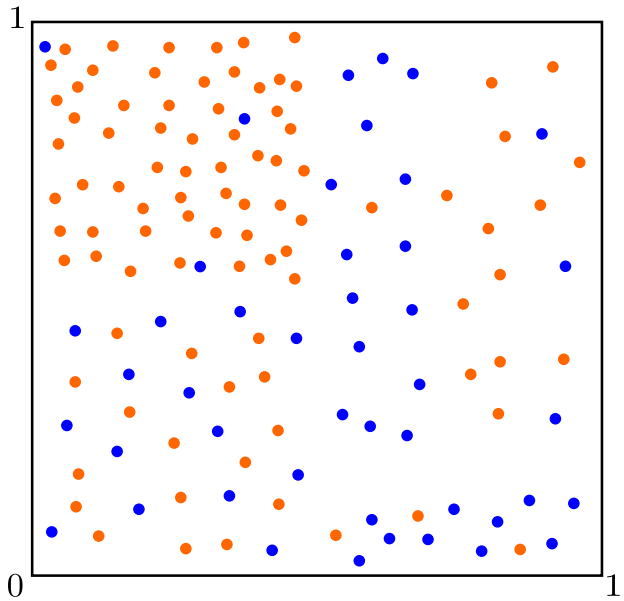


Decision tree building

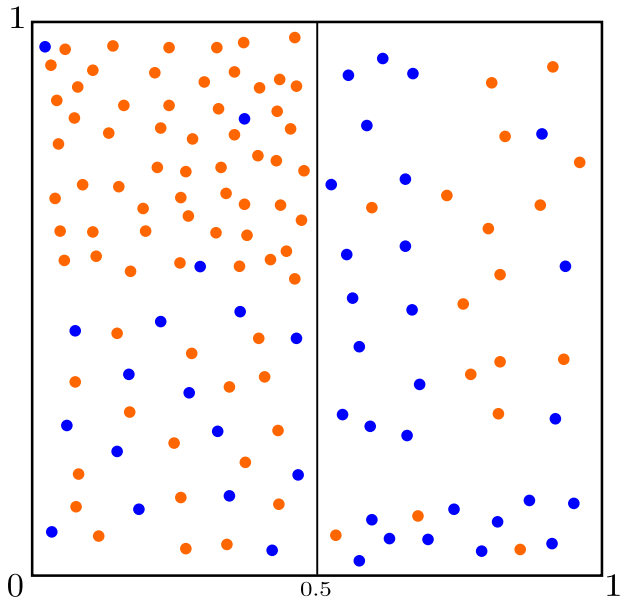
- Requires a splitting rule
- Requires a stopping rule
- Requires a prediction rule
  $\rightarrow$ Average per leaf

Construction of Decision trees - classification



$k = 0$

Construction of Decision trees - classification



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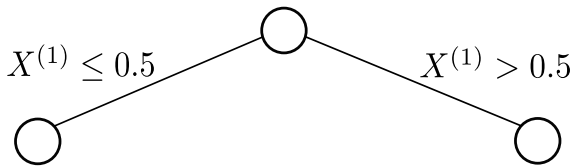
$k = 1$



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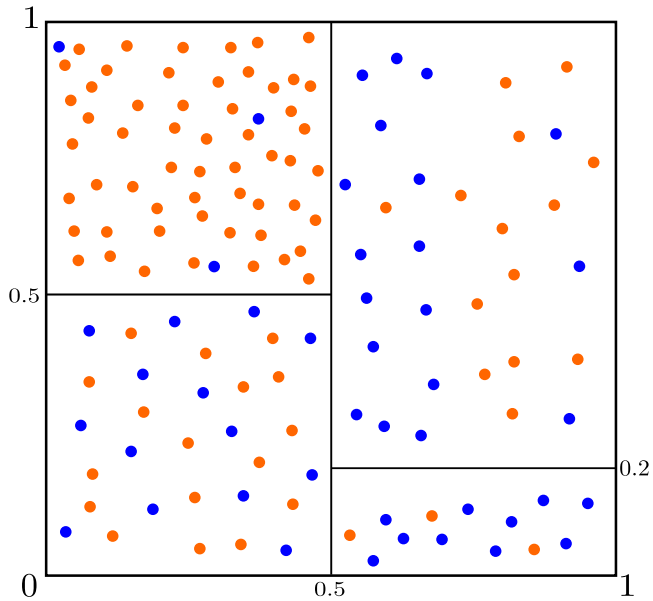
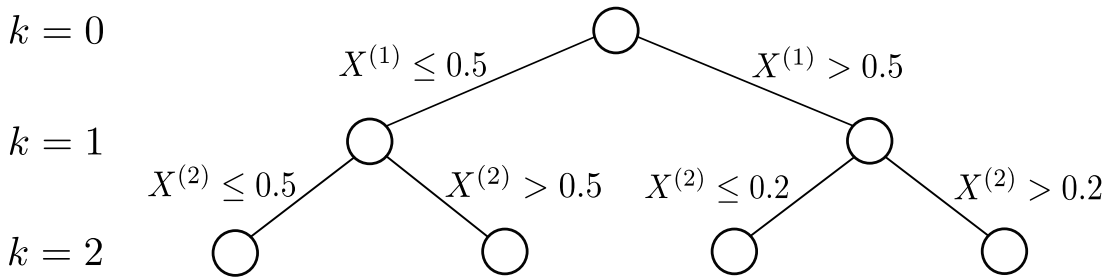
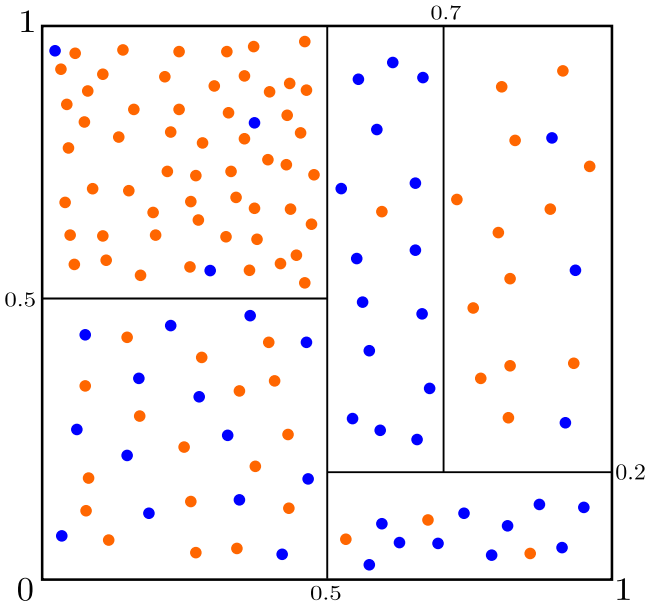
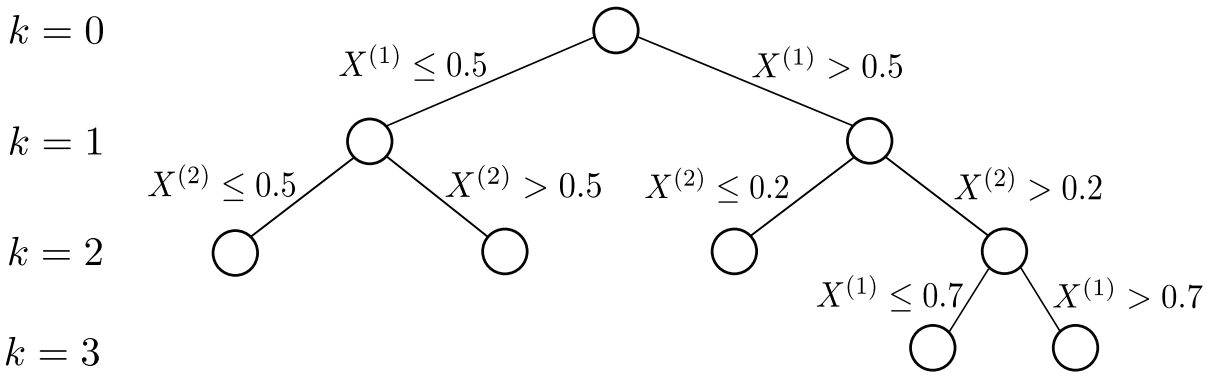




Construction of Decision trees - classification





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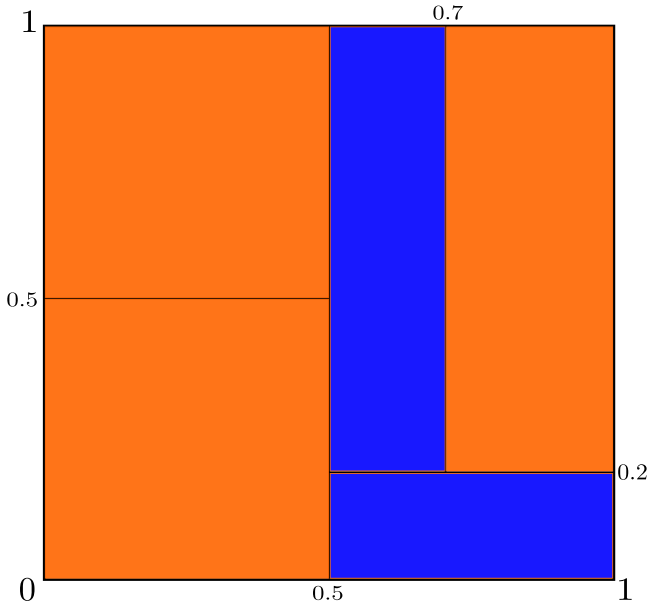
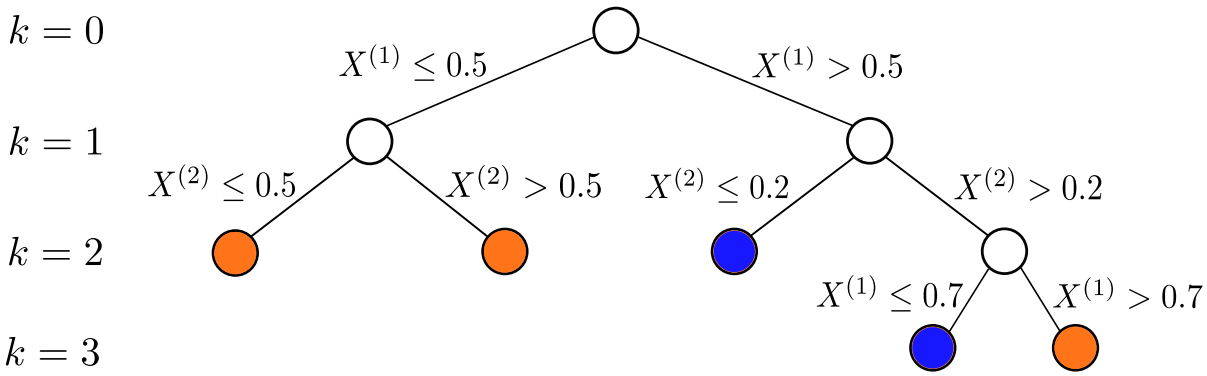
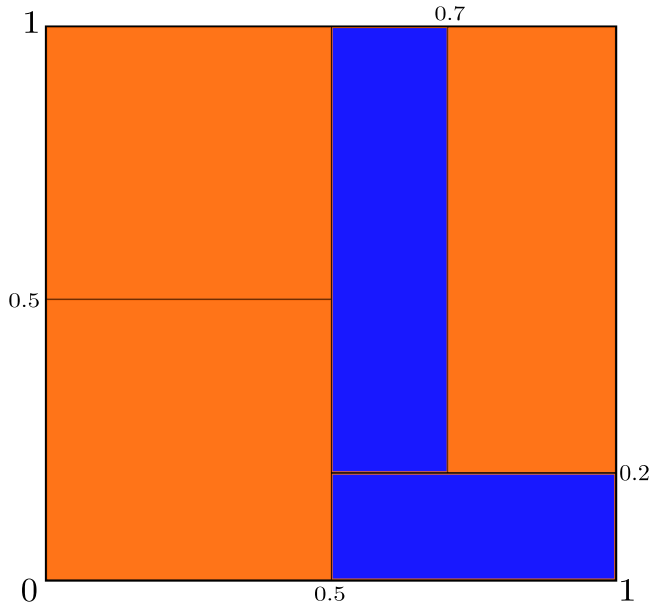




Construction of Decision trees - classification



Decision tree building

- Requires a splitting rule
- Requires a stopping rule
- Requires a prediction rule
  $\rightarrow$ Majority vote per leaf

Outline

Outline

Splitting criterion

Finding the best split in a cell A requires an impurity criterion Imp. Based on this criterion, one can define the impurity reduction associated to a split (j, s) as

$$\begin{aligned} &\Delta Imp(j, s; A) \\ =&Imp(A) - p_L Imp(A_L) - p_R Imp(A_R), \end{aligned} \tag{1}$$

where p_L (resp. p_R) is the fraction of observations in A that fall into A_L (resp. A_R).

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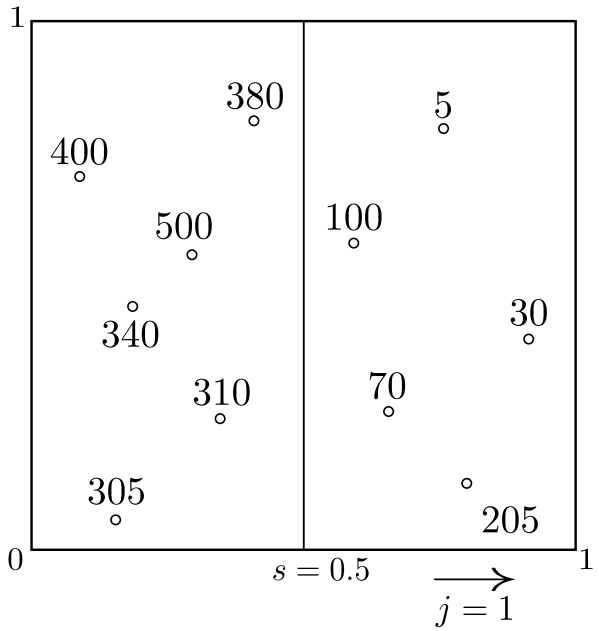

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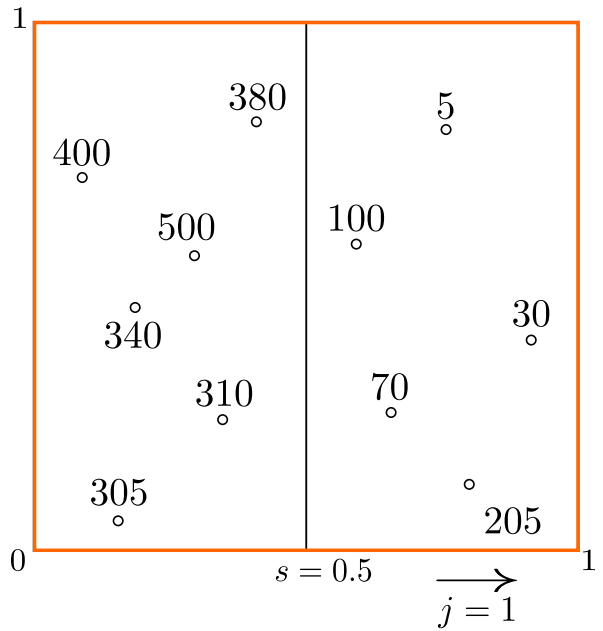

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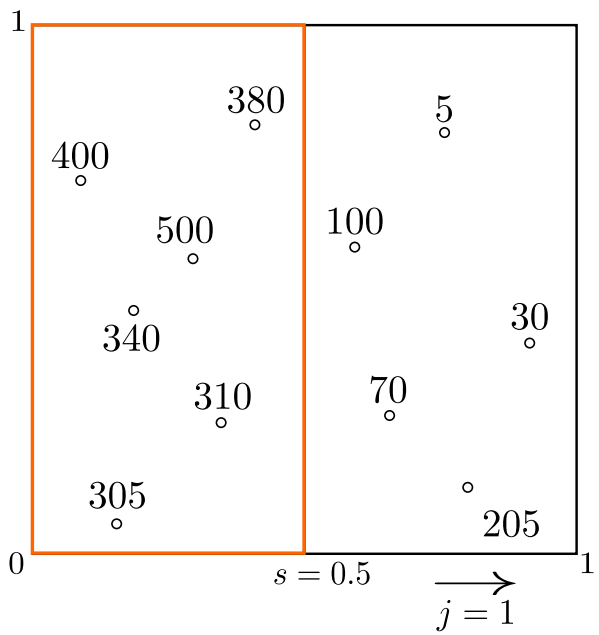

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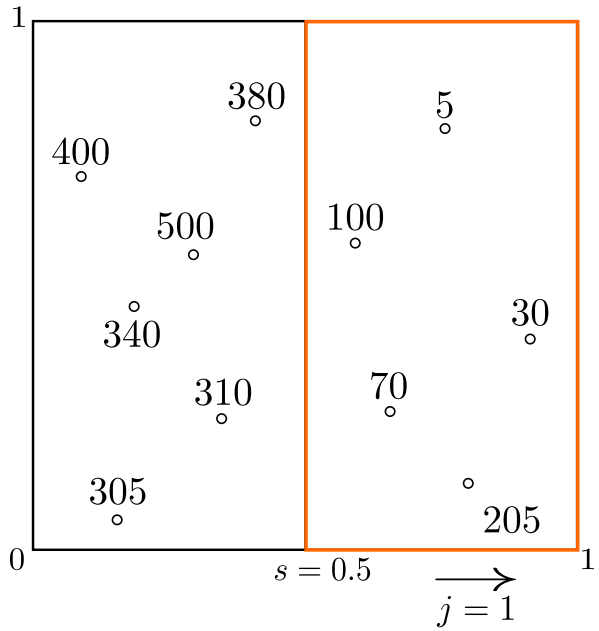

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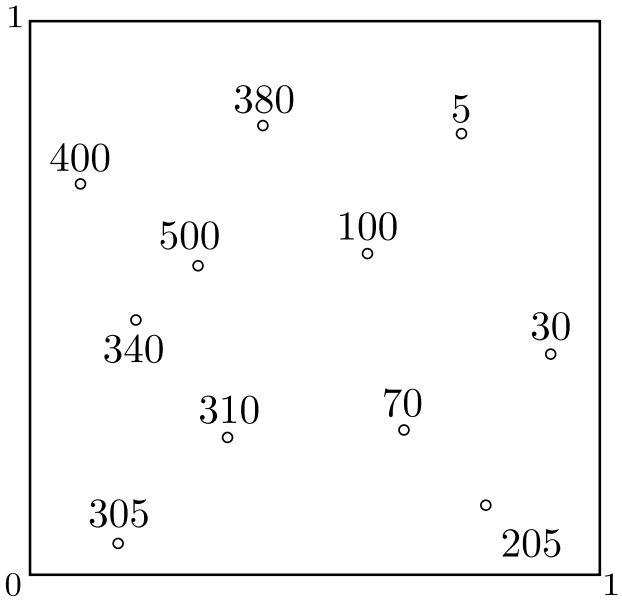
The best split $(j^\star, s^\star)$ is then chosen as

$$(j^\star, s^\star) \in \underset{j,s}{\operatorname{argmax}}\, \Delta Imp(j, s; A). \tag{2}$$

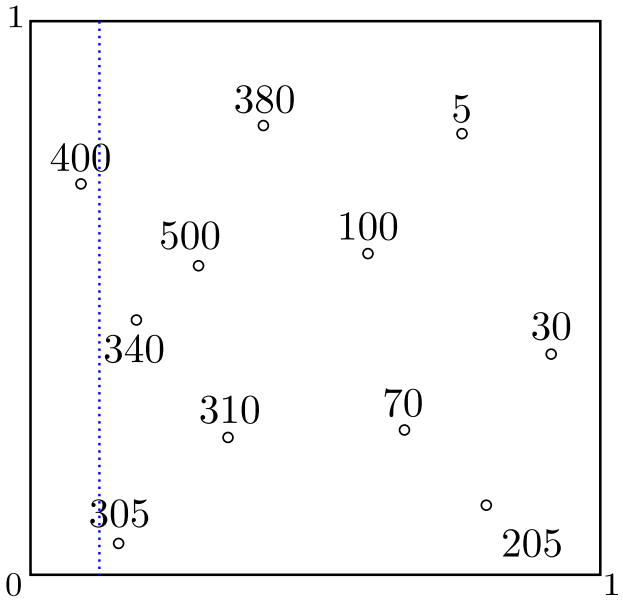
An instance of $Imp(A)$ in regression: the empirical variance of the Y_is in A.

Finding the best split - an example



- Consider splits at the middle of two consecutive observations
- For each split, compute the decrease in impurity between the parent node and the two resulting nodes.

Finding the best split - an example



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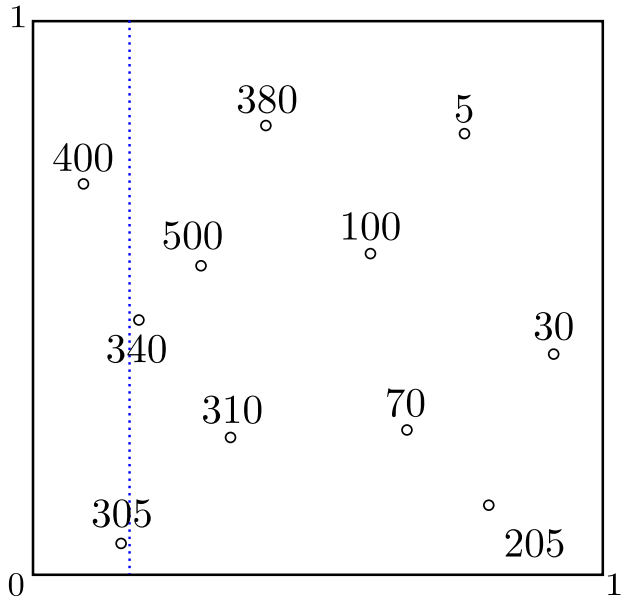

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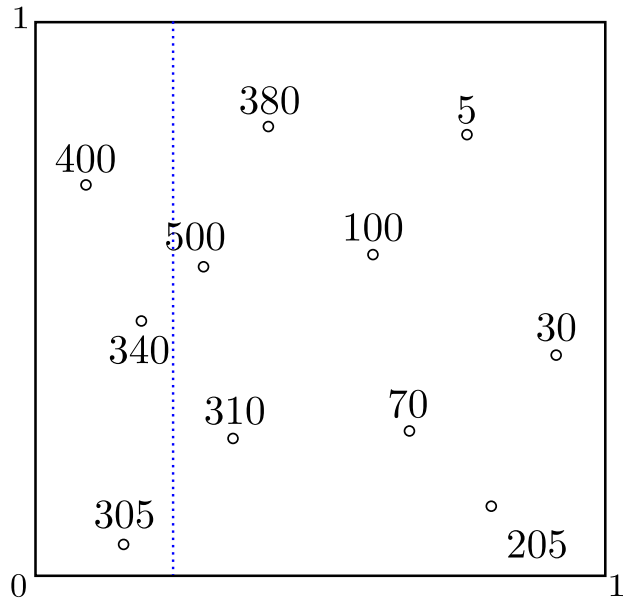

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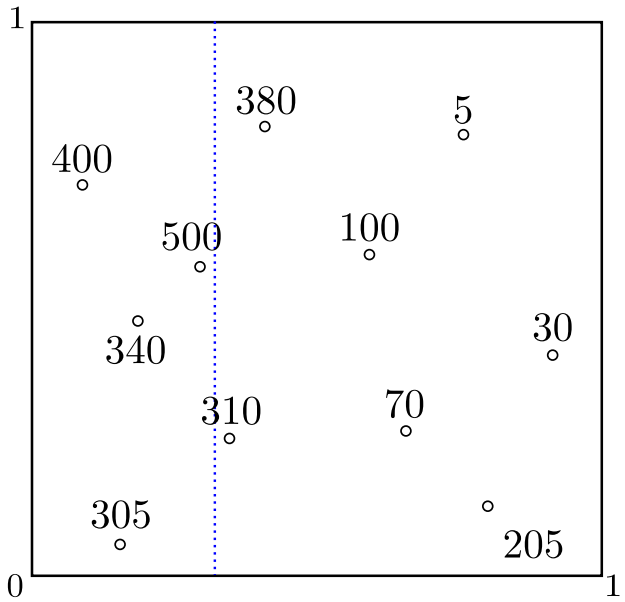

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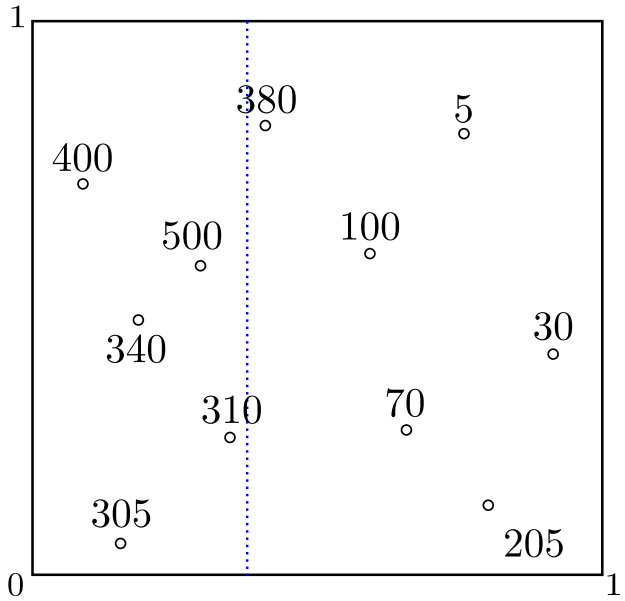

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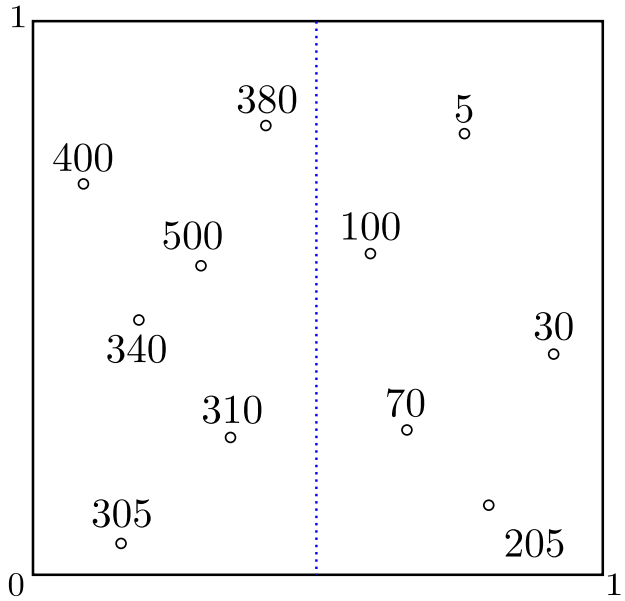

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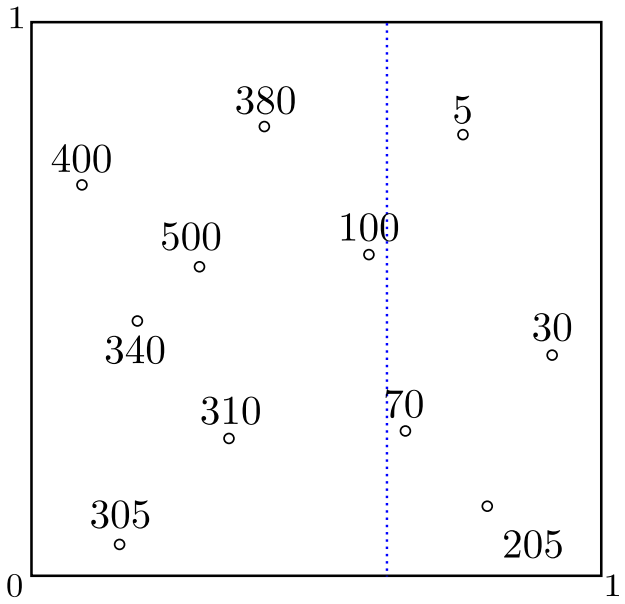

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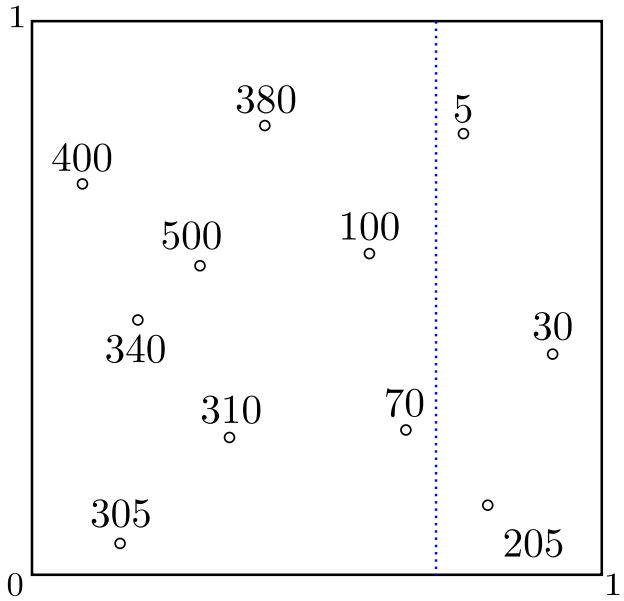

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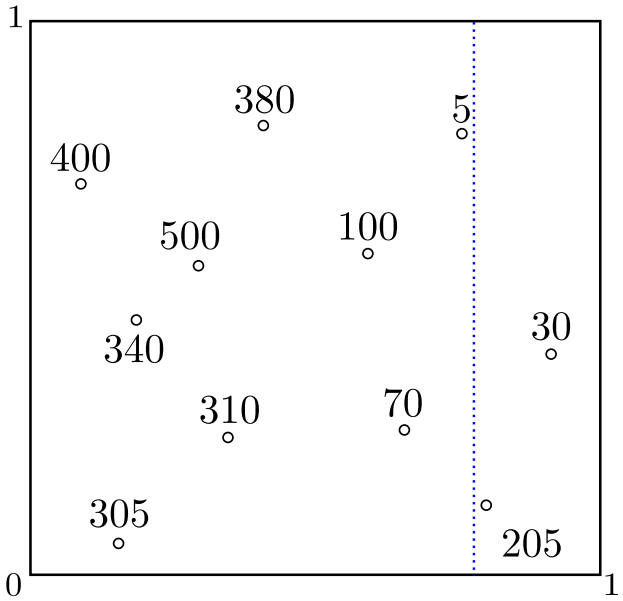

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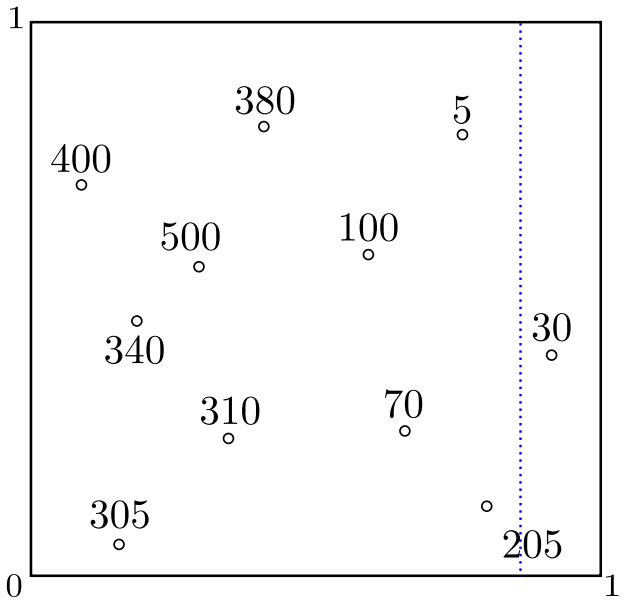

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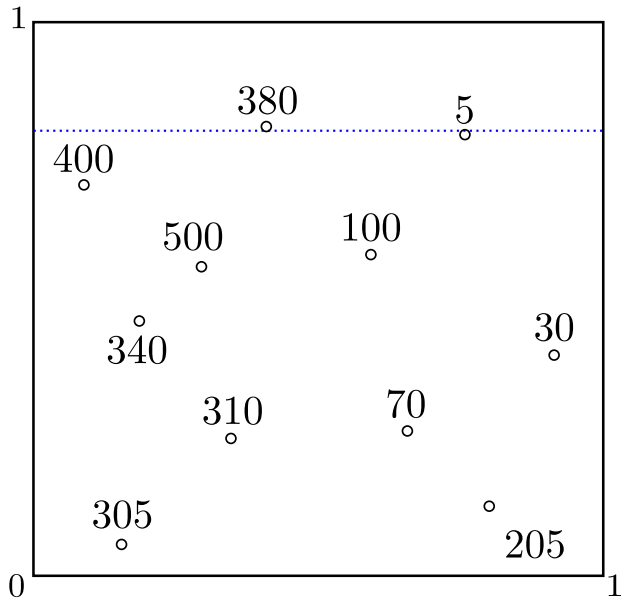

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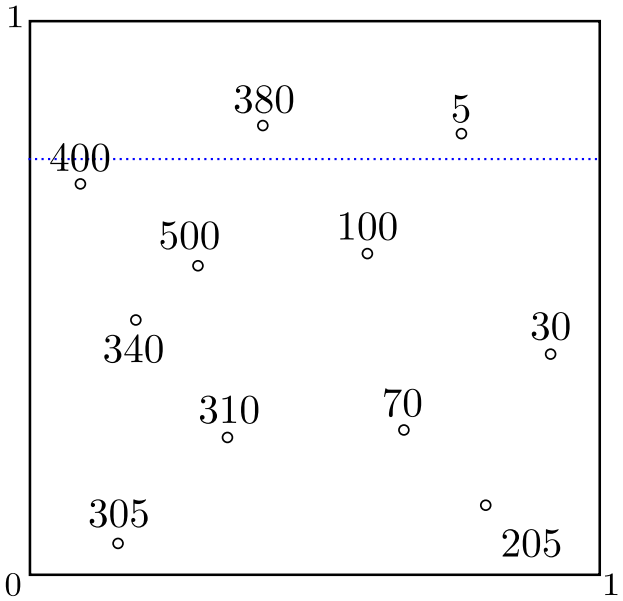

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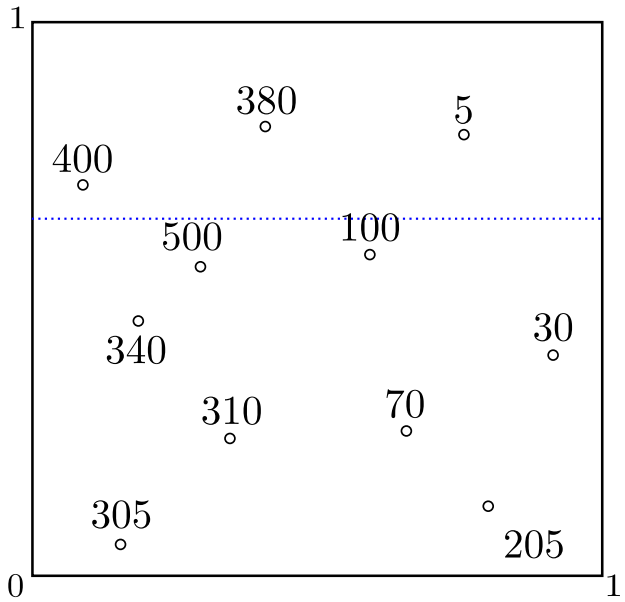
Finding the best split - an example



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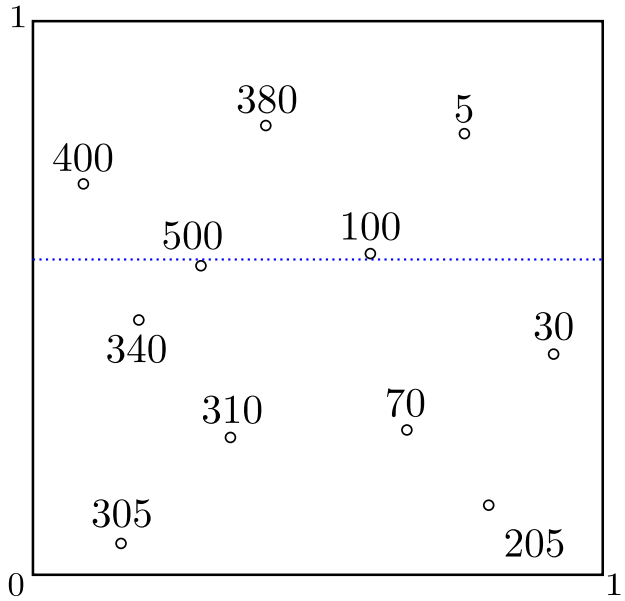

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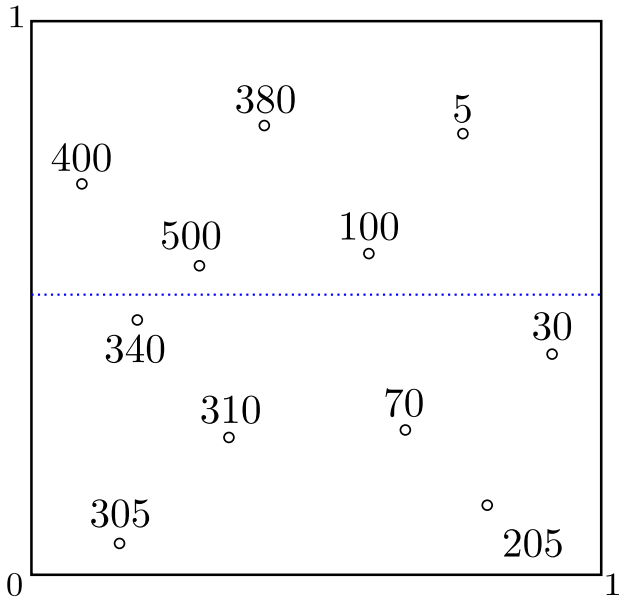

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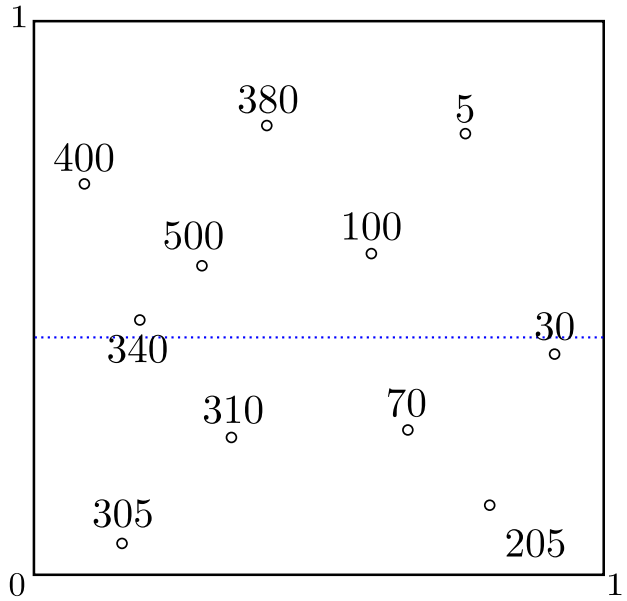

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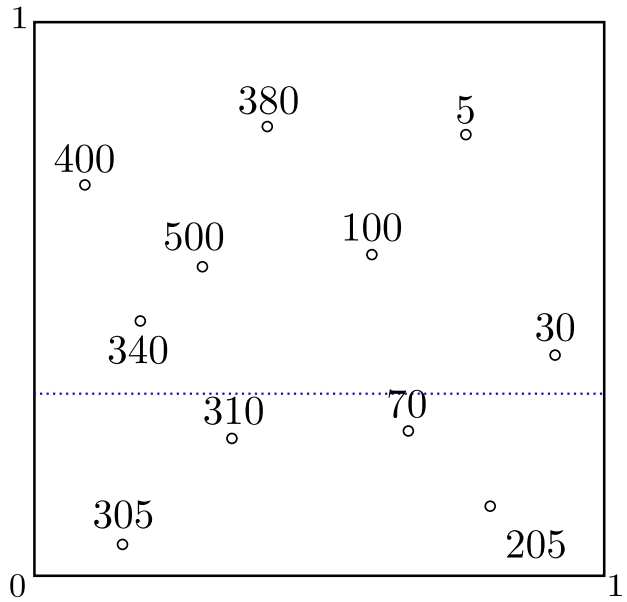
Finding the best split - an example



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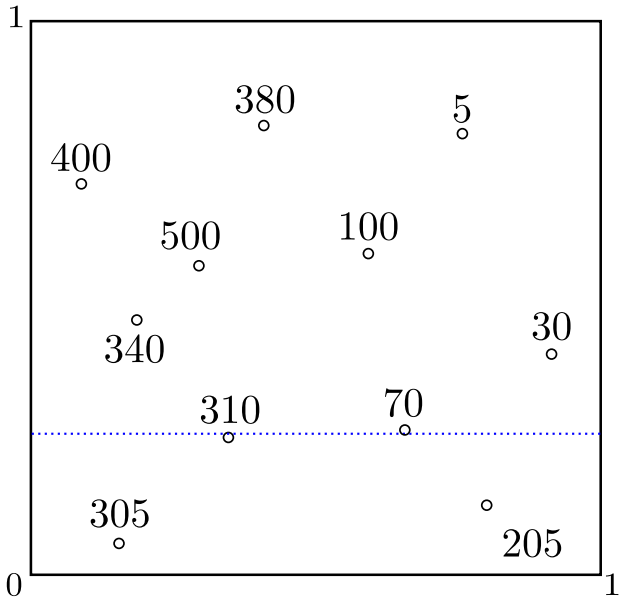

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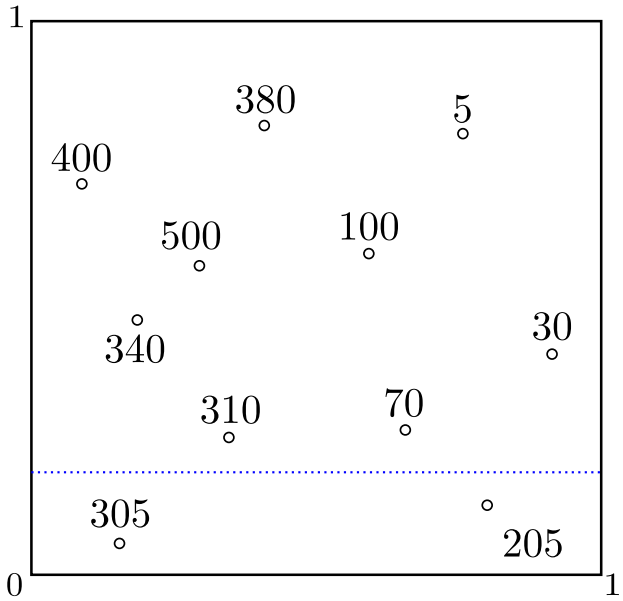

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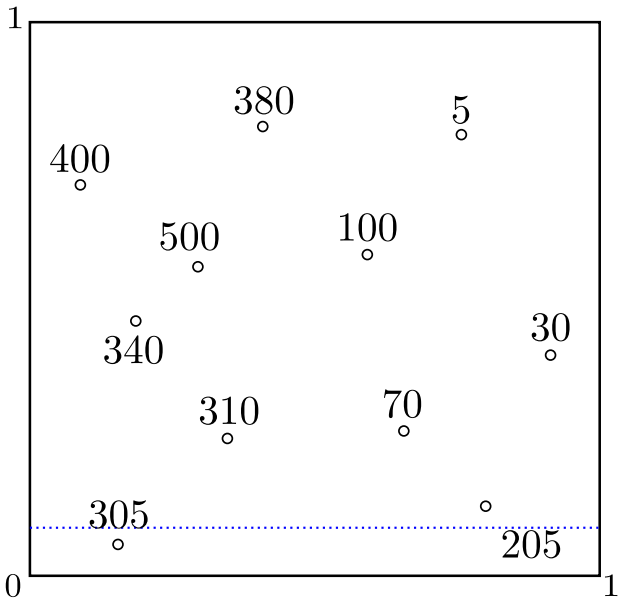

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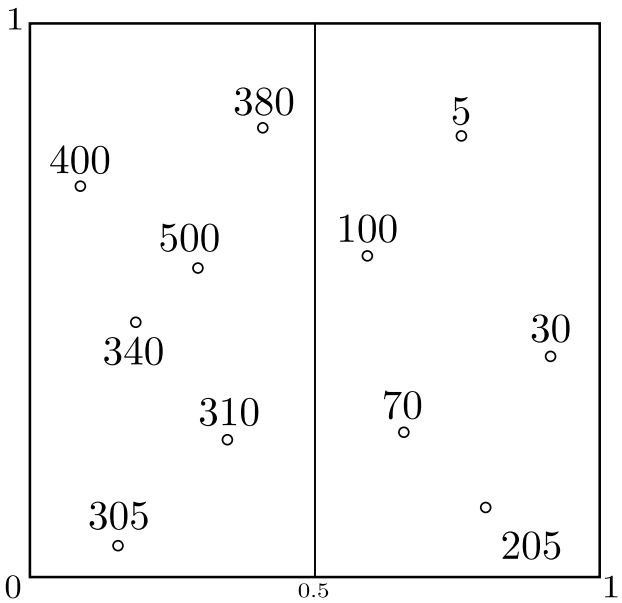

- Consider splits at the middle of two consecutive observations
- For each split, compute the decrease in impurity between the parent node and the two resulting nodes.
- Select the split maximizing the decrease in impurity

Impurity criteria

For **regression**, letting $N_n(A)$ the number of observations in the cell A and $\bar{Y}_A$ the mean of the Y_is in A:

- Variance

$$Imp_V(A) = \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2, \tag{3}$$

- Mean absolute deviation around the median

$$\begin{aligned} &Imp_{L_1}(A) \\ =&\frac{1}{N_n(A)} \sum_{i, X_i \in A} |Y_i - \mathrm{Med}(Y_i : X_i \in A)|. \end{aligned} \tag{4}$$

Impurity criteria

For **classification**, letting $p_{k,n}(A)$ the proportion of observations in A such that $Y = k$:

- Misclassification error rate

$$Imp_{err}(A) = 1 - \max_{1 \leq k \leq K} p_{k,n}(A) \quad (3)$$

- Gini

$$Imp_G(A) = \sum_{k=1}^{K} p_{k,n}(A)(1 - p_{k,n}(A)). \quad (4)$$

- Entropy

$$Imp_H(A) = -\sum_{k=1}^{K} p_{k,n}(A) \log_2(p_{k,n}(A)). \quad (5)$$

Splitting criterion and risk of the method

Consider the variance as impurity measure:

$$Imp(A) = \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2. \qquad (6)$$

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$$Imp(A) = \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2. \tag{6}$$

For any split (j, s) in any cell A resulting in cells A_L and A_R, the impurity reduction takes the form

$$\begin{aligned} &\Delta Imp(j, s; A) \\ =&Imp(A) - p_L Imp(A_L) - p_R Imp(A_R) \\ =&\frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_A)^2 \\ &- \frac{1}{N_n(A)} \sum_{i, X_i \in A} (Y_i - \bar{Y}_{A_L} \mathbb{1}_{X_i \in A_L} - \bar{Y}_{A_R} \mathbb{1}_{X_i \in A_R})^2. \end{aligned} \tag{7}$$

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This corresponds to the square loss of a predictor, which is piecewise constant on A_L and A_R, whose values equal the mean of Y_i's in each cell.

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Optimal partition. Finding the tree partition with the minimal quadratic risk on the training set.

- Statistically sound
- Computationally infeasible

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Greedy partition. At each step, finding the split with the minimal quadratic risk on the training set.

- Not the best predictive performances
- Computationally cheap

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General rule. Choose the splitting criterion corresponding to the risk you want to minimize.

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Classification

- The entropy impurity is related to the cross-entropy loss
- The Gini impurity is not related to any loss, as it does not correspond to a majority vote but rather a random one
- The misclassification error rate is related to $0-1$ loss, which should not be used, as detailed hereafter.

Classification - which impurity to use?

We can choose between

- Misclassification rate

$$Imp_{err}(A) = 1 - \max_{1 \leq k \leq K} p_{k,n}(A) \qquad (6)$$

- Gini

$$Imp_G(A) = \sum_{k=1}^{K} p_{k,n}(A)(1 - p_{k,n}(A)). \qquad (7)$$

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Classification - which impurity to use?

In a binary classification setting, impurities can be rewritten as

- Misclassification rate

$$Imp_{err}(A) = 1 - \max_{k \in \{0,1\}} p_{k,n}(A) \tag{6}$$

- Gini

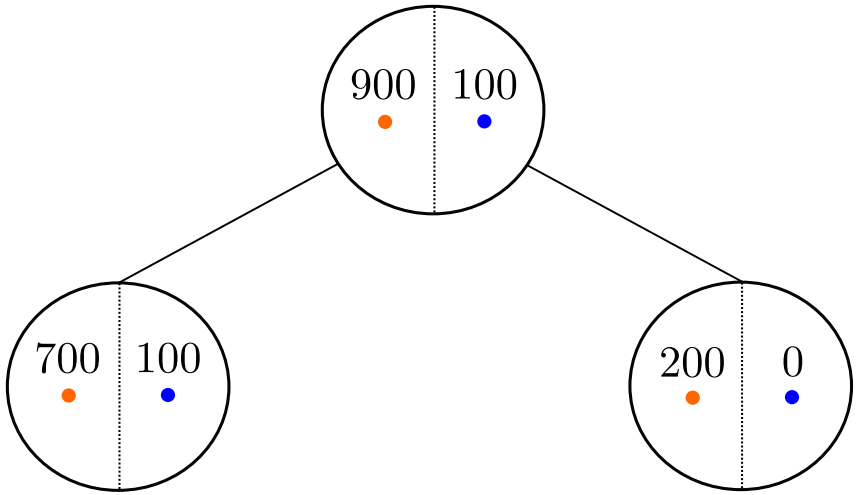
$$Imp_G(A) = 2p_{0,n}(A)(1 - p_{0,n}(A)) \tag{7}$$

- Entropy

$$\begin{aligned} Imp_H(A) = &- p_{0,n}(A) \log_2(p_{0,n}(A)) \\ &- (1 - p_{0,n}(A)) \log_2(1 - p_{0,n}(A)) \end{aligned} \tag{8}$$

Classification - which impurity to use?

Let us take an example:



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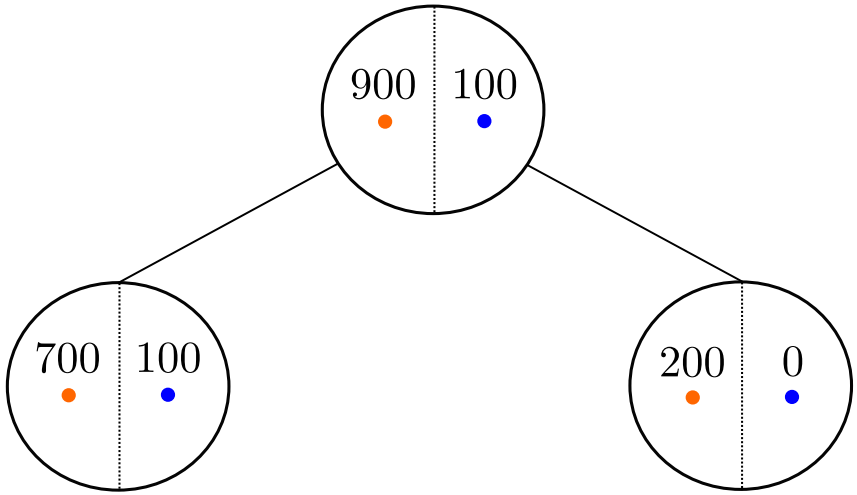

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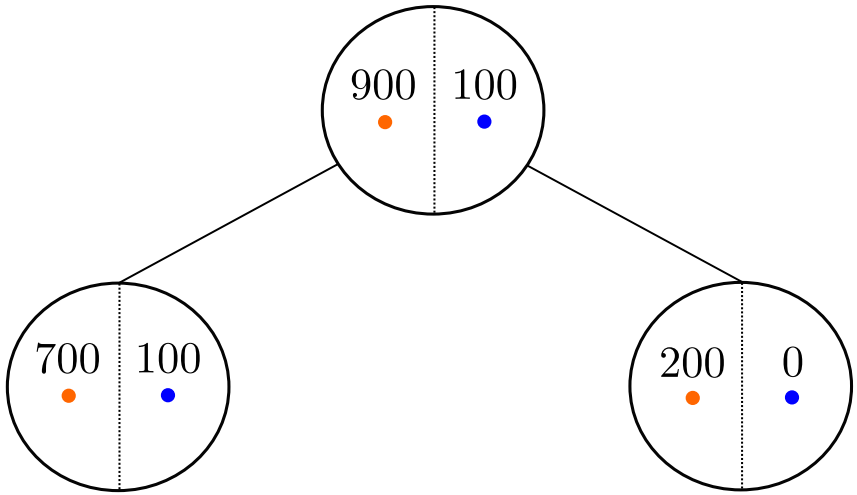

- Since $\Delta Imp_{err} = 0$, the split appears to be non-informative.
- But the right node is pure! The decrease in impurity for the two other criterion is

$$\Delta Imp_G(A) = 0.005$$
$$\text{and} \quad \Delta Imp_H(A) = 0.01. \qquad (6)$$

Classification - which impurity to use?

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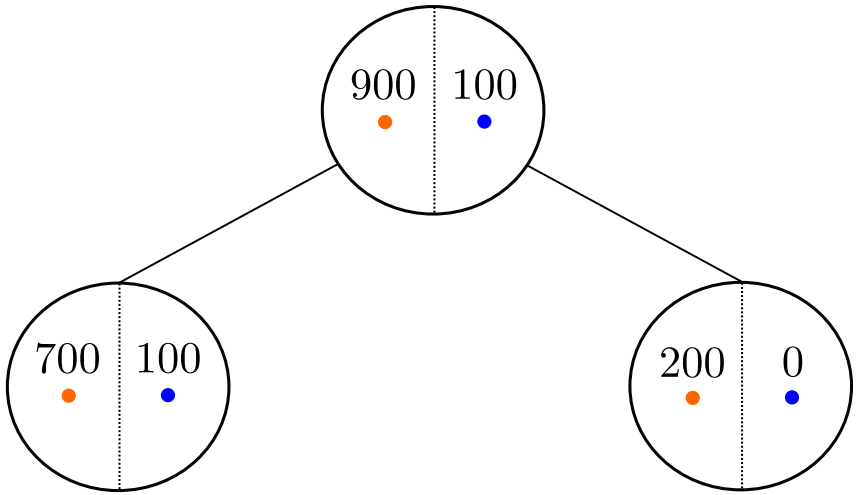

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This phenomenon results from the fact that the misclassification rate in the binary setting is not strictly concave, contrary to the Entrope/Gini criterion. More explanation here[a]

[a] https://tushaargvs.github.io/assets/teaching/dt-notes-2020.pdf

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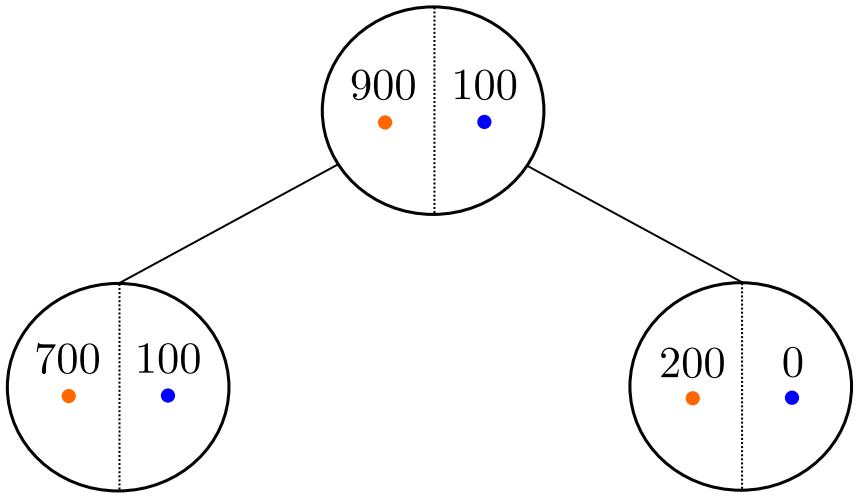

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Misclassification criterion is not precise enough to be used for building trees.

Outline

Decision tree

Now that we have defined a splitting rule, let us see the rest of the tree construction.

Decision tree building

- Splitting rule (Variance in regression, Gini or Entropy in classification)

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- The cell has already been split `max-depth` times (∞, by default)

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- Prediction rule

Prediction rule:

- Regression - Average of labels per leaf

$$\hat{t}_n(x) = \sum_{i=1}^{n} Y_i \frac{\mathbb{1}_{X_i \in A_n(x)}}{N_n(A_n(x))} \qquad (6)$$

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- Classification - Majority vote per leaf

$$\hat{t}_n(x) = \underset{k \in \{1,\dots,K\}}{\operatorname{argmax}} \sum_{i=1}^{n} \frac{\mathbb{1}_{Y_i = k} \mathbb{1}_{X_i \in A_n(x)}}{N_n(A_n(x))} \tag{7}$$

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- Prediction rule (average or majority vote per leaf)

Outline

Handling different types of features

There exist three main types of features:

- Continuous (blood pressure)
- Ordinal (Glasgow score)
- Nominal (Medical treatments)

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Ordinal features. Construction can be directly extended to ordinal features: splits are exactly of the same form $X^{(j)} \leq s$.

Nominal features. For nominal feature, it makes no sense to consider such splits: there is no natural order on treatments.

Nominal features

A **nominal features** $X^{(j)}$ can take different discrete values that are not ordered. For example, $X^{(j)}$ can be the type of treatment, which is surgical, chemical, or nothing (three different modalities).

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Exhaustive search Letting $\mathcal{C}$ the set of all modalities of a variable, any split along this variable is of the form C versus C^c for any $C \subset \mathcal{C}$.

- All partitions of modalities in two groups is admissible
- Computationally costly / infeasible to evaluate all these splits for variables with high cardinality (number of modalities)

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Common practice - One-hot encoding Creating as many new (dummy) variables as modalities. In our example, our treatment variable would become

$(1,0,0)$ for surgical treatments, $(0,1,0)$ for chemical treatments,
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- More limited number of splits, computationally appealing but decreases the model predictivity.

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One-hot encoding is the most common encoding method.

A clever encoding: Target encoding

Nominal variables. A classic way to handle them is via one-hot encoding. Sadly, it limits the predictivity of the model.

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- Choose an impurity (misclassification rate, entropy or Gini)
- Consider a nominal variable X_j that can take L modalities. Reorder it so that the empirical probabilities in a given cell A satisfy

$$\begin{aligned} &\mathbb{P}_n[Y=1|X_j=C_1, X\in A] \\ \leq &\mathbb{P}_n[Y=1|X_j=C_2, X\in A] \\ \leq &\ \dots \\ \leq &\mathbb{P}_n[Y=1|X_j=C_L, X\in A]. \end{aligned} \tag{6}$$

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- Then the best split (that maximizes the decrease in impurity) is of the form

$$X_j \in \{C_1, \dots, C_\ell\} \quad \text{vs} \quad X_j \in \{C_{\ell+1}, \dots, C_L\}. \tag{7}$$

This is a result from Fisher 1958

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Summary. Finding the optimal split by reordering and then evaluating $L-1$ splits instead of $2^{L-1}-1$ splits for exhaustive search (and L splits with suboptimal decision for one-hot encoding).

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Extension to regression. The same procedure holds in regression by considering the average values of Y for each modality (instead of the probabilities).

Outline

Generalization / Overfitting

By default, a tree is fully grown, i.e., there is only one observation per leaf.

What is the training error of such trees?

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Pruning strategies are always/often preferred!

$\rightarrow$ Stopping the tree construction when the splitting criterion is low is not a valid strategy.

Pruning strategies

Two types of pruning strategies exist:

- Reducing Error, consists in removing branches of the fully-grown tree, based on the error computed on an extra data set (validation set). Simple but implies that less data are used for the training of the tree (first step).
- Cost-complexity pruning (CART) is based on a penalization of the decision tree error via the number of leaves.

Pruning strategies

Cost-complexity pruning. Let T_0 be the trained fully-grown tree. We denote by $R(T)$ the risk of any tree T, defined as either the misclassification rate (1 - accuracy) or the weighted impurity of each one of its leaves:

$$R(T) = \sum_{A \in \text{Leaf}(T)} p_A Imp(A), \tag{8}$$

where p_A is the proportion of observations falling into A (usually $1/n$).

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As mentioned before, for a fully-grown tree T_0, $R(T_0) = 0$ and then does not give a good measure of predictive performances of T_0.

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For all $\alpha > 0$, we define the cost-complexity measure $R_\alpha(T)$ as

$$R_\alpha(T) = R(T) + \alpha|\text{Leaf}(T)|, \tag{9}$$

where $|\text{Leaf}(T)|$ is the number of leaves in T.

A cross-validation procedure can then be used to select the best value for α, therefore producing an shallower tree than T_0.

Outline

Final algorithm

Tree construction

- Input: a dataset, an impurity measure.
- At each node A, select the best split via
$$(j^\star, s^\star) \in \underset{j \in \{1,\dots,d\}, s \in \text{range}(X^{(j)})}{\text{argmax}} \Delta Imp(j, s; A).$$
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Tree prediction Tthe tree prediction at x_{new} is given by the average / majority vote among the training observations falling into the same leaf as x_{new}.

Pro/cons

Benefits

- Work in classification and regression
- Can handle categorical and continuous features
- Interpretable
- Invariant by monotonic transformation of the data
- Missing values
- Numerical complexity : $nd \log n$
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Drawbacks

- Non-robust to small changes in data
- Limited approximation capacity (thresholded nature)

[Fis58] Walter D Fisher. “On grouping for maximum homogeneity”. In: *Journal of the American statistical Association* 53.284 (1958), pp. 789–798.

1. Random forests
   - Bagging and split randomization
   - Random forest algorithm
   - Out-of-bag error
   - Variable importance

2. Tree Boosting
   - Motivation
   - General Boosting algorithm
   - Gradient Boosting Decision Trees

Tree ensemble methods

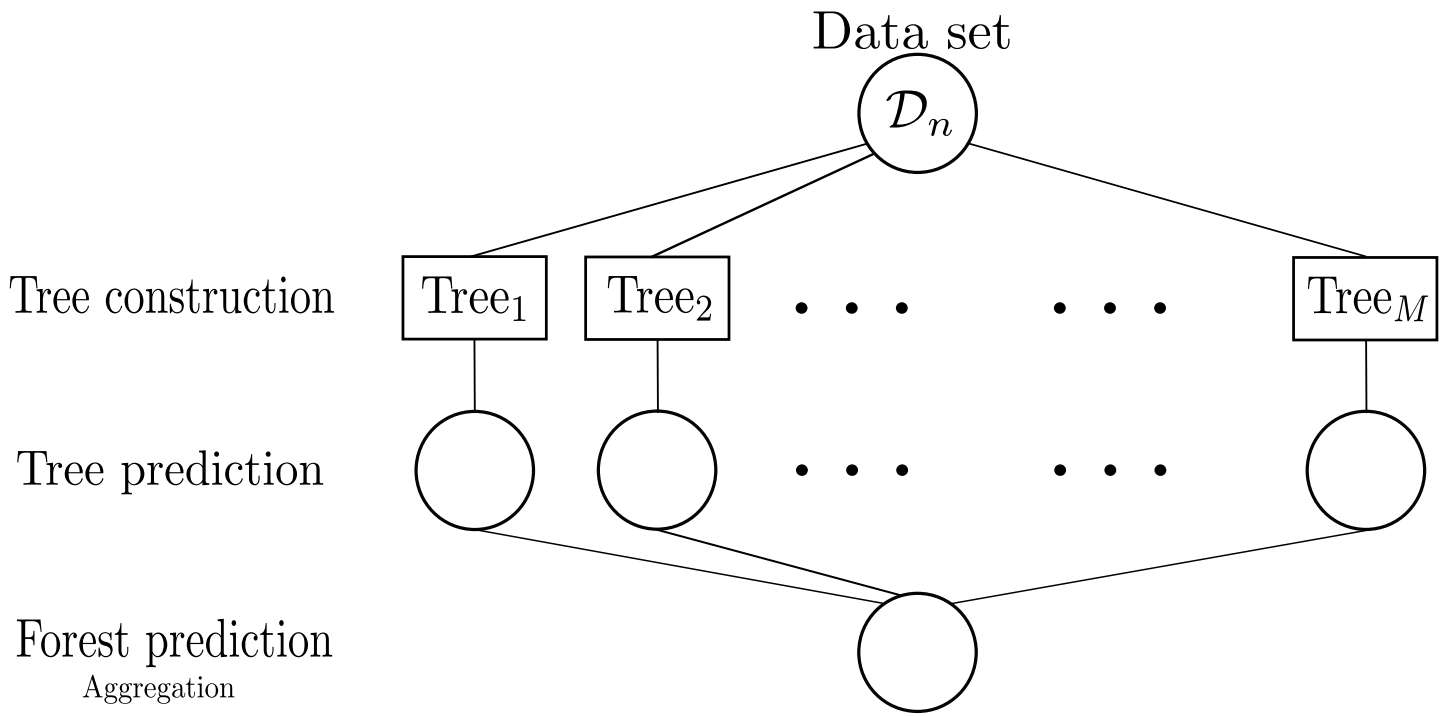
Consist in aggregating the predictions of several decision trees:

- More flexible methods / useful for modelling complex input-output relations
- More robust than individual trees to changes in data

Tree ensemble methods

How to do that?

- Random forests (parallel methods)



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How to do that?

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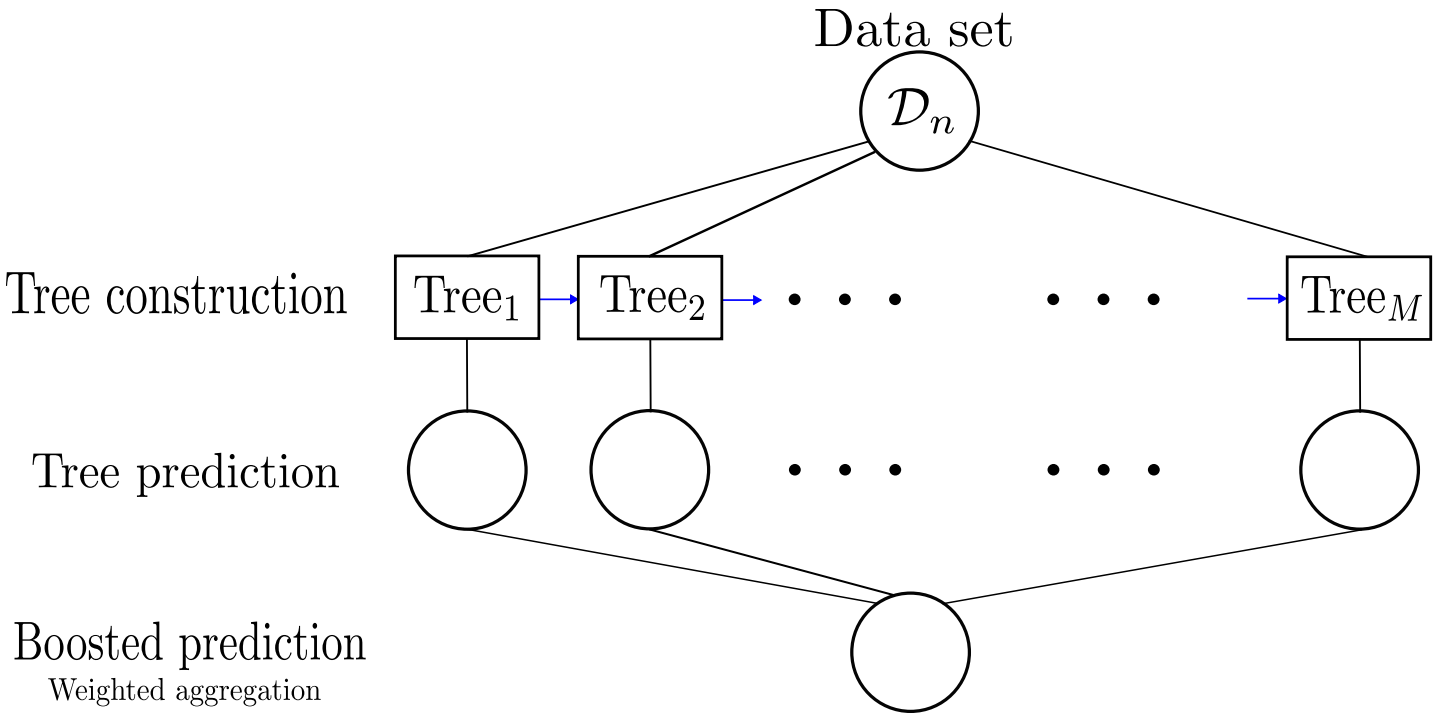
- Tree boosting (sequential methods)



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Tree construction in random forests

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For trees in random forests, no pruning strategy

Such trees have a small bias (fully-grown) but a large variance (one point per leaf).

They cannot be used as single estimators!

Bagging - Averaging predictors via data set resampling

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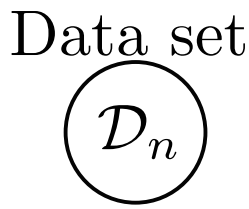
Bootstrap. A sampling scheme that consists in drawing n observations with replacement among the n original ones. Applied once, bootstrap creates one new data set, called a bootstrapped data set.

Bagging - Averaging predictors via data set resampling



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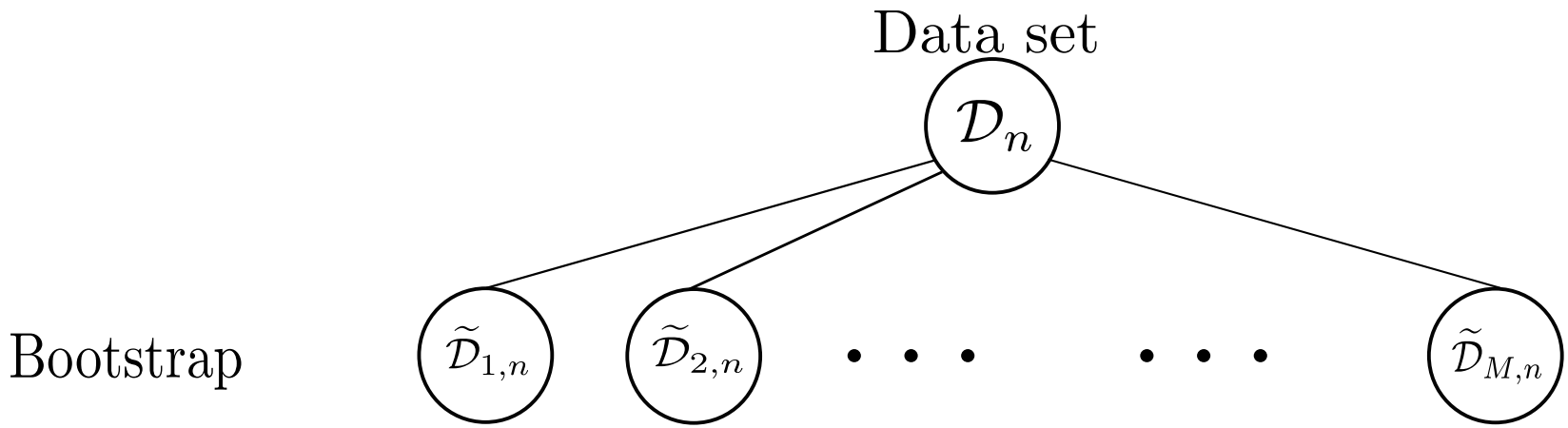

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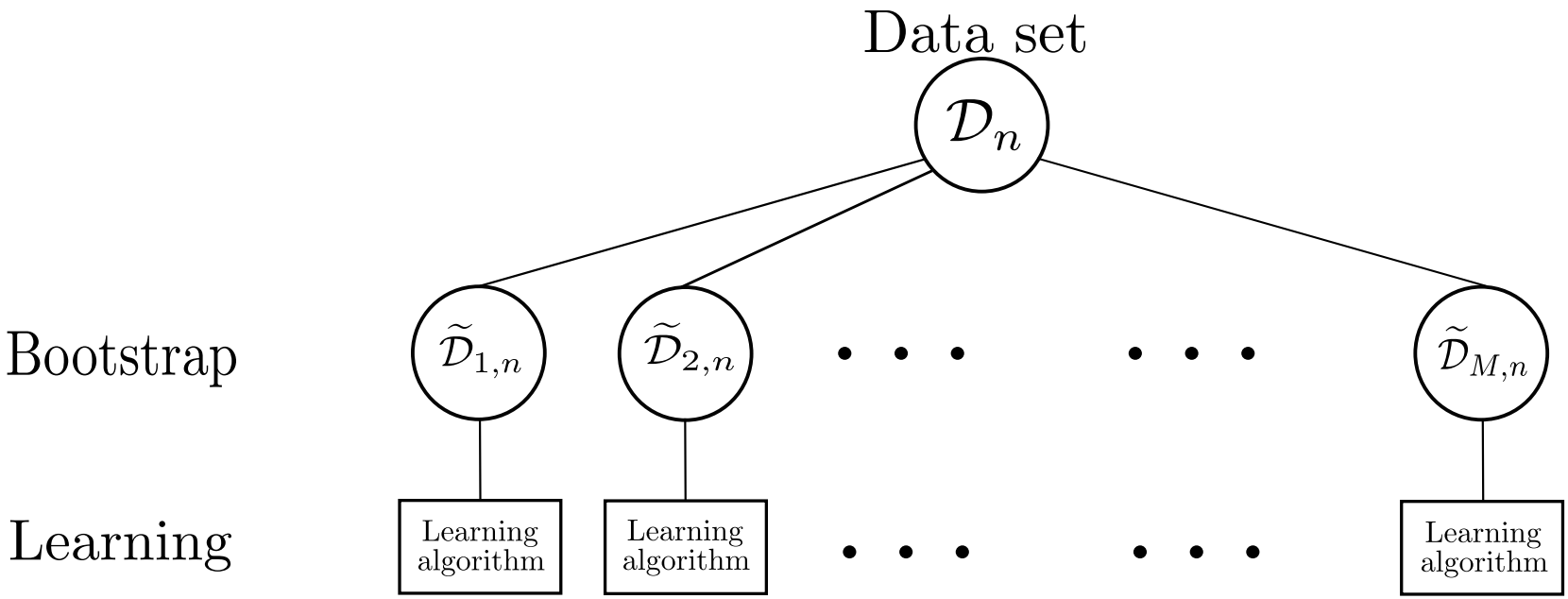

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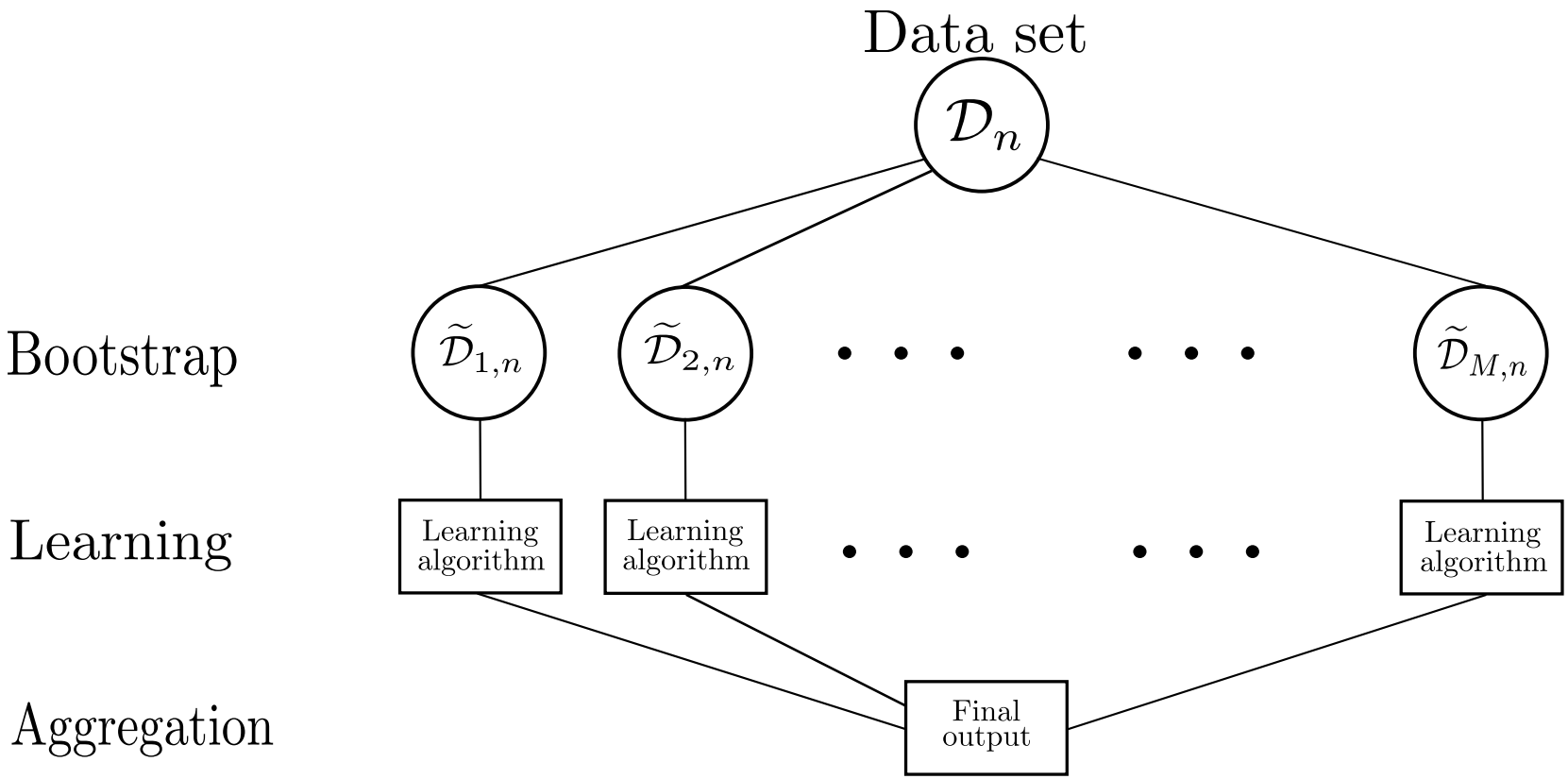

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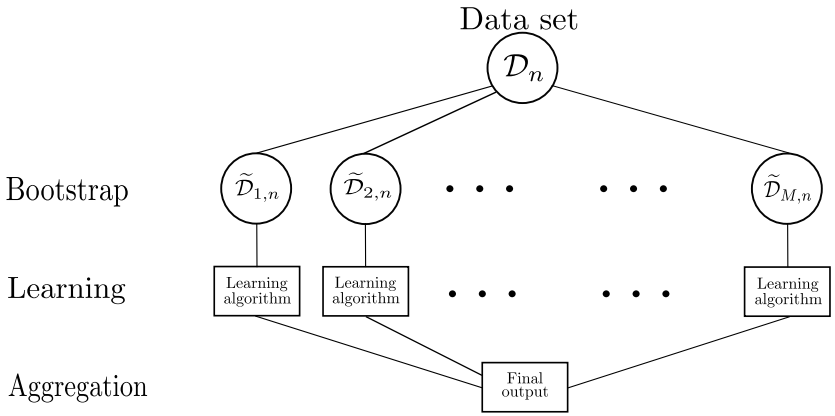

Interests:

- Increase stability - data modification has less impact on the final predictor
- Parallel method - computationnally efficient
- Can be applied to a wide range of learning algorithm (for example, decision trees!)

Inconvenient: individual predictors may be too correlated (built on similar observations).

Split randomization in tree construction

Random forests

Two randomization ingredients:

- Bagging
- Split randomization

Split randomization in tree construction

Regular split selection. In each cell of a tree, select the best split, by optimizing the splitting criterion along all directions.

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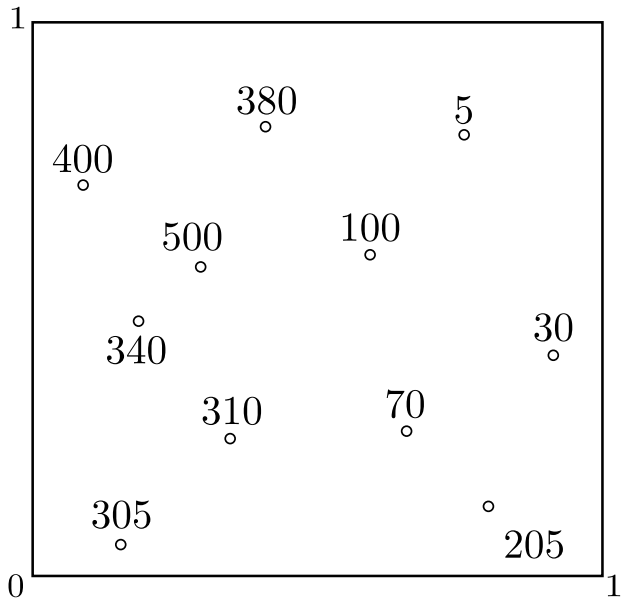

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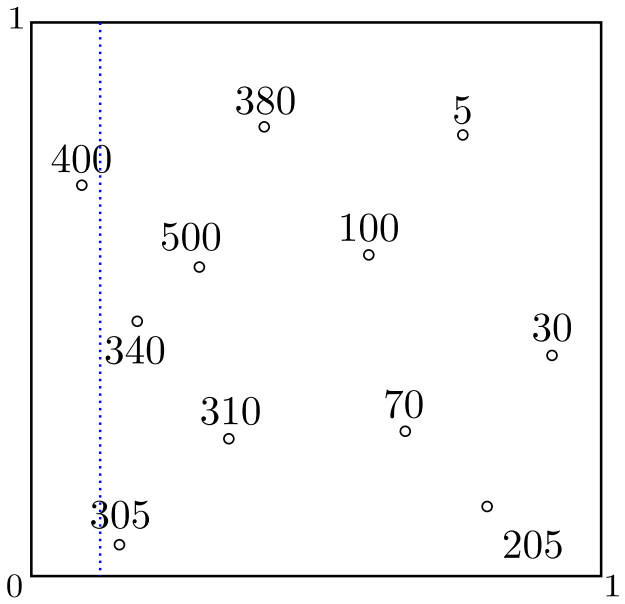

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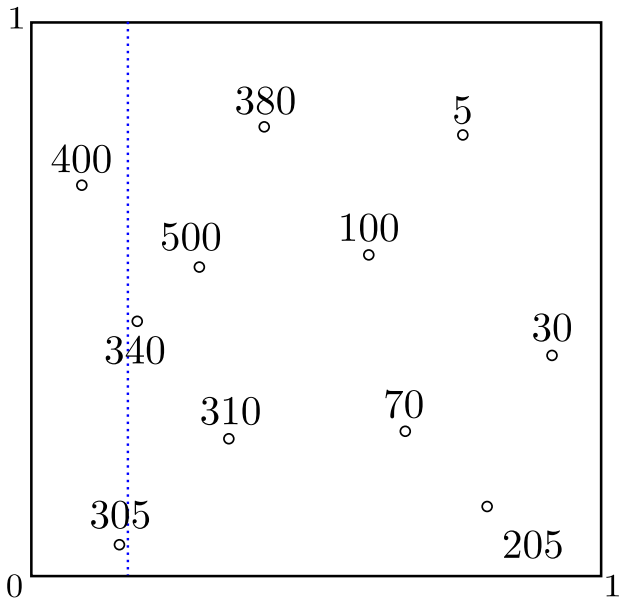

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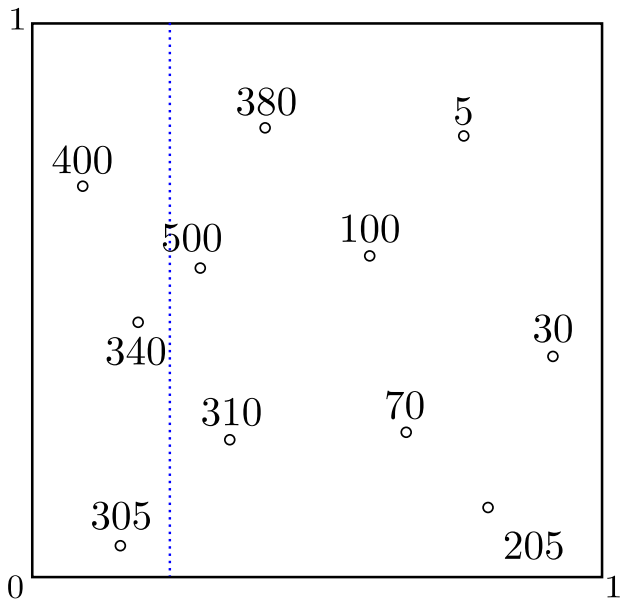

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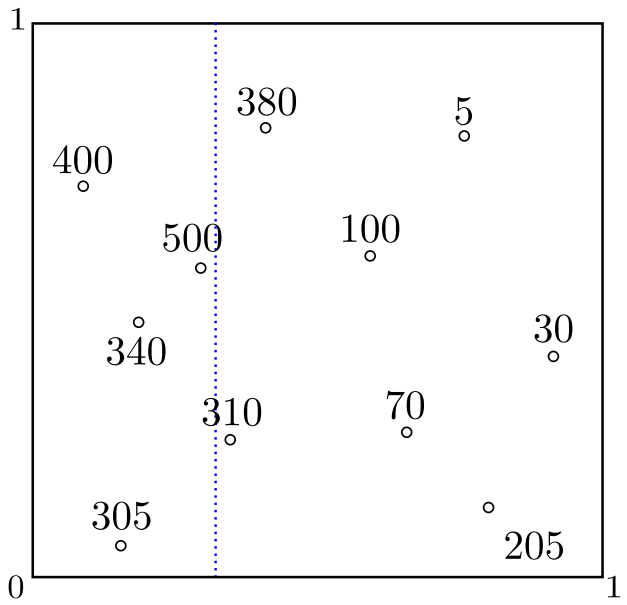

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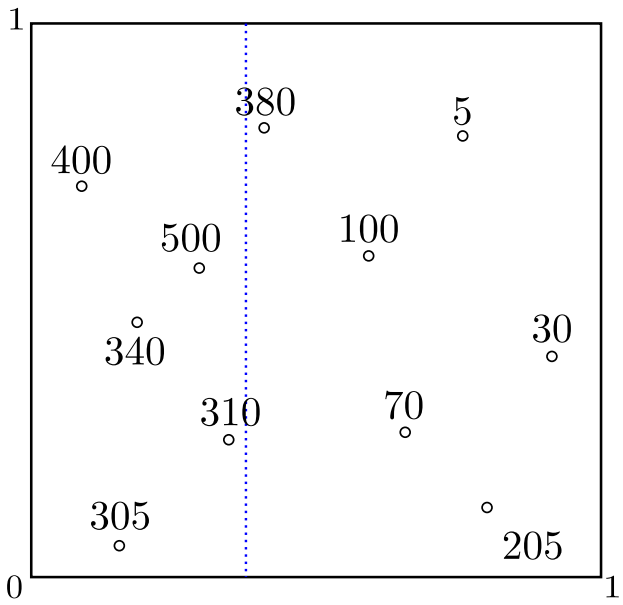

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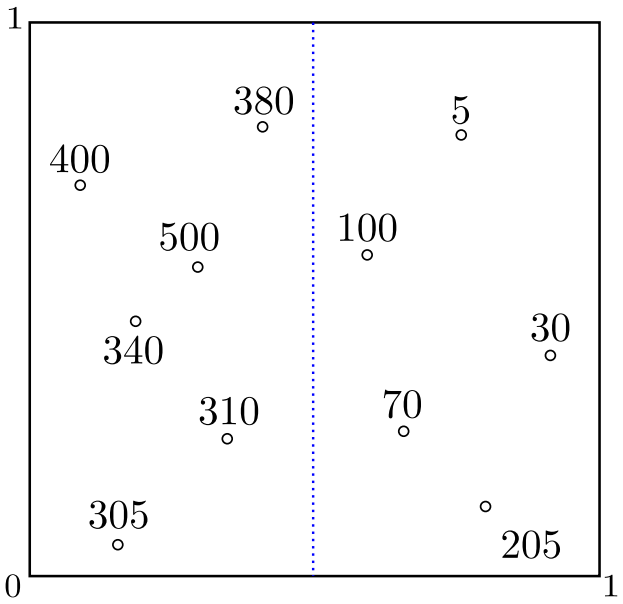

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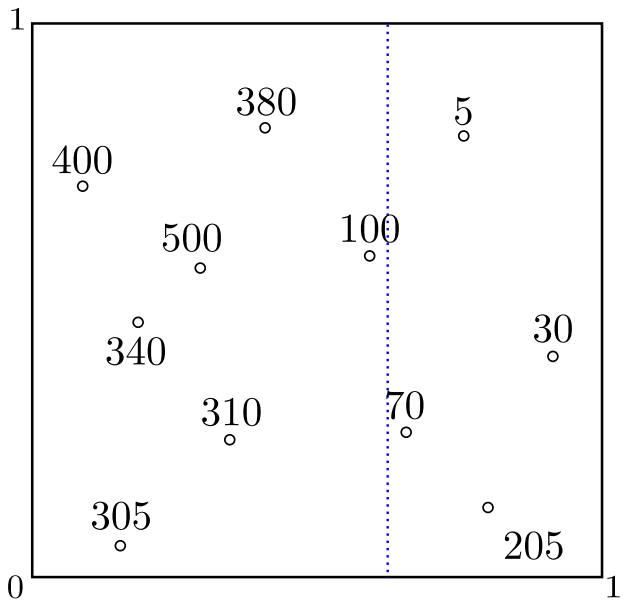

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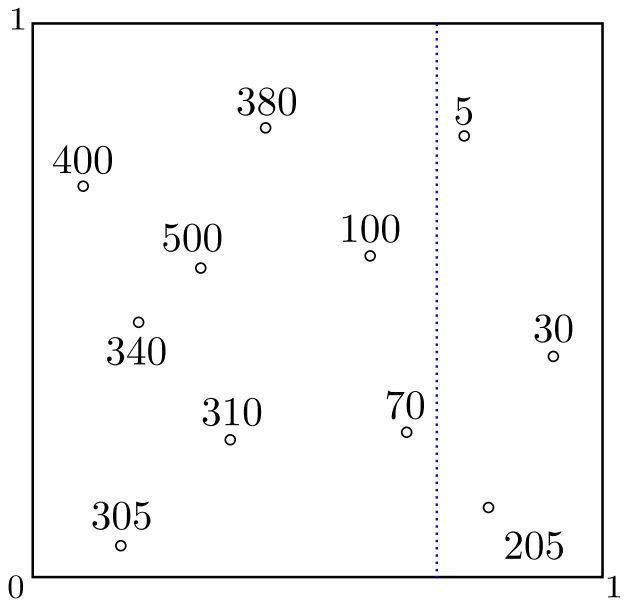

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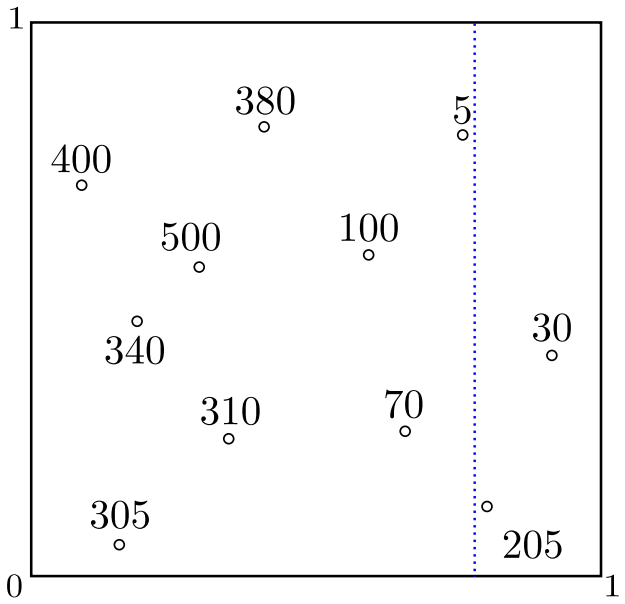

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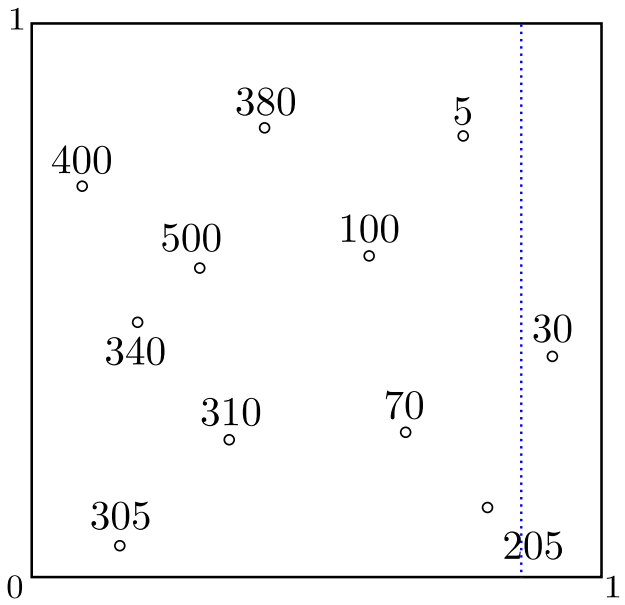

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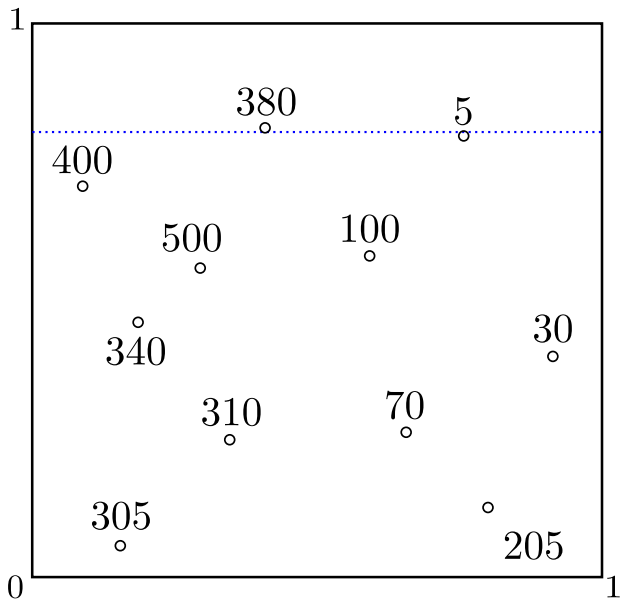

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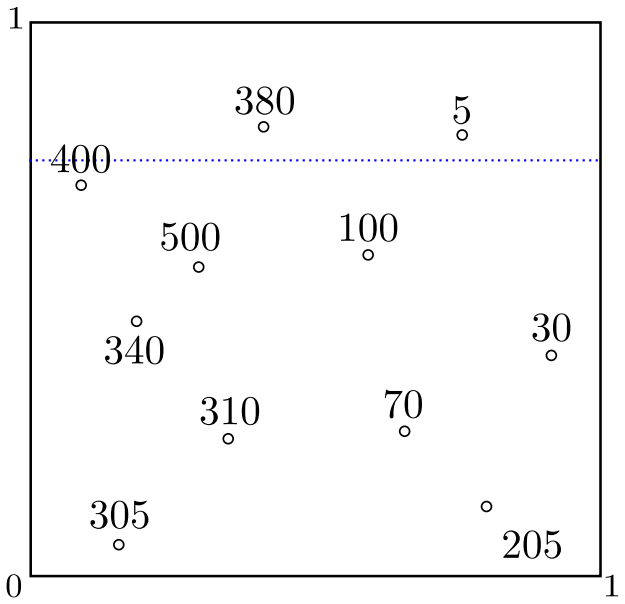

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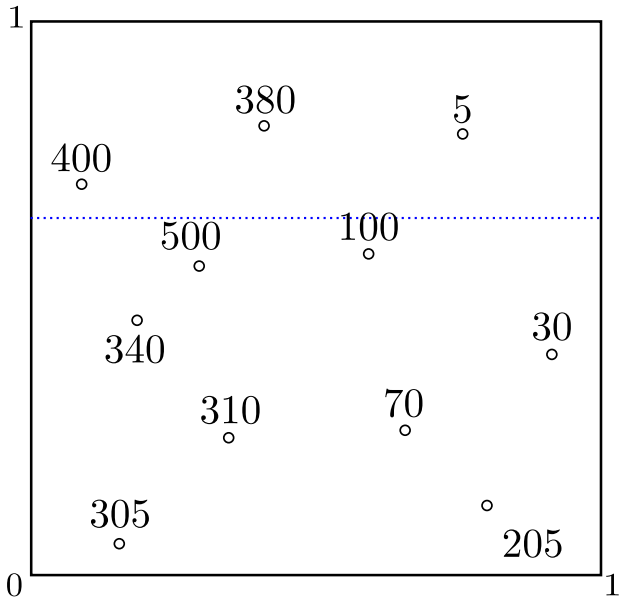

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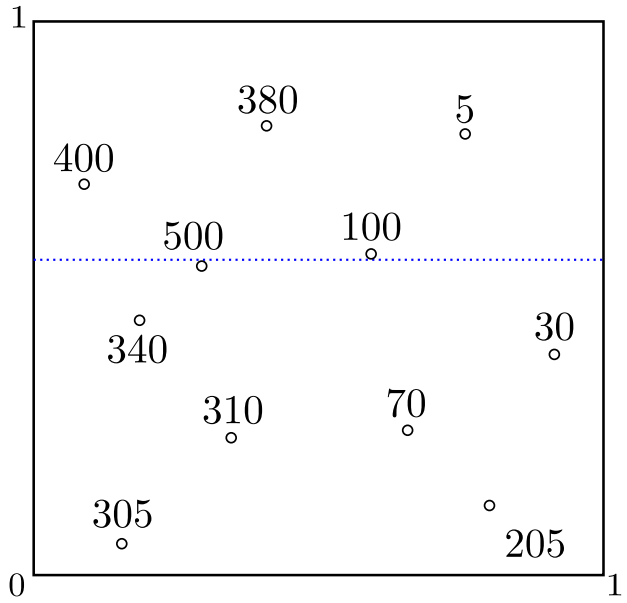

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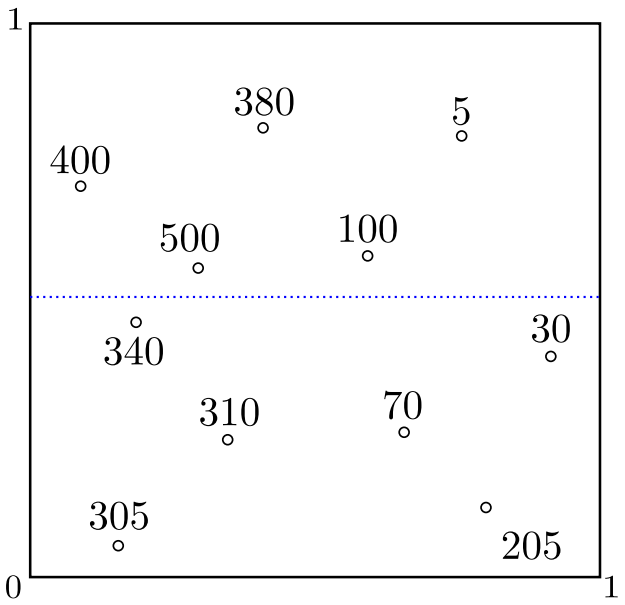

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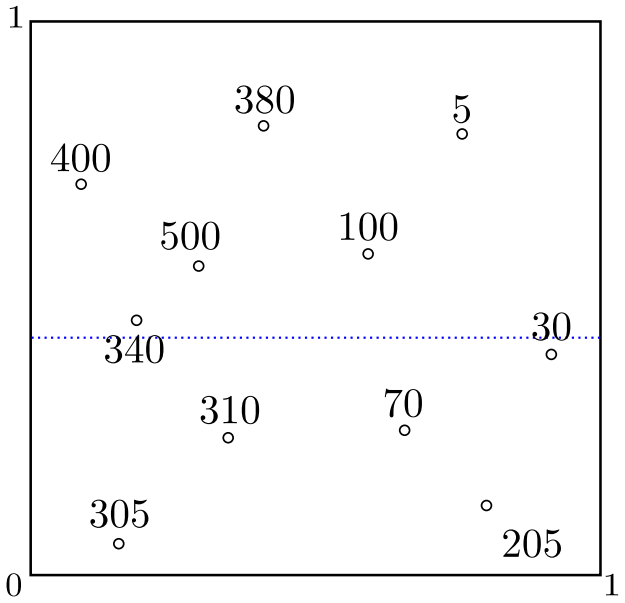

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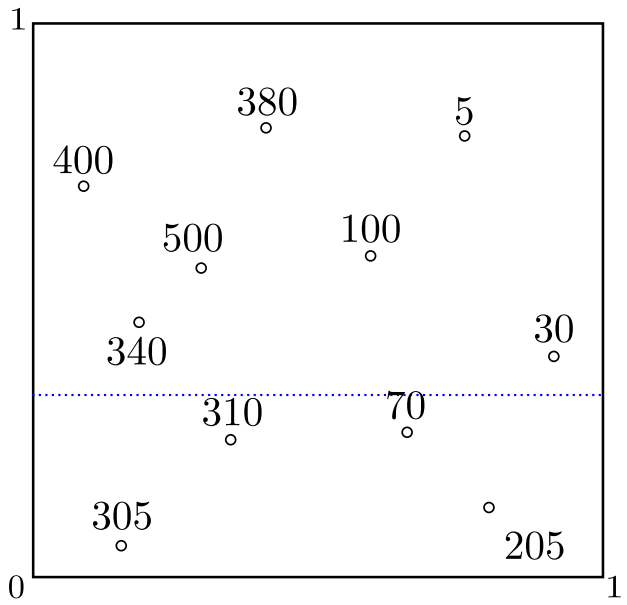

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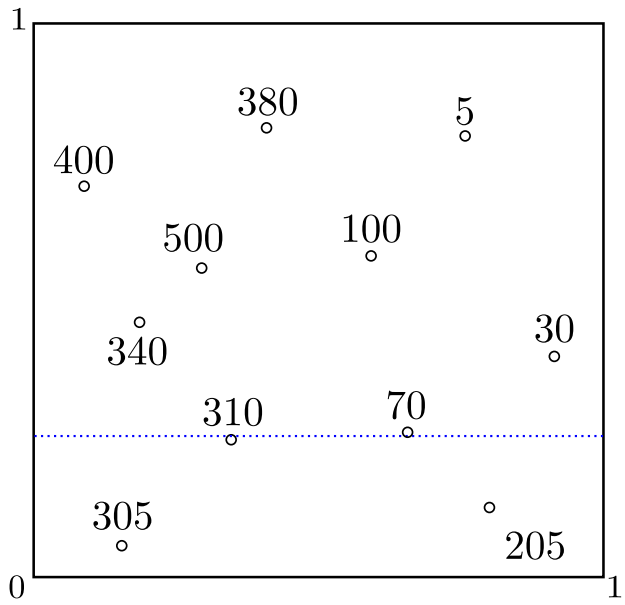

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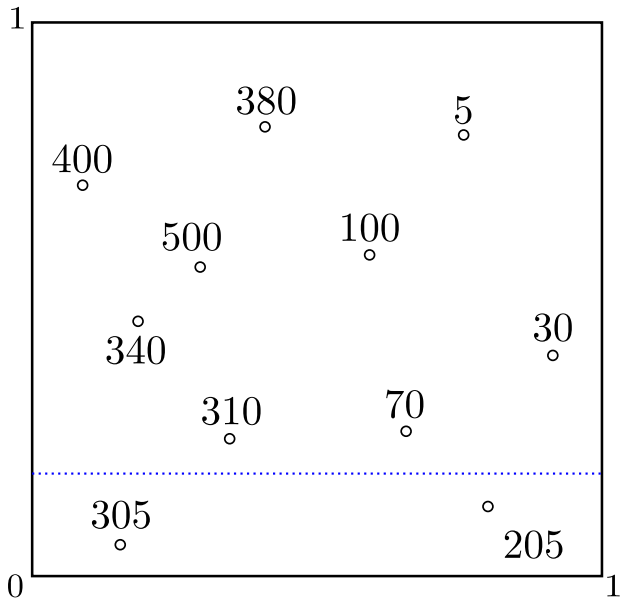

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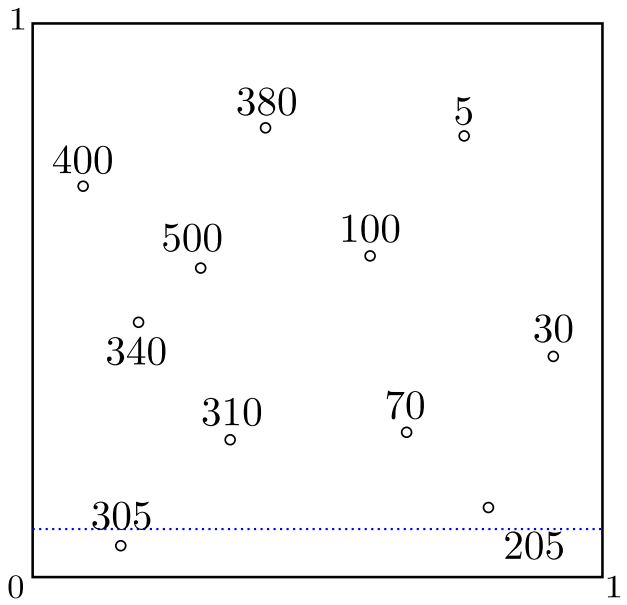

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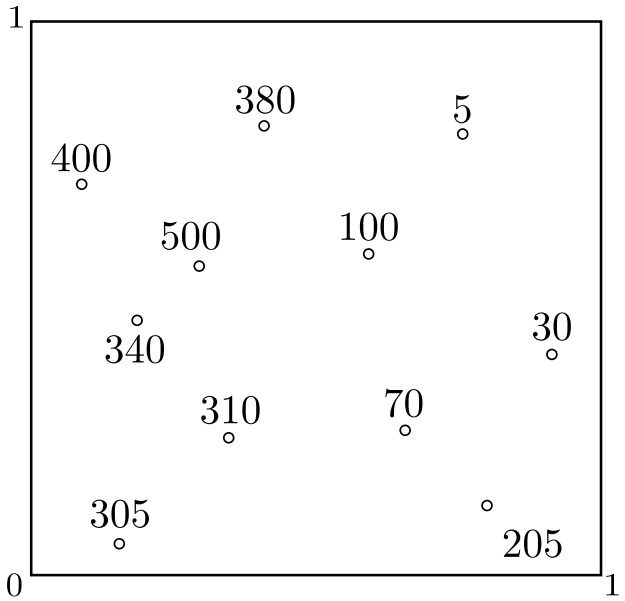

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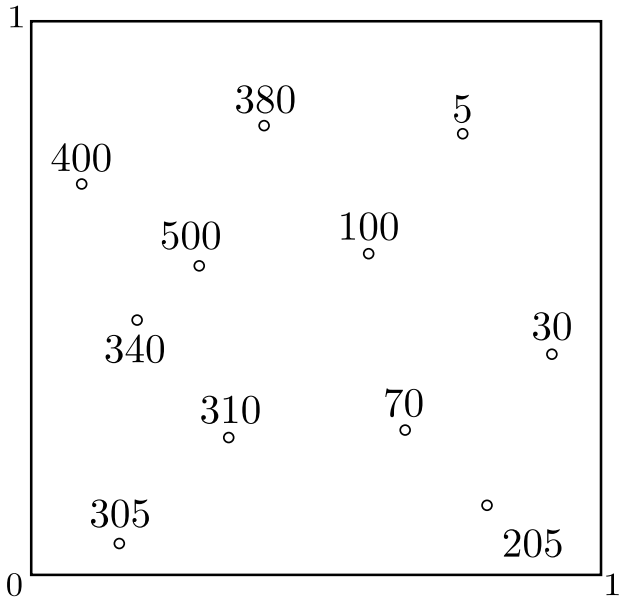

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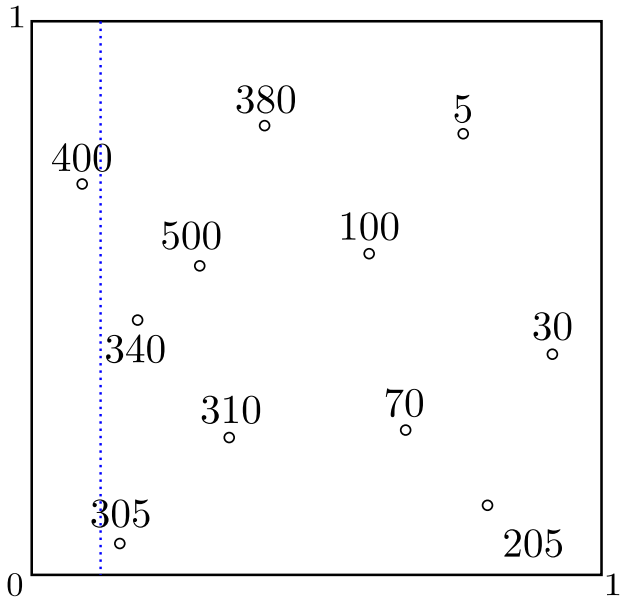

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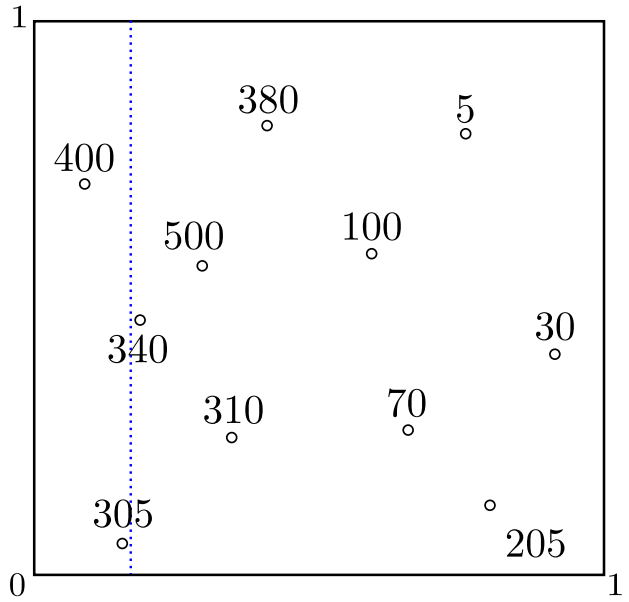

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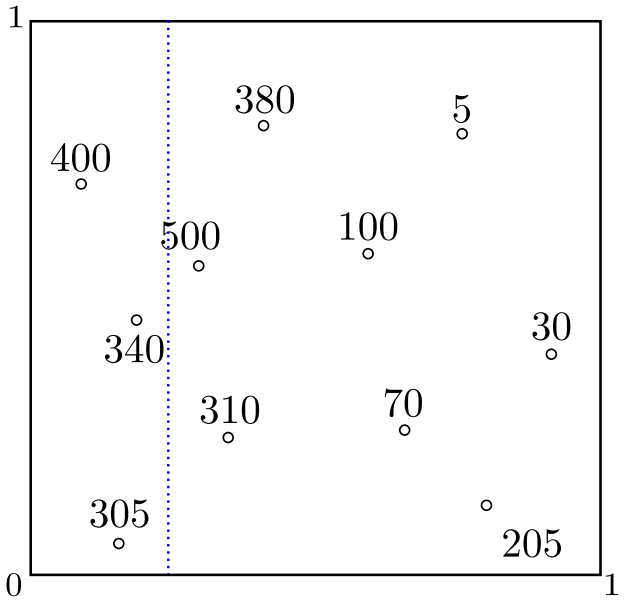

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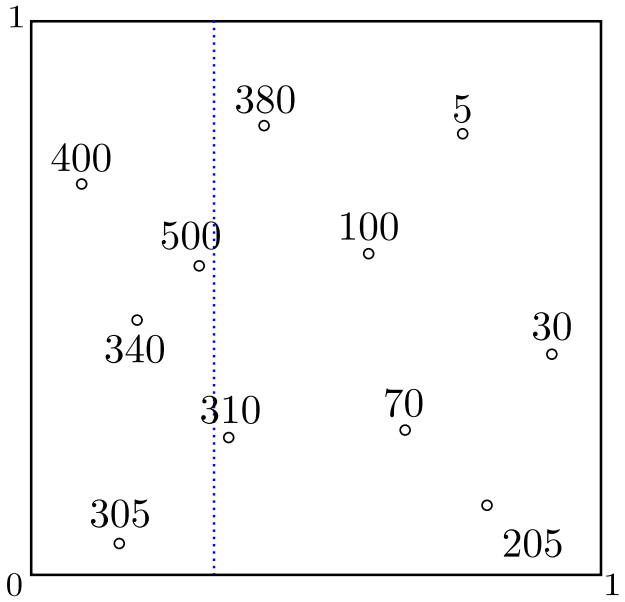

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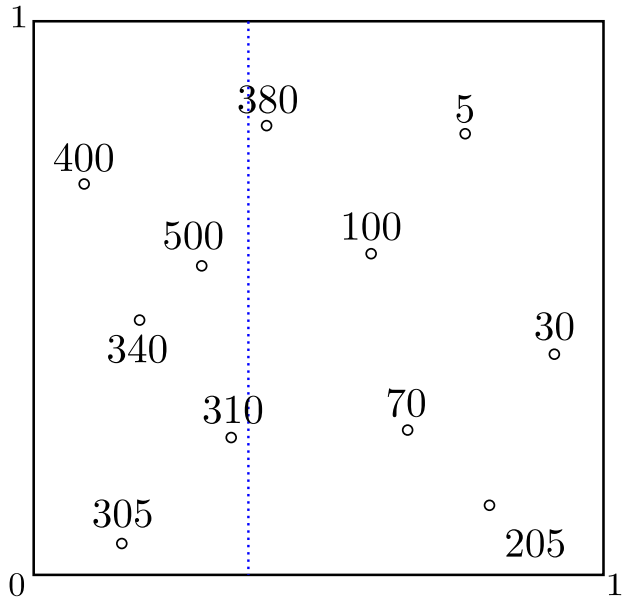

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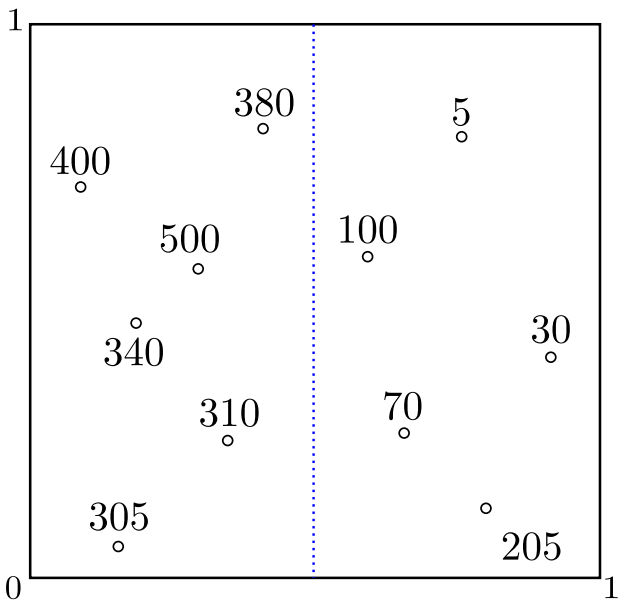

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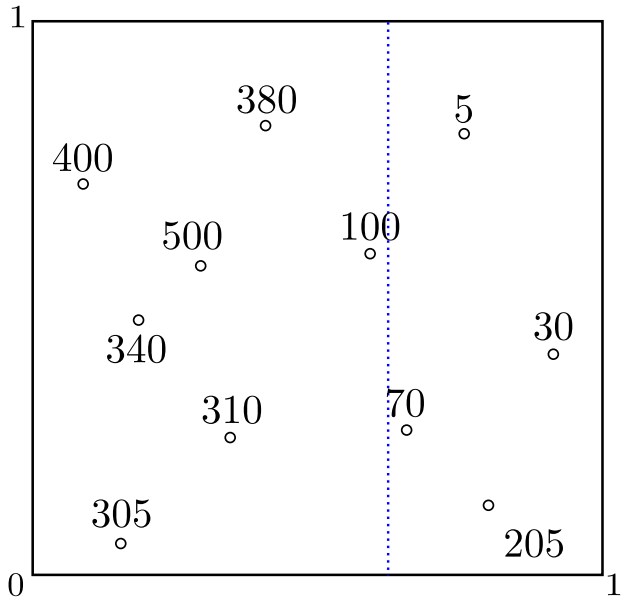

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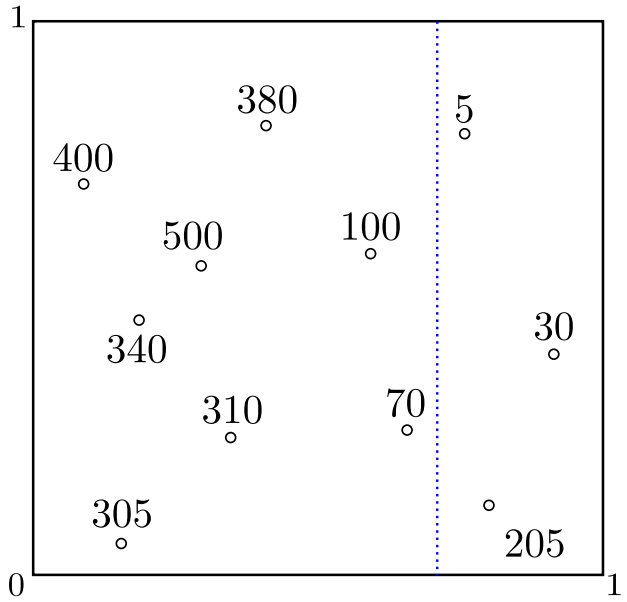

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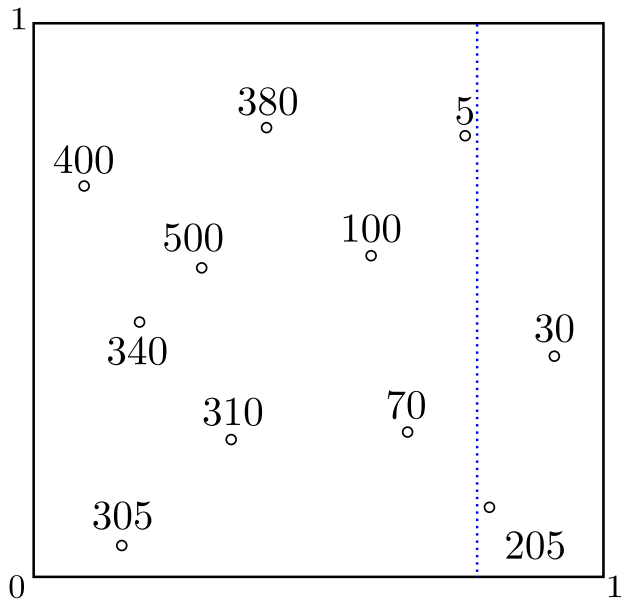

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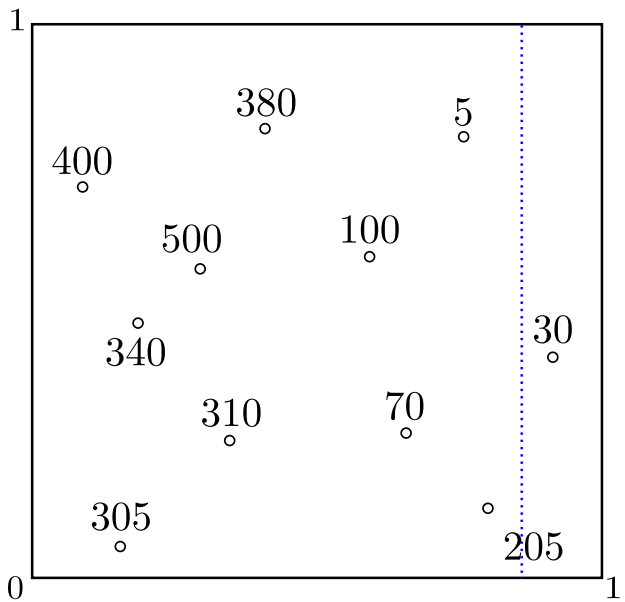

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In each cell of a tree, select **uniformly at random a prespecified number of directions**. Select the best split (by optimizing the splitting criterion) **along these directions only**.

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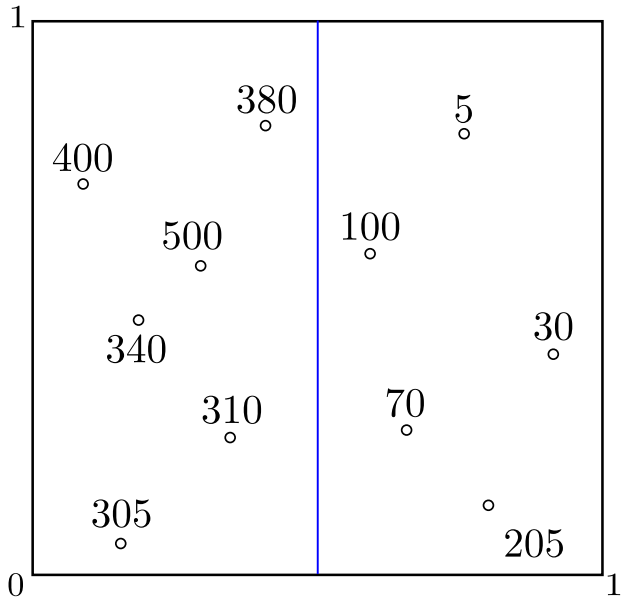

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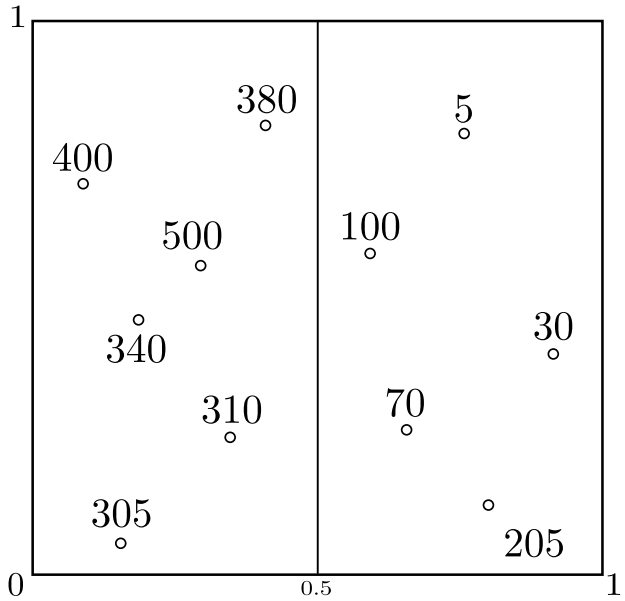
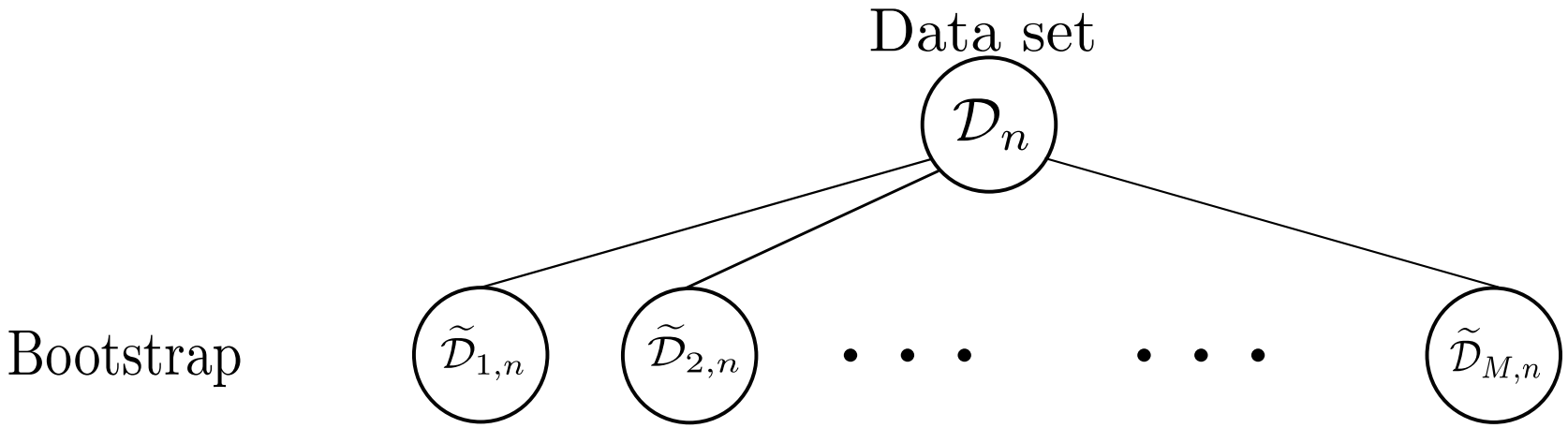


The same procedure is repeated on the resulting cells, with a new random choice of the splitting directions.

Outline

Construction of random forests

Construction of random forests



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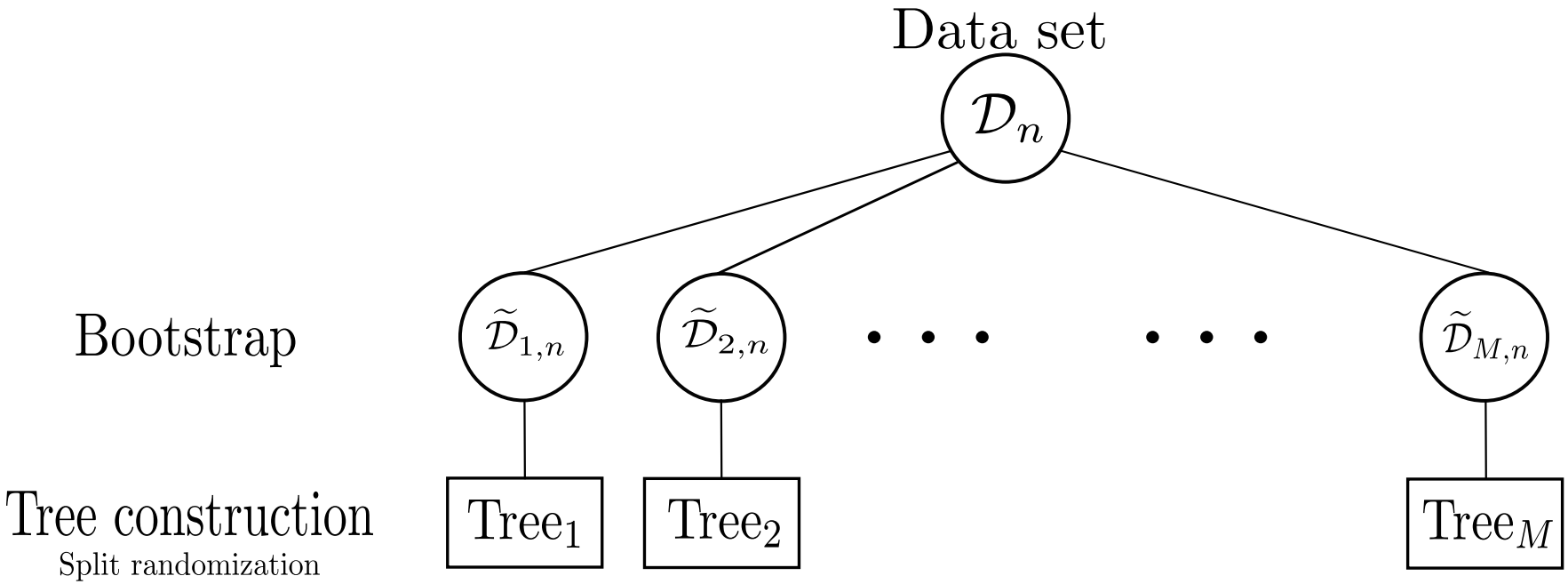

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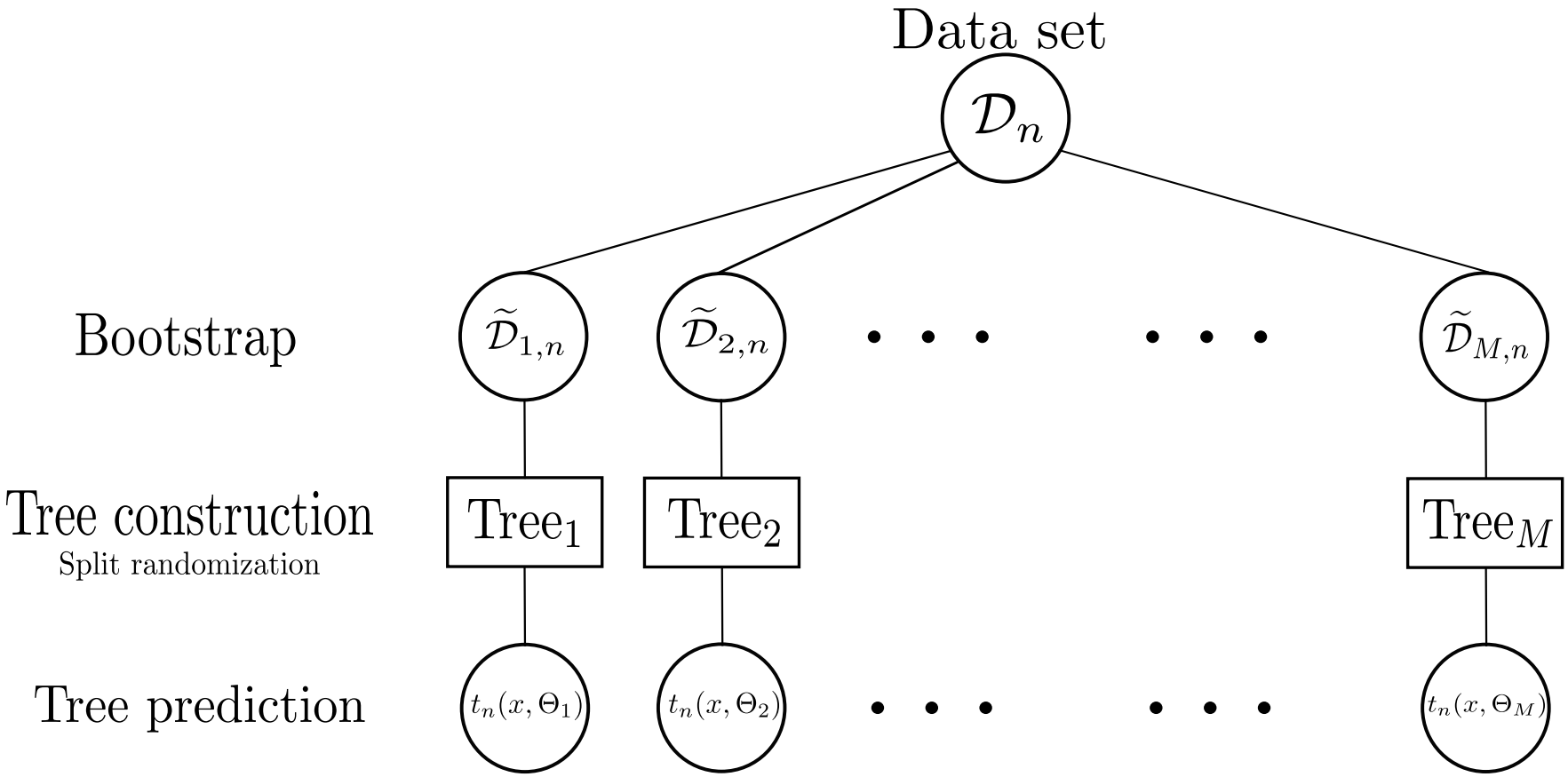

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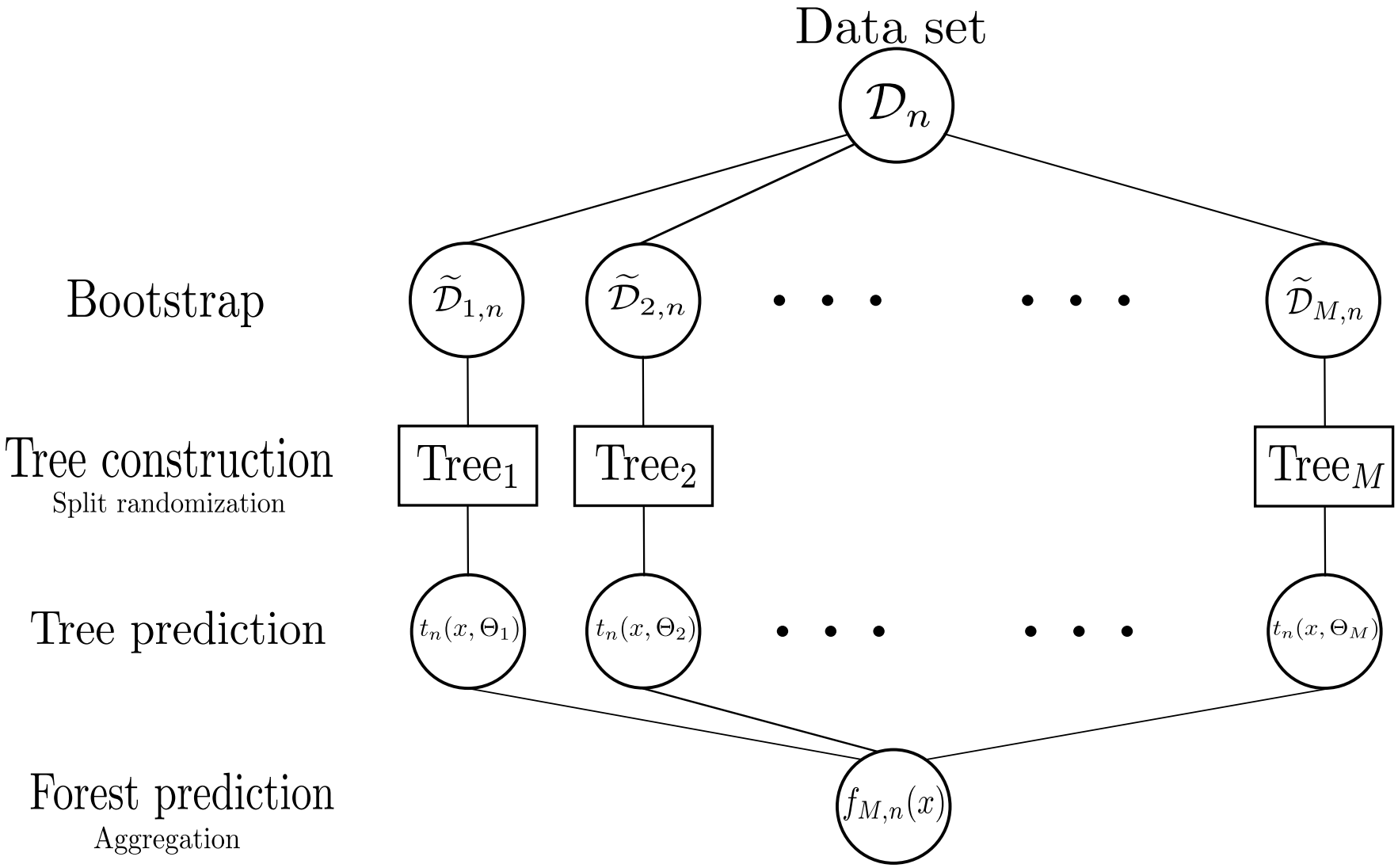

Construction of Breiman forests

- Build in parallel **`n-estimators`** CART as follows.

CART

Bootstrap - Select **`max-samples`** observations with replacement among the original sample $\mathcal{D}_n$. Use only these observations to build the tree.

For each cell,

Select randomly **`max-features`** coordinates among $\{1, \ldots, d\}$;
Choose the best split along previous directions, based on the choosen `criterion` (impurity measure).

Stop splitting each cell when all observations inside it have the same label or when a stopping criterion is met:

there are less than **`min-sample-leaf`** observation in the leaf
resulting cells would contain less than **`min-sample-split`** observation
cell is already split **`max-depth`** times
there are already **`max-leaf-nodes`** leaves

- Compute the forest prediction by averaging the predictions of all trees.

List of all random forest hyperparameters

See `Scikit-learn` documentation for more details: `RandomForestRegressor` / `RandomForestClassifier`.

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List of all hyperparameters in the forest:

- `n-estimators` = 100
- `criterion`='gini'
- `max-depth`=None,
  `min-samples-split` = 2,
  `min-samples-leaf` = 1,
  `min-weight-fraction-leaf` = 0.0,
  `min-impurity-decrease` = 0.0,
  `max-leaf-nodes`=None

  → By default, trees are fully grown with no pruning strategy
- `max-features`='sqrt' (classif.) 'None' (regression).
- `bootstrap`=True, `max-samples`=None

List of all random forest hyperparameters

See `Scikit-learn` documentation for more details: `RandomForestRegressor` / `RandomForestClassifier`.

Remarks.

- Due to bootstrap and split randomization, running twice RF may lead to different results. Increasing the number of trees limits this difference.
- Fixing a `random-state` makes two runs of RF identical.
- Beware, by default, split randomization is used in classification but not in regression!

Role of each hyperparameter

Number of trees.

- Larger values are better
- No statistical tradeoff between low and high values
- Limited by computational power - growing many trees is expensive
- Default values (several hundreds / thousands) usually do a good job

Role of each hyperparameter

Bootstrap size / tree shape.

- Control the bias/variance tradeoff: small bootstrap size / shallow trees lead to predictors with a large bias but a small variance
- Use small bootstrap size or shallow tree if data are very noisy
- Use default setting for modelling very complex phenomenon

$\rightarrow$ Precise tuning can help but default values are good in general

Role of each hyperparameter

Split randomization

- Most complex parameter to tune
- Small values of `max-features` lead to very different trees

  $\rightarrow$ `max-features`=1 corresponds to drawing randomly the splitting direction
- Large values of `max-features` lead to similar trees

  $\rightarrow$ `max-features`=d corresponds to building the same tree (if no bootstrap is used)
- No precise heuristic, can be tuned by cross-validation.

Outline

Out-of-bag error

Idea. Evaluate the error of a random forest using the fact that each observation has not been used in all tree constructions and can thus be used as test points for such aggregated trees.

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General procedure (short):

- Consider that a forest has been trained on the data set $\mathcal{D}_n$.
- For each observation $i \in \{1, \dots, n\}$,
  - Consider the bootstrap samples that do not contain this observation.
  - For the trees that are not built using observation i, compute the predictions at X_i and aggregate them. Compute the loss of such an aggregated prediction.
- Compute the Out-of-bag error by averaging the losses over all observations.

Out-of-bag error

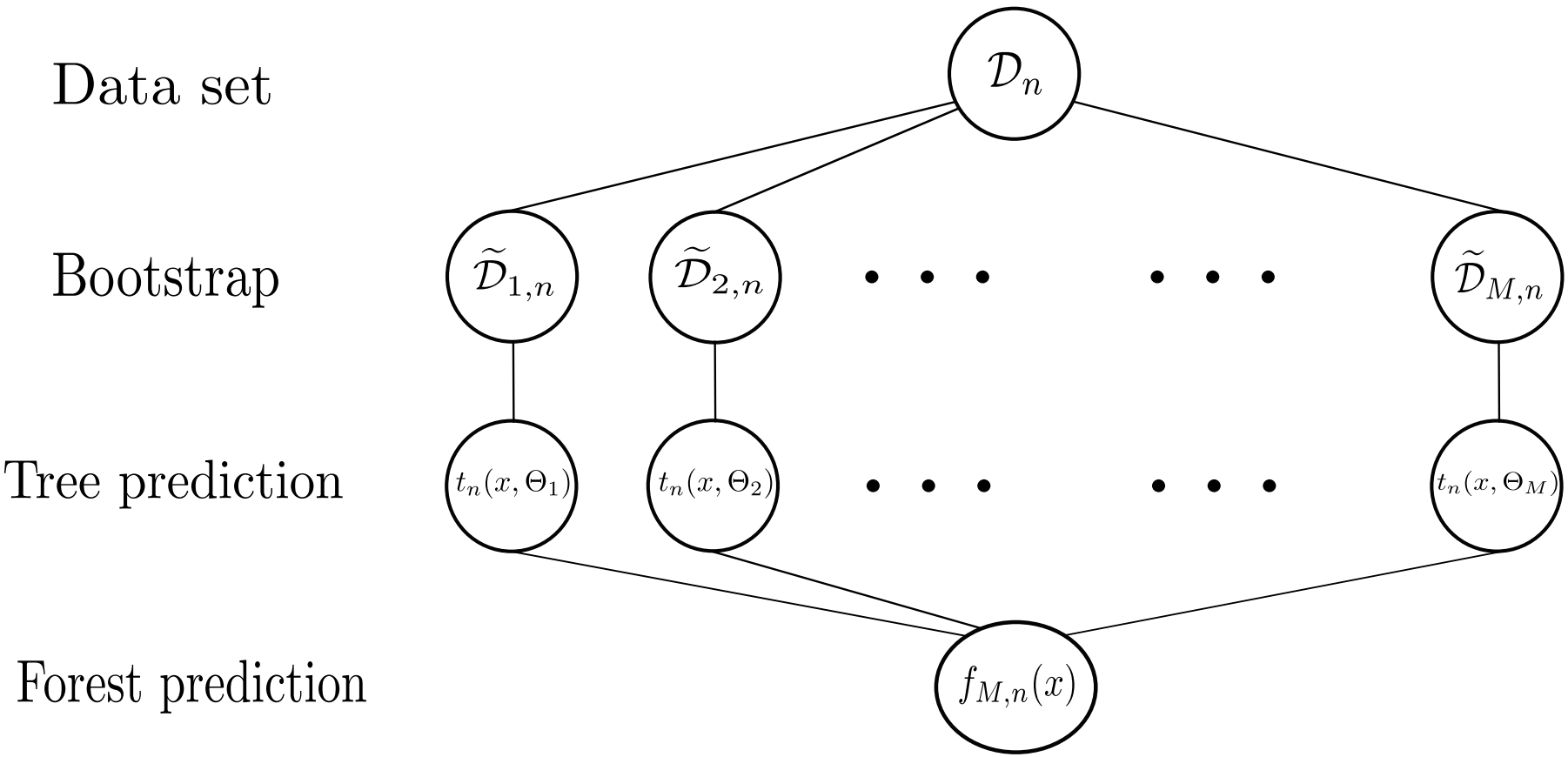
Benefits:

- No need for dividing the data set into a train and a test set
- Easily parallelizable
- Asymptotically equivalent to the risk of the forest for large M.

Drawback:

- Do not compute exactly the error of the whole forest but rather the aggregated error of some trees in the forest.

Out-of-bag procedure



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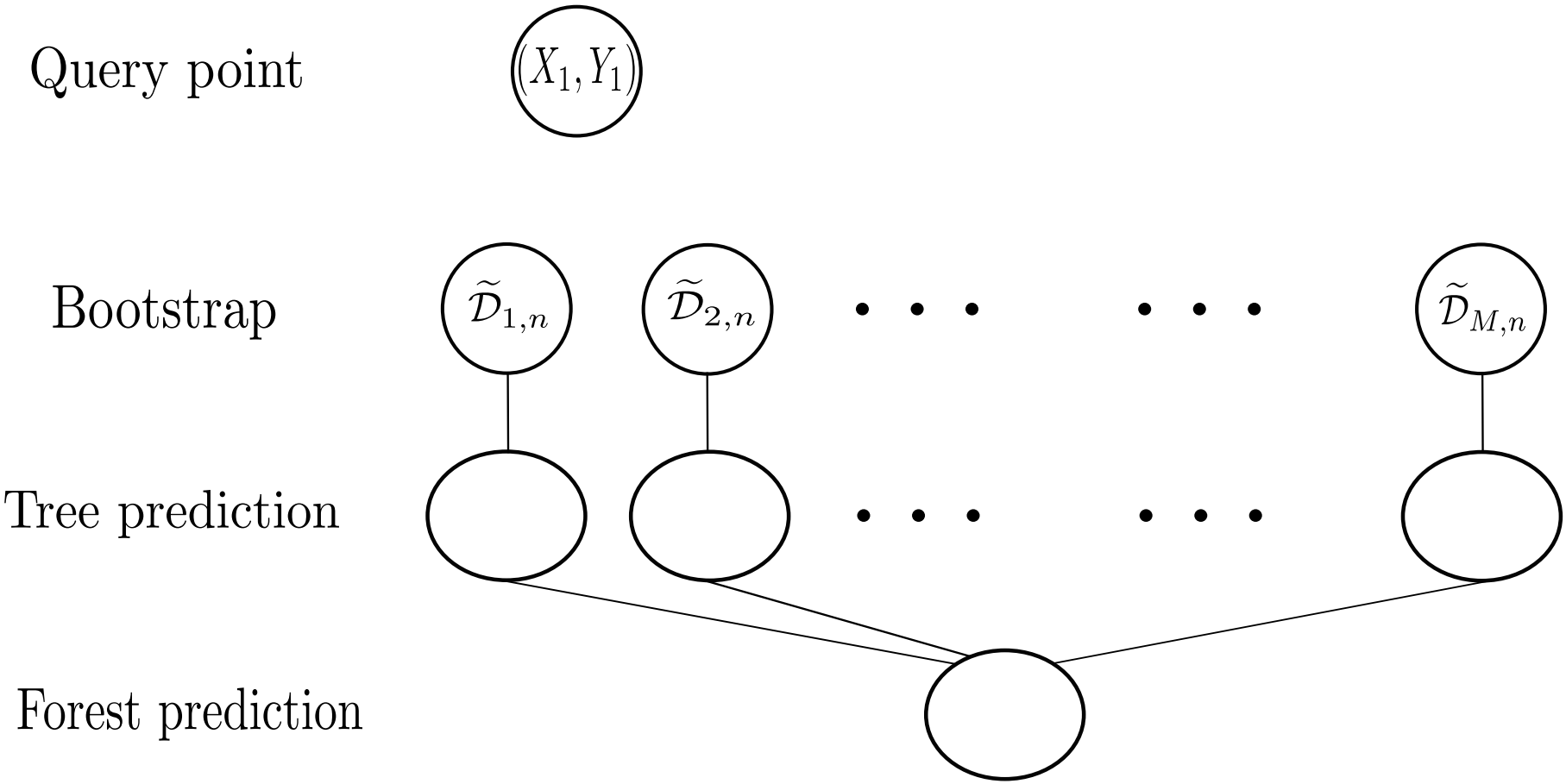

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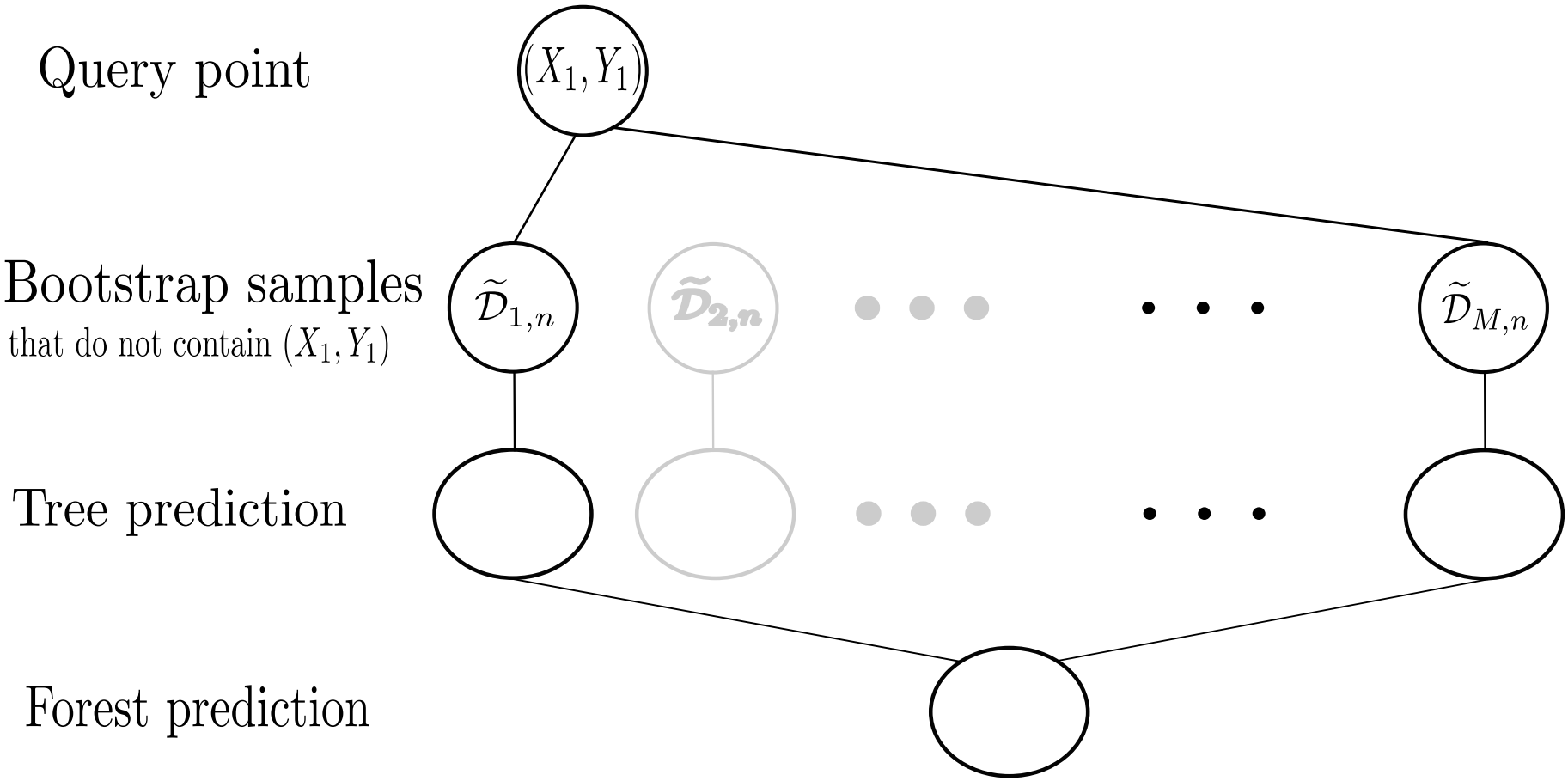

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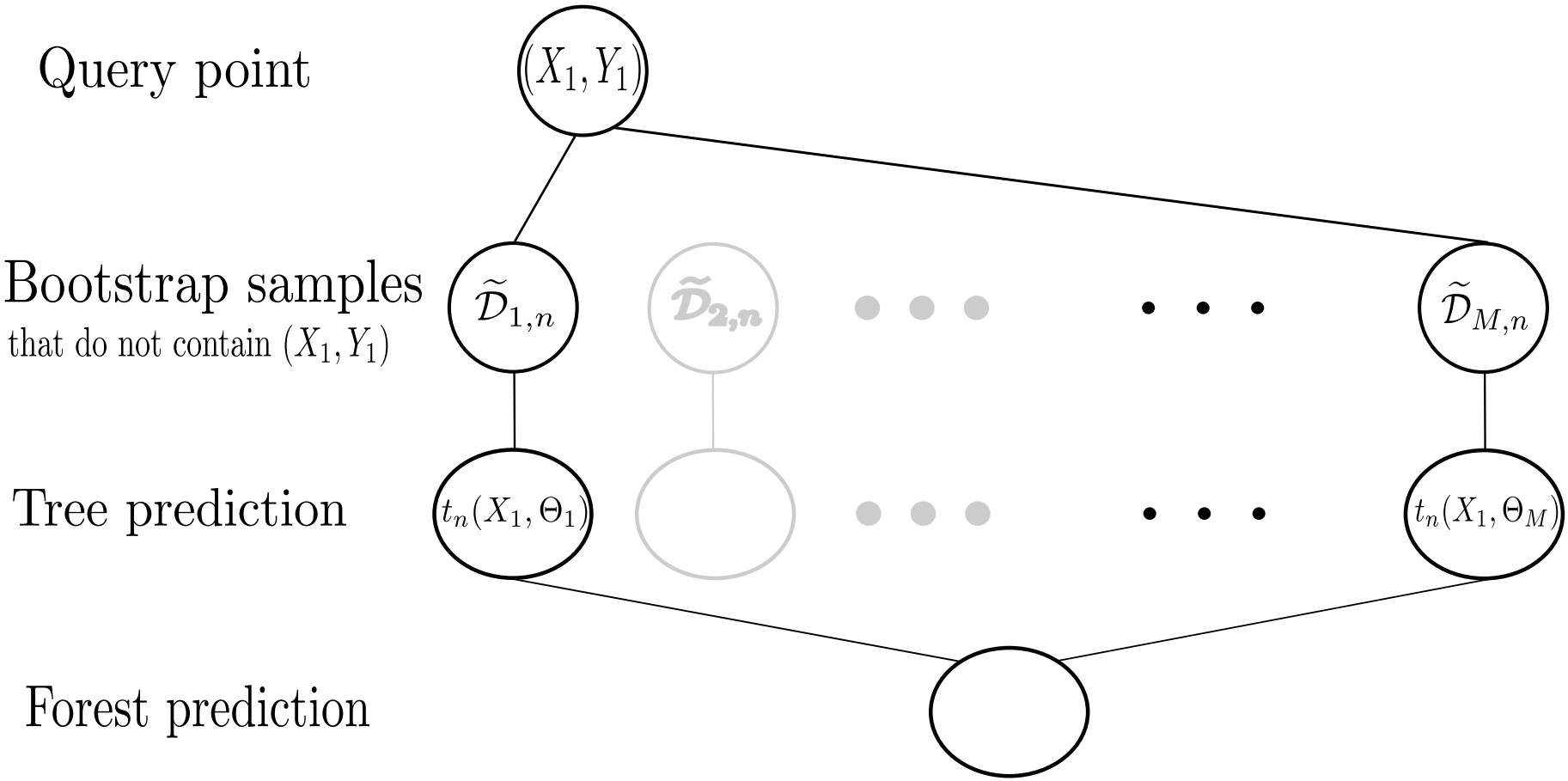

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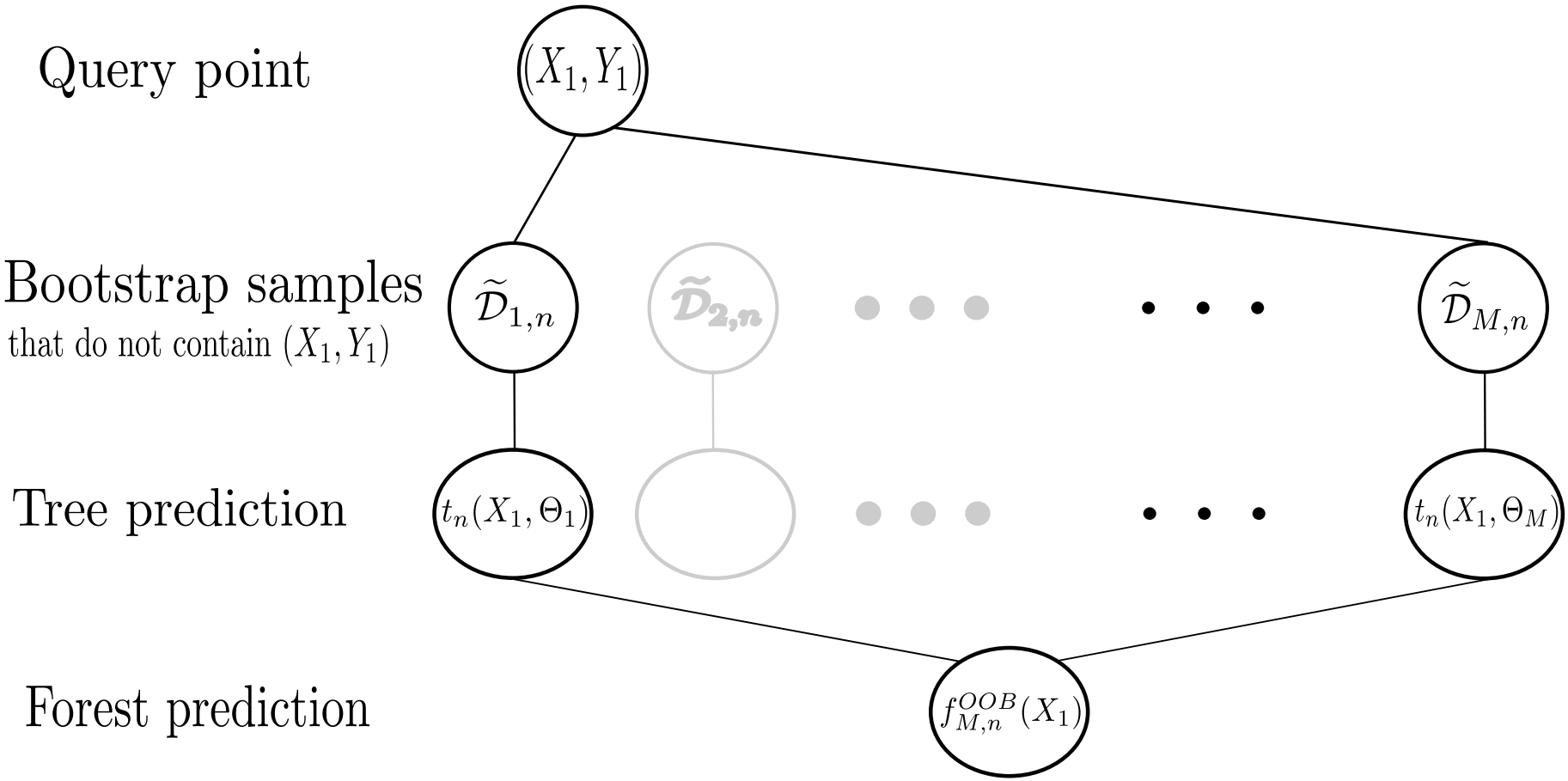

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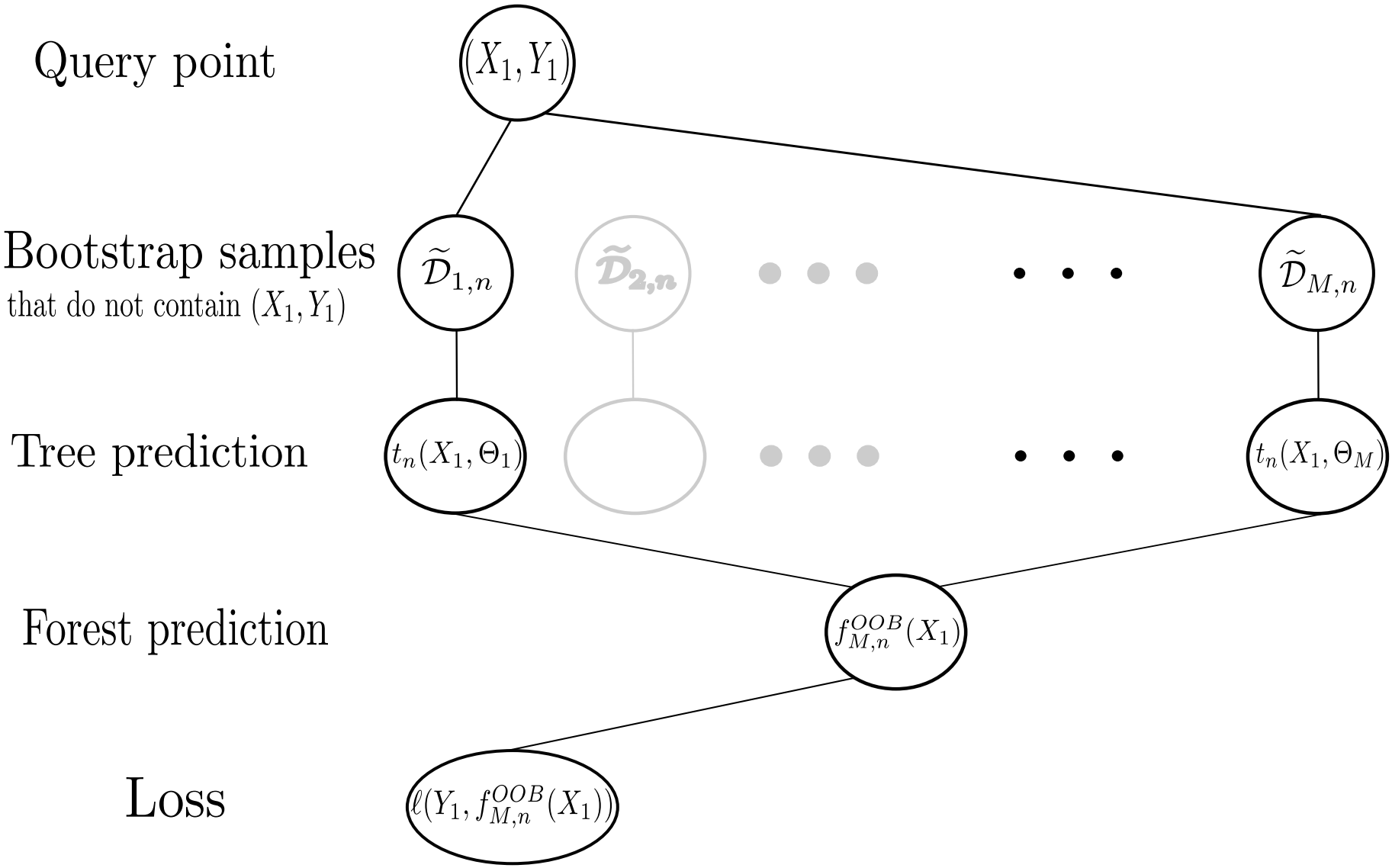

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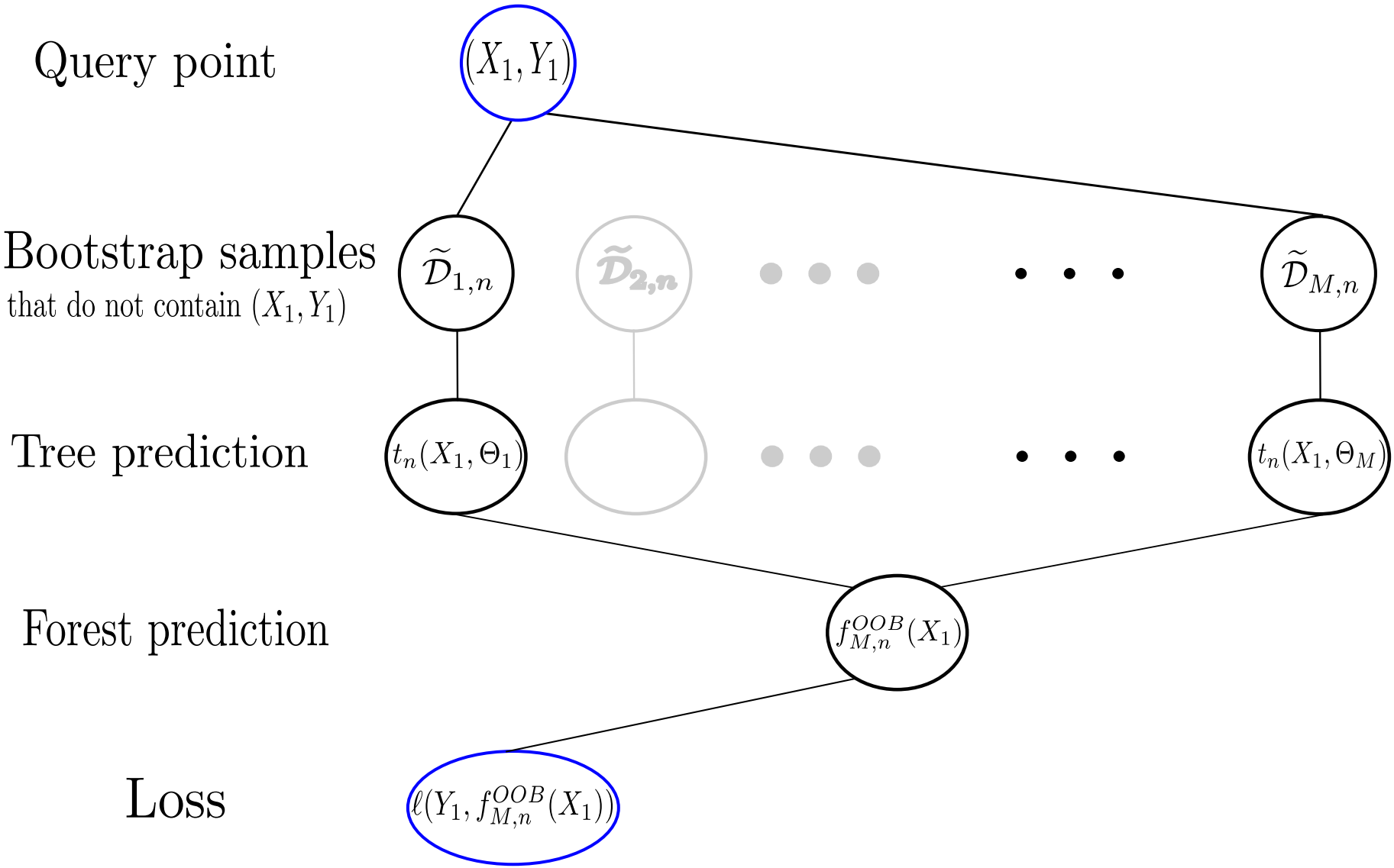

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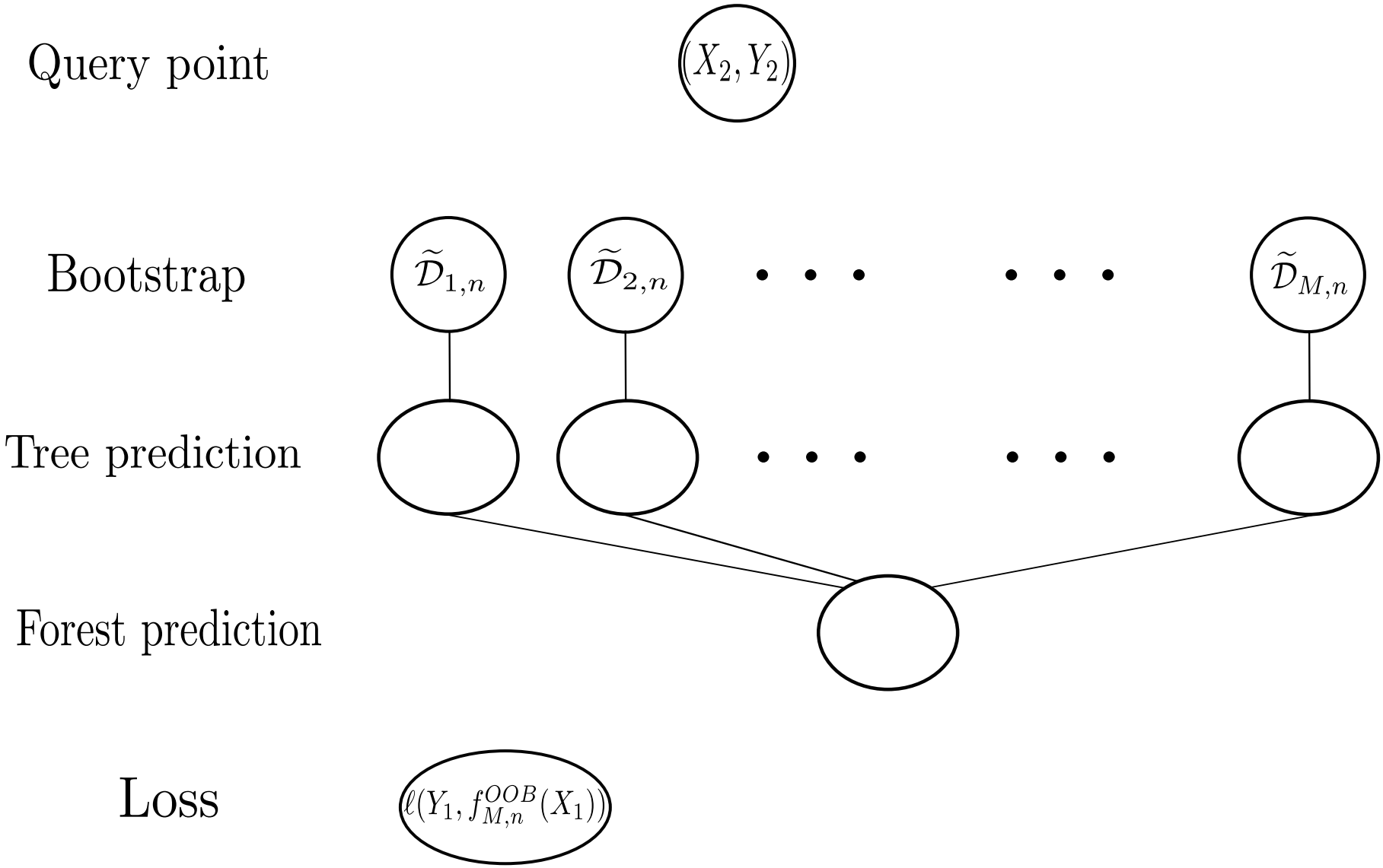

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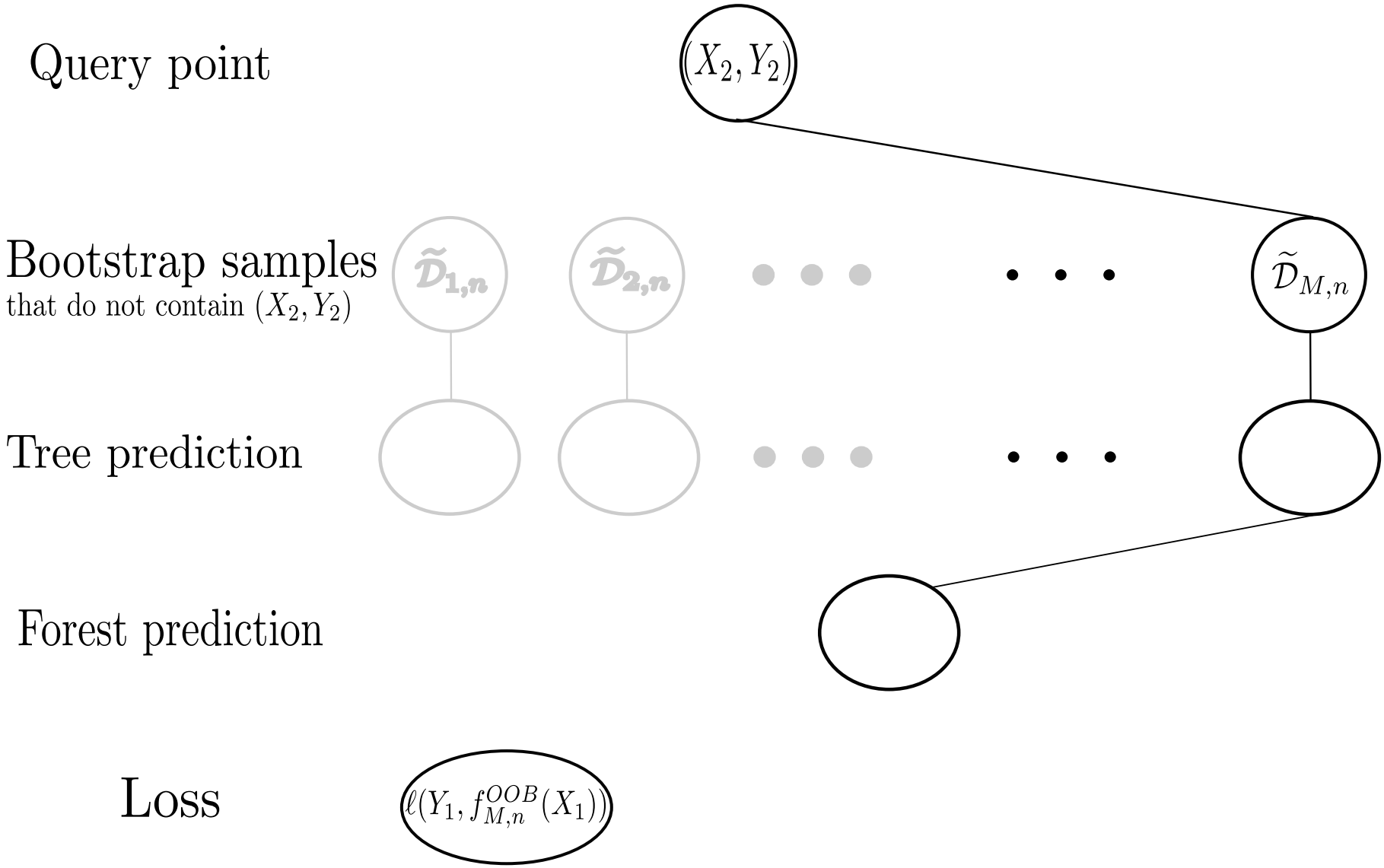

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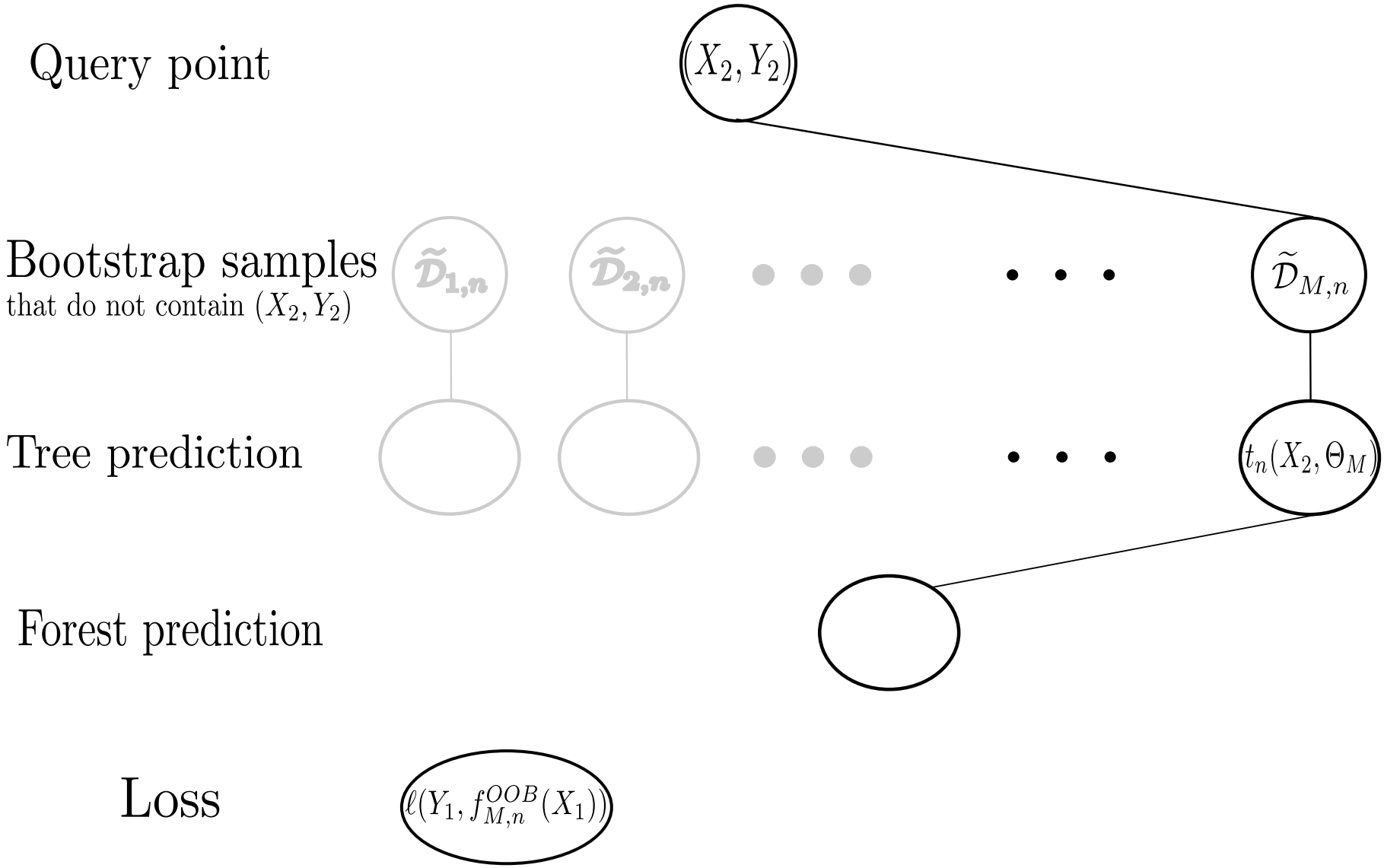

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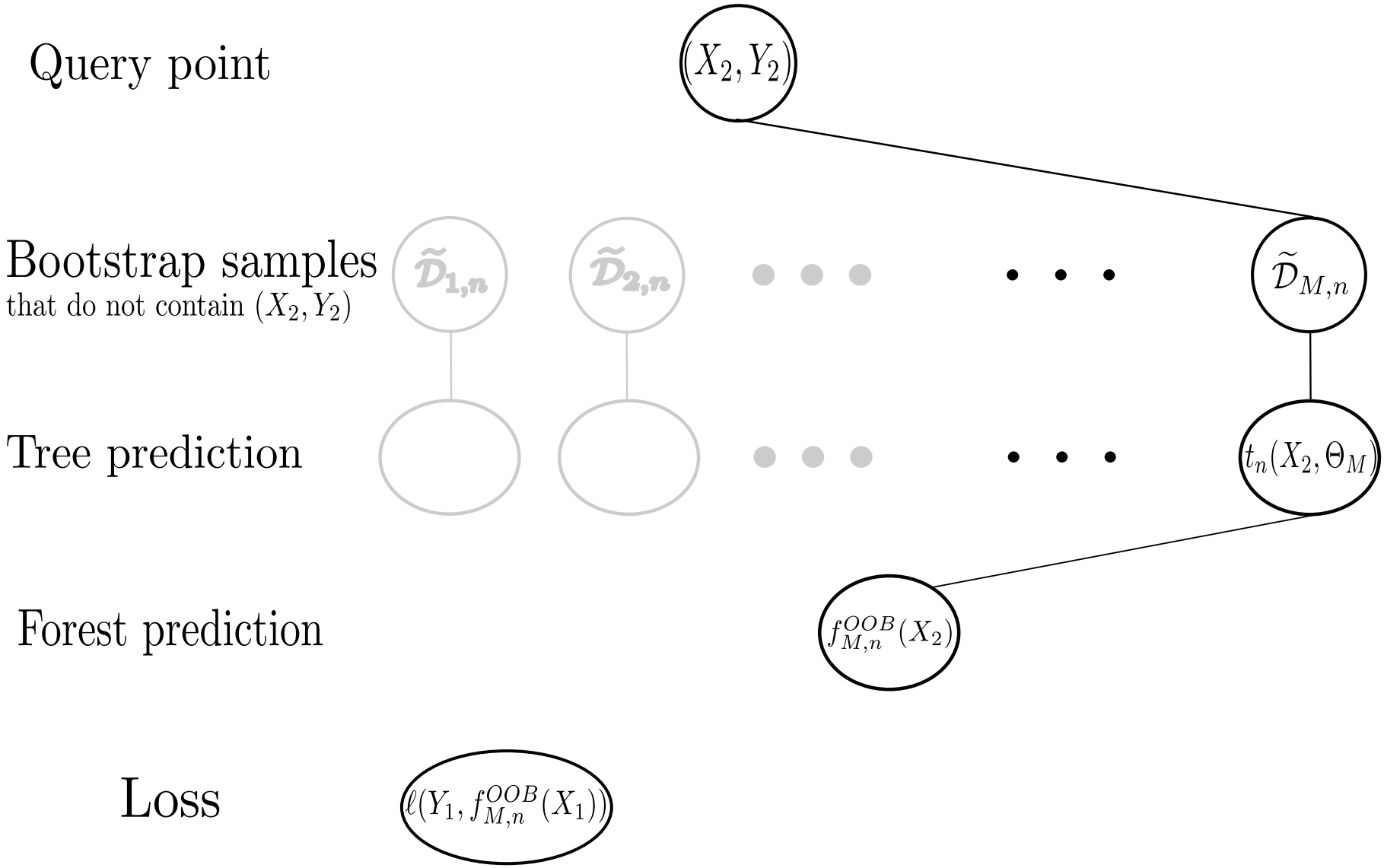

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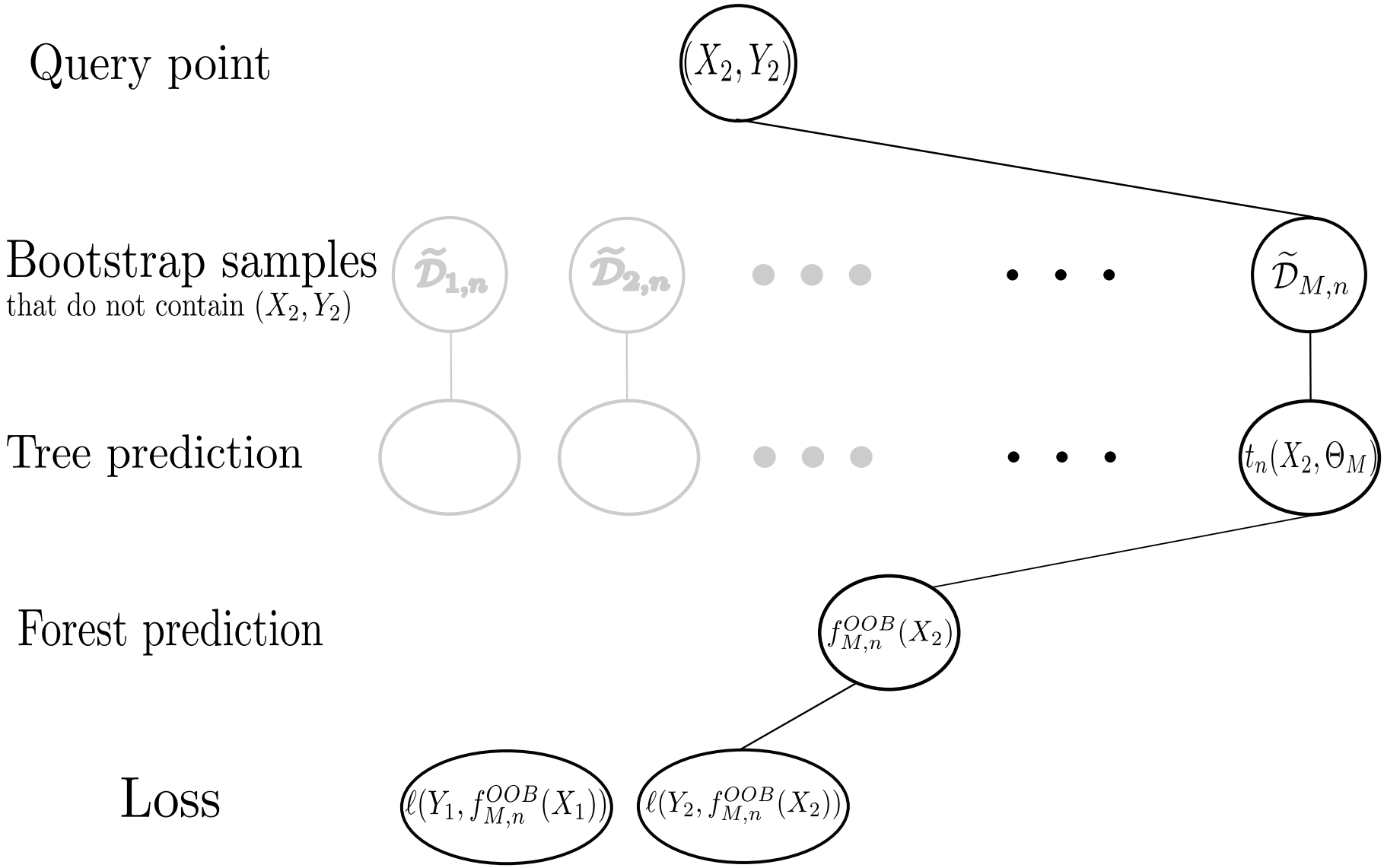

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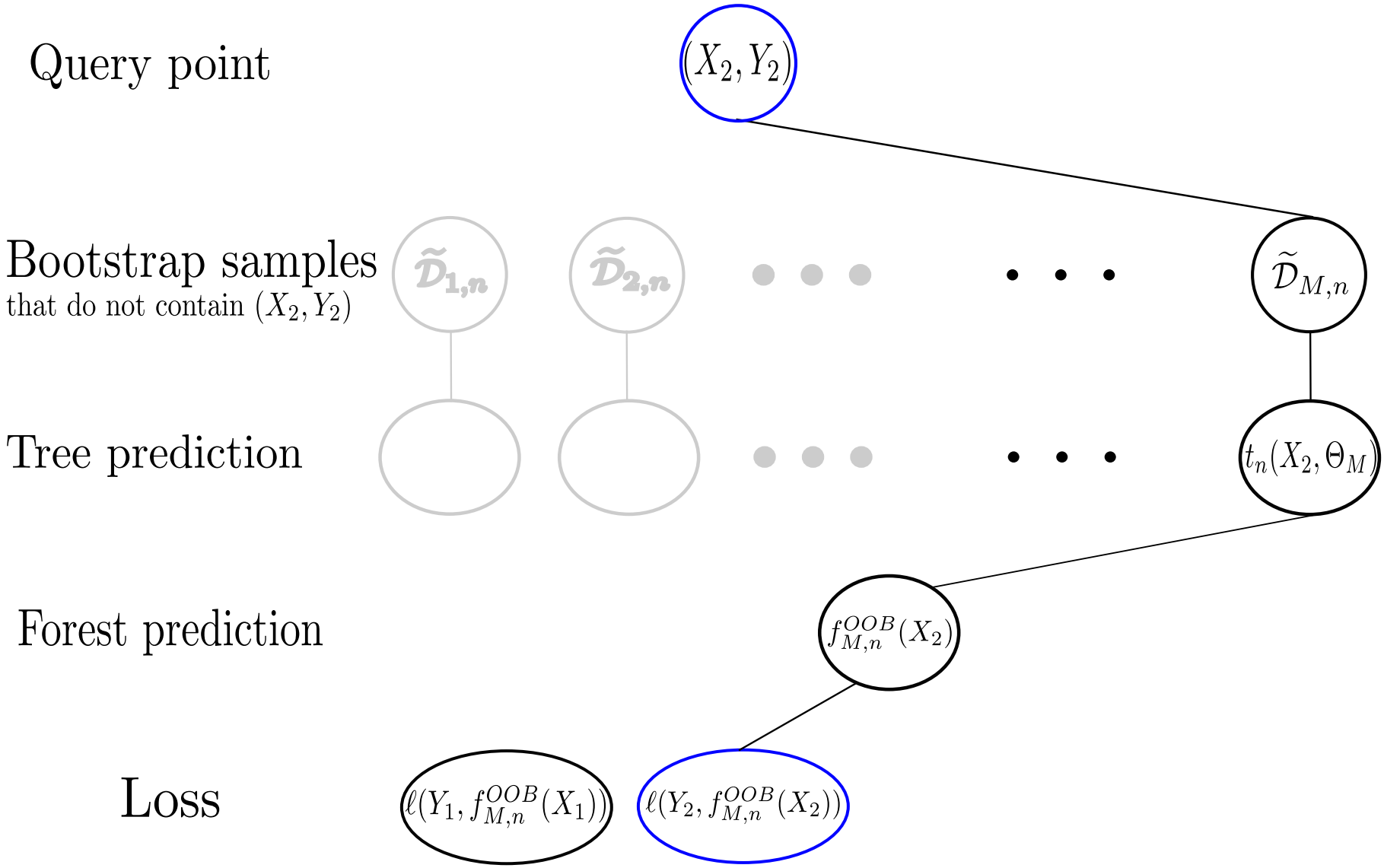

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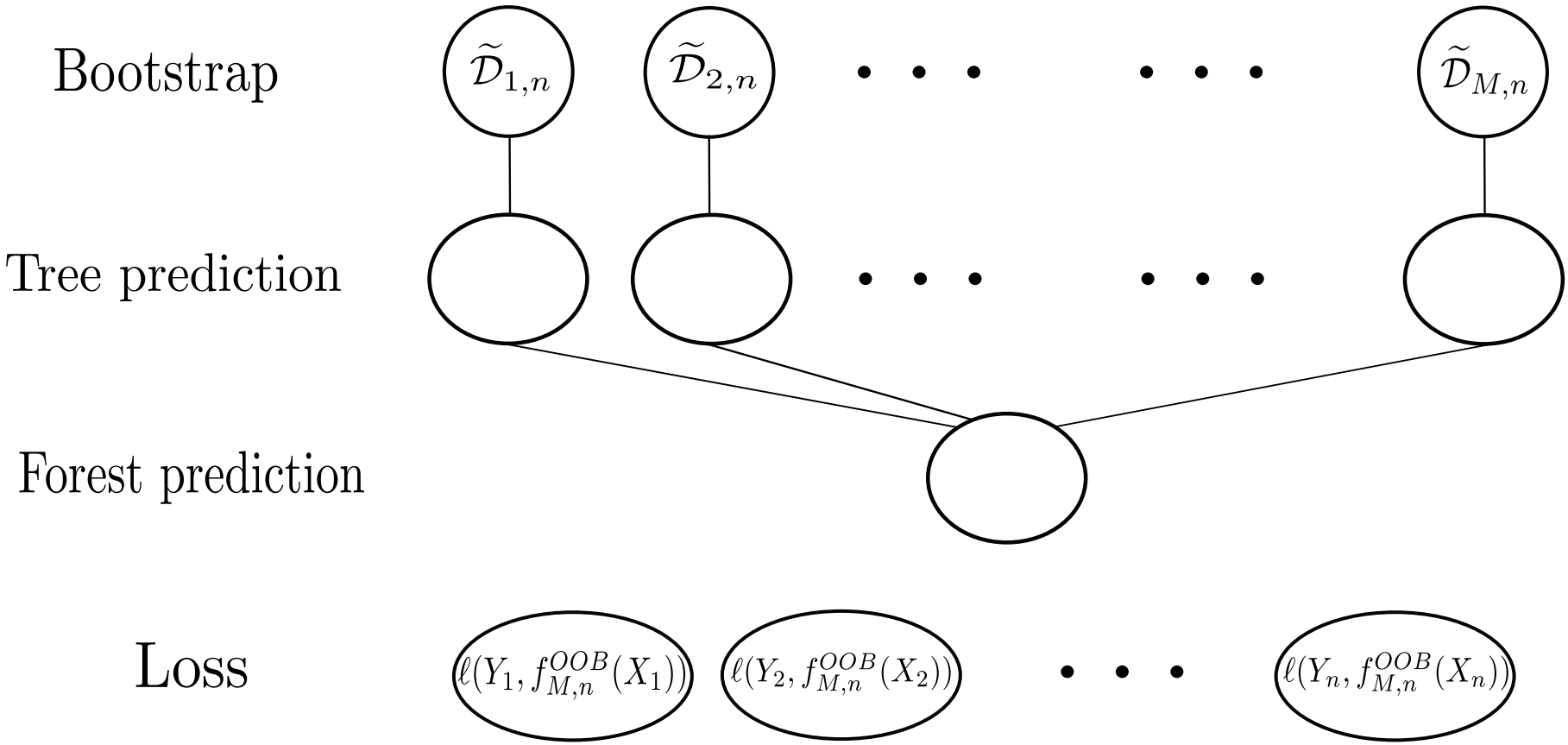

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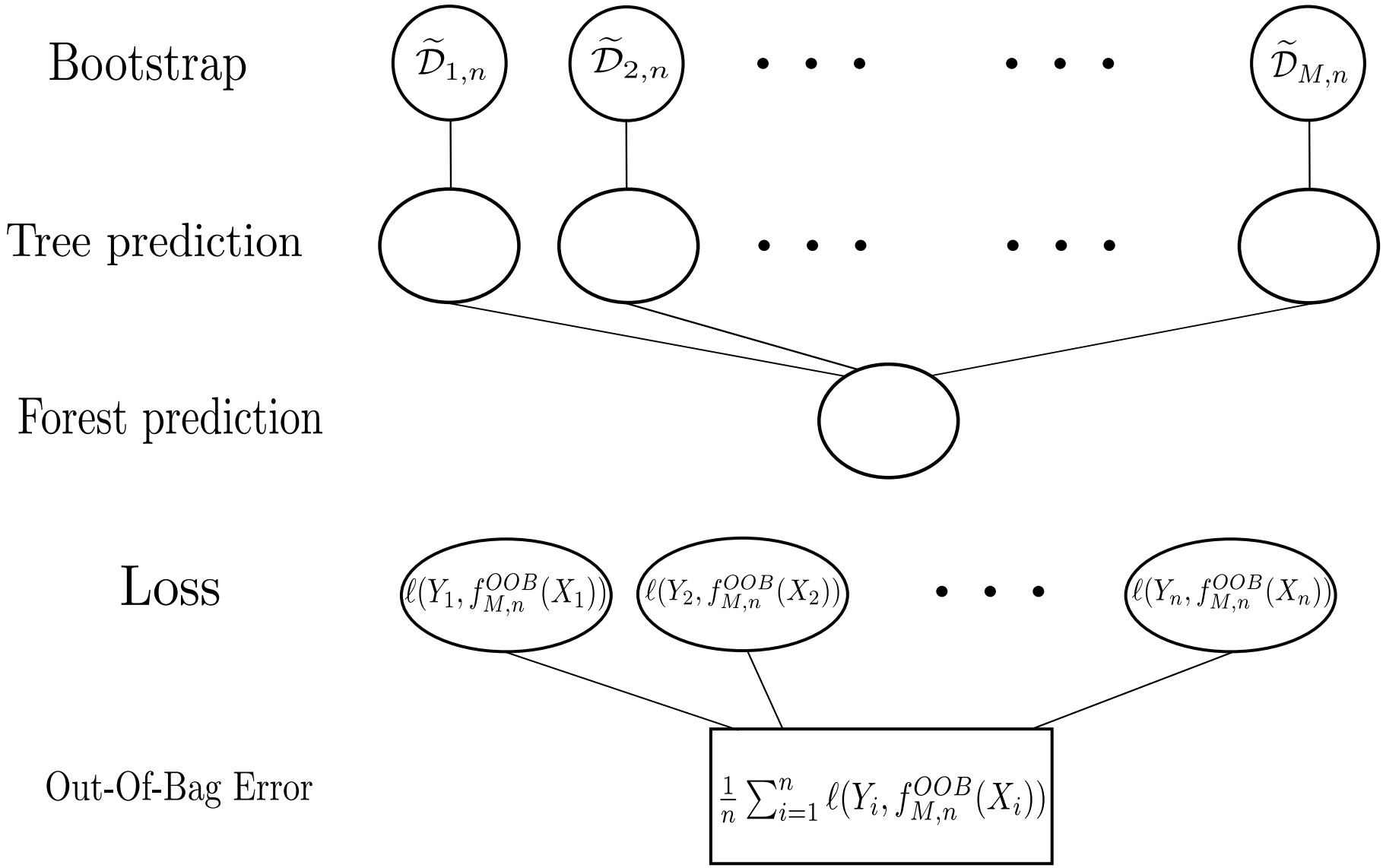

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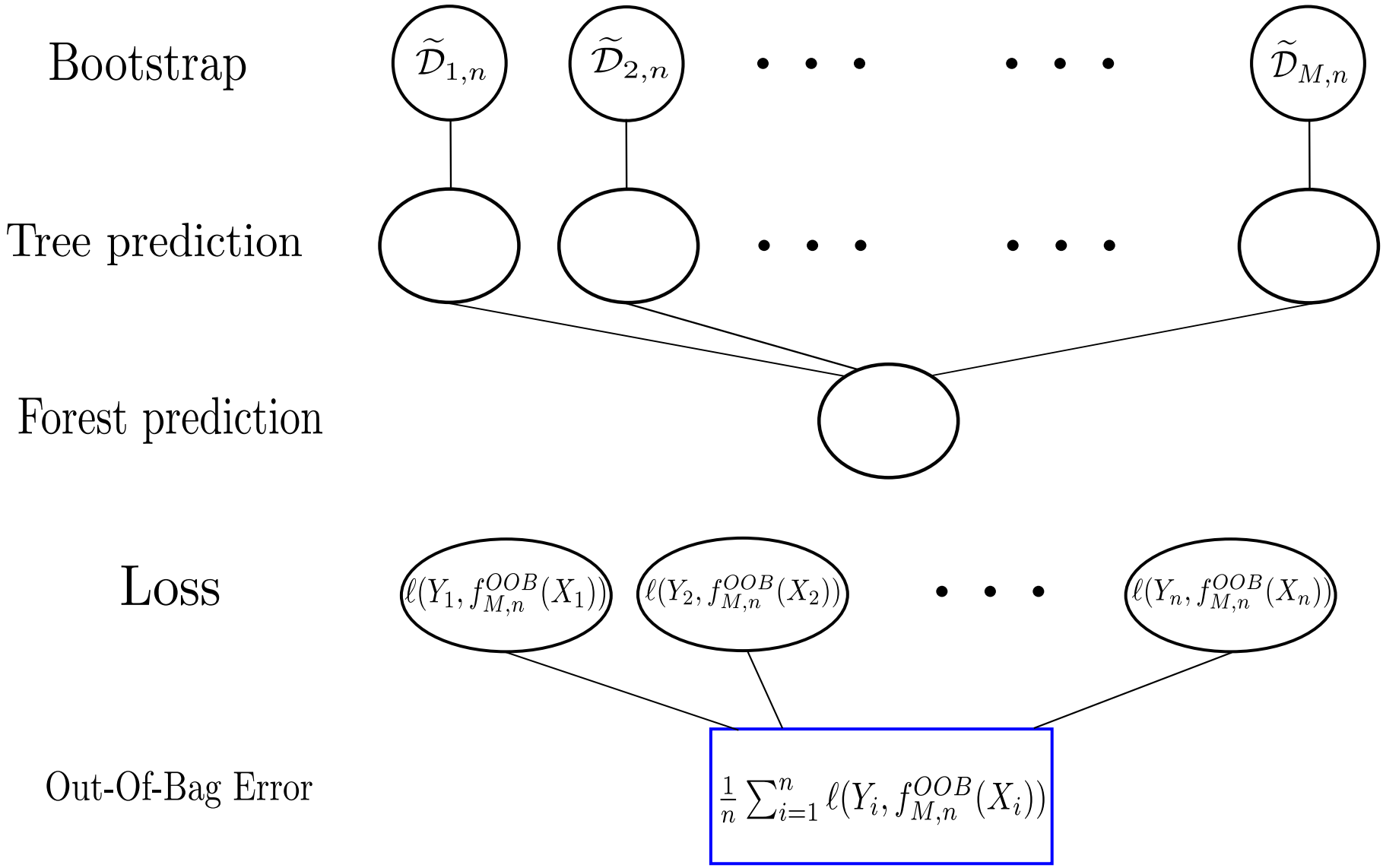


Out-of-bag (detailed procedure)

Consider that a forest has been trained on the data set $\mathcal{D}_n$.

- For each observation $i \in \{1, \ldots, n\}$,
  - Consider the bootstrap samples that do not contain this observation, that is the set $\Lambda_{i,n} = \{m, (X_i, Y_i) \notin \widetilde{\mathcal{D}}_{m,n}\}$
  - For the trees that are not built using observation i, compute the prediction at X_i and aggregate them as

$$f_{M,n}^{(OOB)}(X_i) = \frac{1}{|\Lambda_{i,n}|} \sum_{m \in \Lambda_{n,i}} t_n(X_i, \Theta_m) \mathbb{1}_{|\Lambda_{n,i}|>0} \quad \text{in regression,}$$

$$= \underset{k \in \{1,\ldots,K\}}{\text{argmax}} \sum_{\ell \in \Lambda_{n,i}} \mathbb{1}_{t_n(X_i,\Theta_\ell)=k} \quad \text{in classification.}$$

  - Compute the associated loss

$$\ell(f_{M,n}^{(OOB)}(X_i), Y_i) = (f_{M,n}^{(OOB)}(X_i) - Y_i)^2 \quad \text{in regression,}$$

$$= \ell(f_{M,n}^{(OOB)}(X_i), Y_i) = \mathbb{1}_{f_{M,n}^{(OOB)}(X_i) \neq Y_i} \text{in classification.}$$

- Compute the Out-of-bag error by averaging the losses over all observations, that is

$$R_n^{OOB} = \frac{1}{n} \sum_{i=1}^{n} \ell(f_{M,n}^{(OOB)}(X_i), Y_i)$$

Outline

Variable importance via random forests

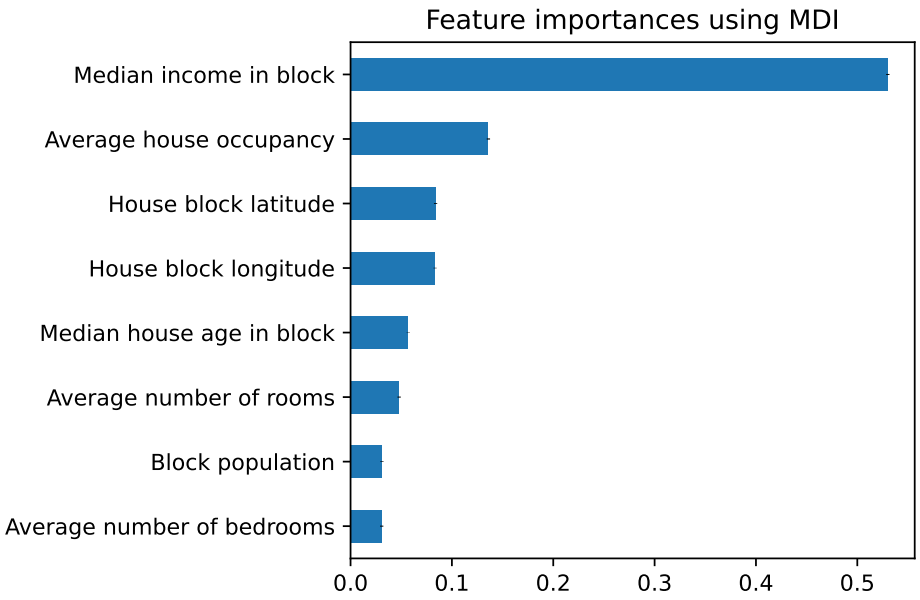
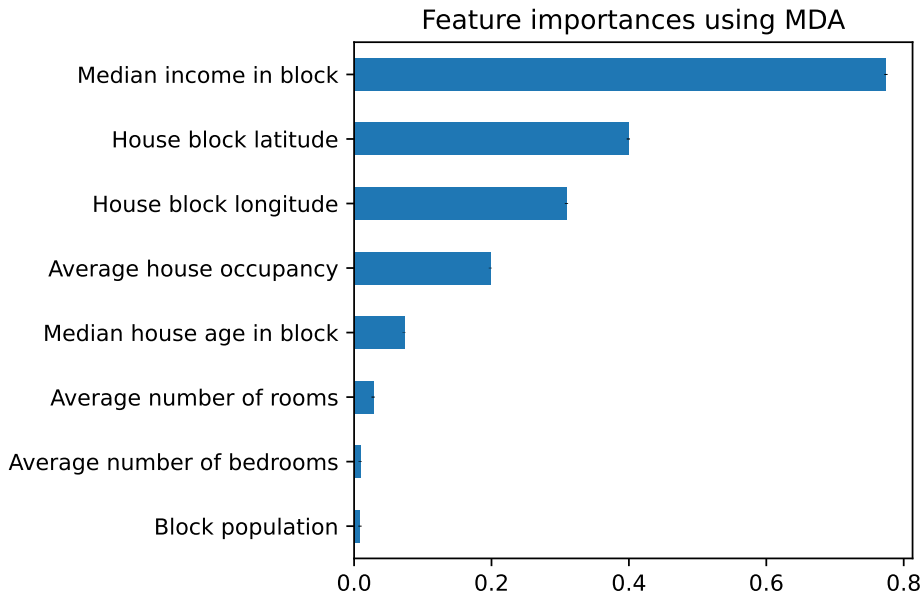


Figure: One of the two variable importance measure, Mean Decrease in Impurity (MDI) computed on the California housing data set.



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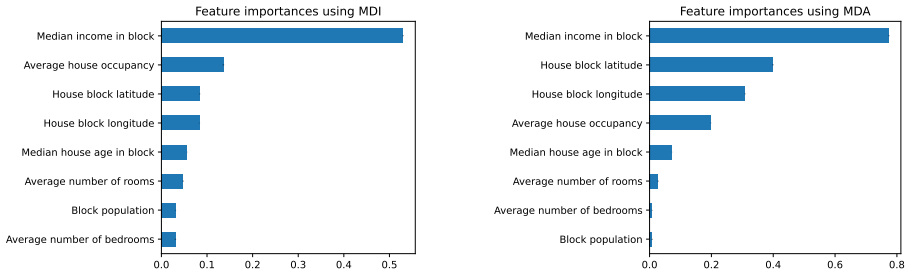
Variable importance via random forests



- Going beyond prediction to understand the black-box model
- Finding the input variables that are the most "linked" to the output
- Here the variable ranking is not exactly the same across these two different measures.

Variable importance - to what aim?

One single good variable importance measure does not exist. It always depend on what it is used for.

A simple example. Assume that $X \in \mathbb{R}^{10}$, $Y \in \mathbb{R}$ and $Y = X_1$ with $X_1 = g(X_2, \ldots, X_{10})$ for some function g.

- (Variable selection) If one is interested in finding the smallest set of variables leading to good predictive performance, the associated variable importance should be large for X_1 and null for $X_2, \ldots, X_{10}$.
- (Link identification) If one is interested in finding all variables linked to the output, the associated variable importance should be large for $X_1, \ldots, X_d$.

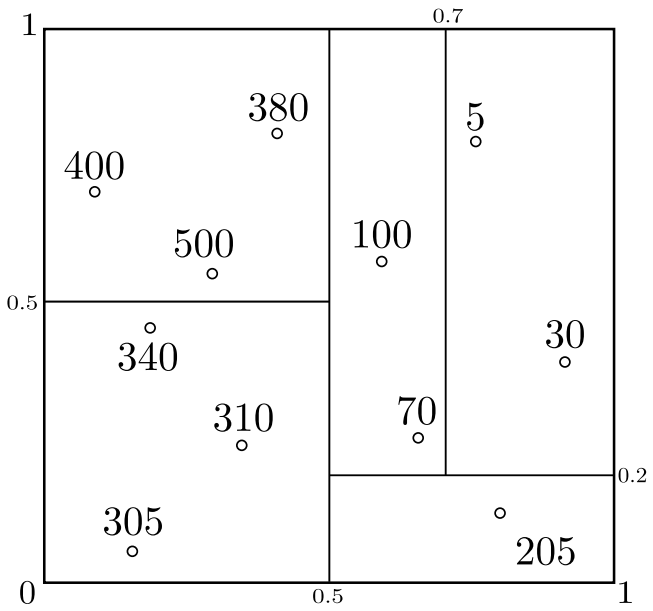
The quality of a variable importance measure depends on its final use (variable selection or link identification).

Variable importance in random forests

Two different measures often computed with random forests:

- Mean Decrease Impurity (MDI) (Breiman, 2002)
  - Tailored for decision tree methods
  - Use the decrease in impurity in each node to compute an aggregated variable importance
- Mean Decrease Accuracy (MDA) (also called *permutation importance*, see Breiman, 2001)
  - Can be used with any supervised learning algorithm (not tree specific)
  - Permute the values of a given feature in the test set and compare the resulting decrease in predictive performance.

Mean Decrease in impurity



$k = 0$

$k = 1$

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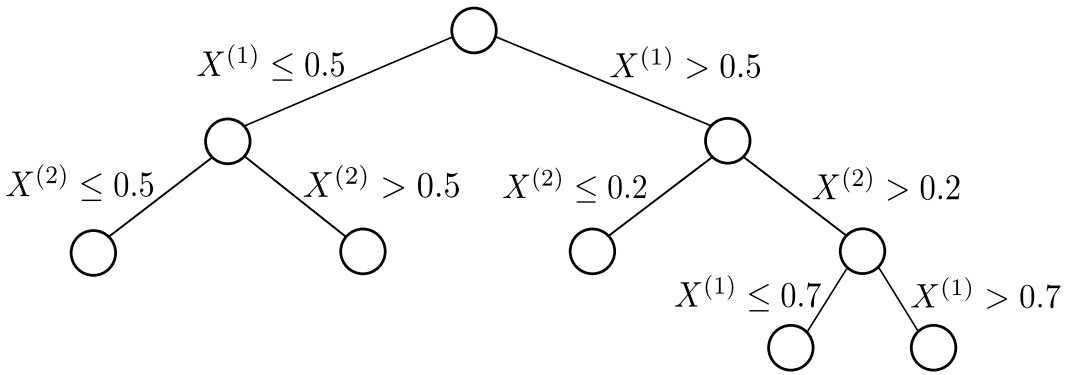
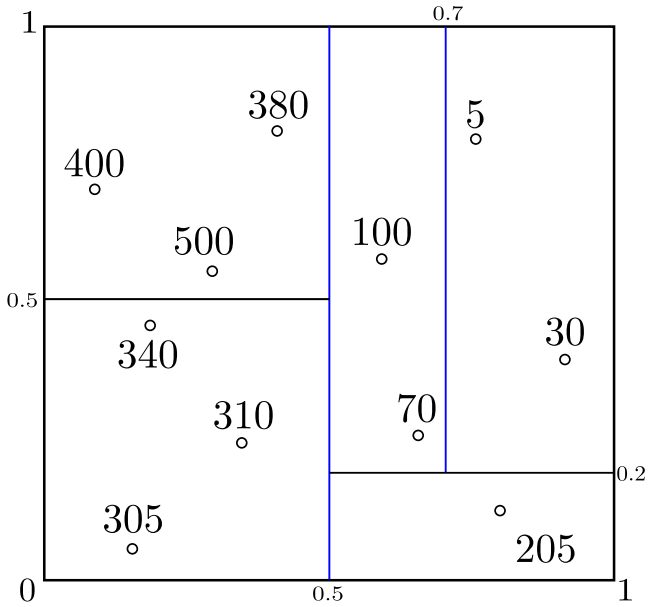
$k = 3$



For this given trained tree $\mathcal{T}$, we want to evaluate the MDI of $X^{(1)}$.

Mean Decrease in impurity



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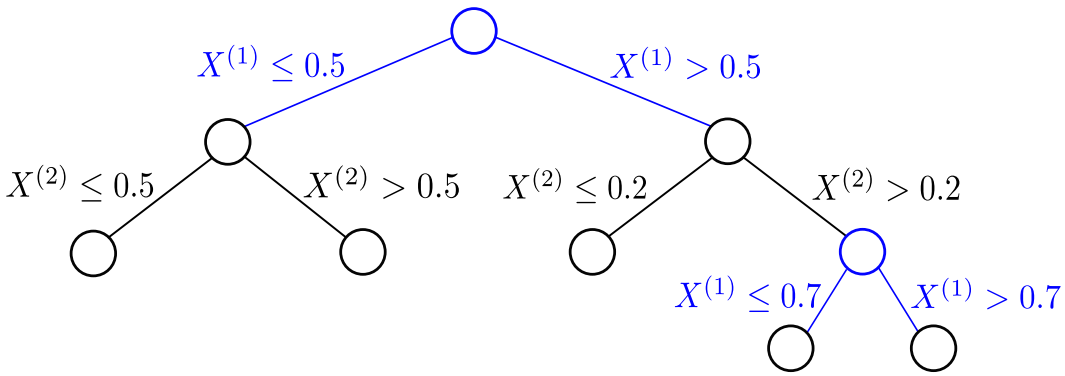

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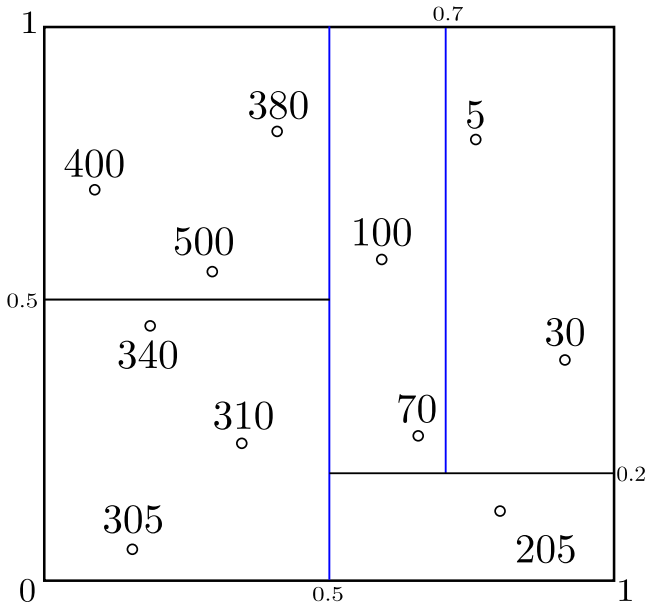

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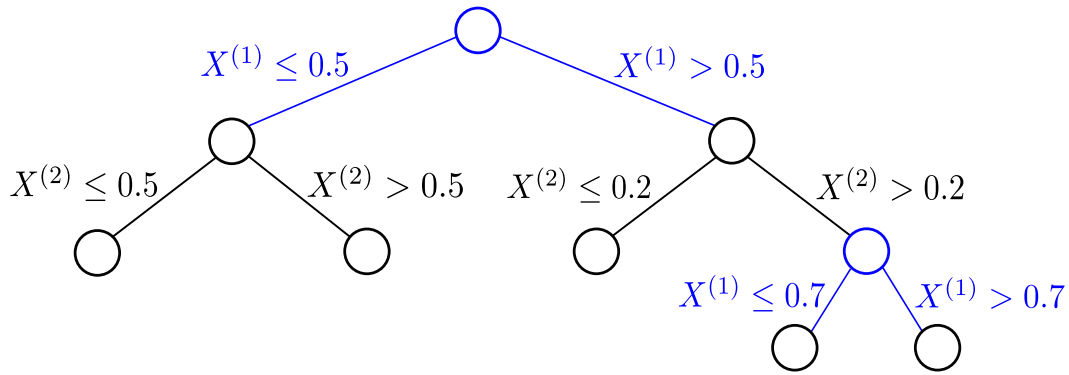

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$$\Delta Imp_n(A) = Imp_n(A) - p_{L,n} Imp_n(A_L) - p_{R,n} Imp_n(A_R),$$

where $p_{L,n}$ (resp. $p_{R,n}$) is the fraction of observations in A that fall into A_L (resp. A_R). For example,

$$Imp_{V,n}(A) = \mathbb{V}_n[Y|X \in A].$$

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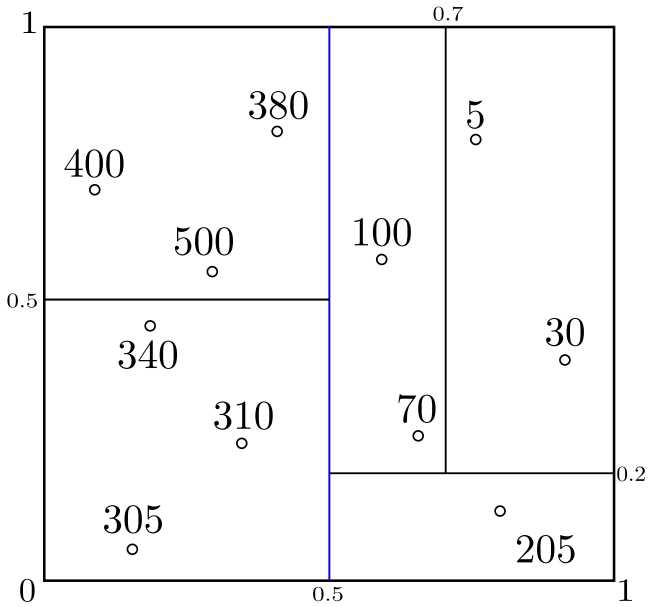

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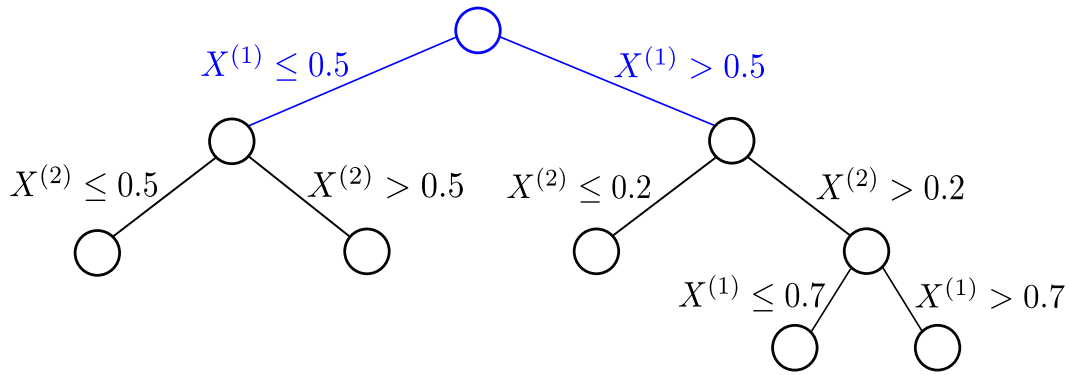

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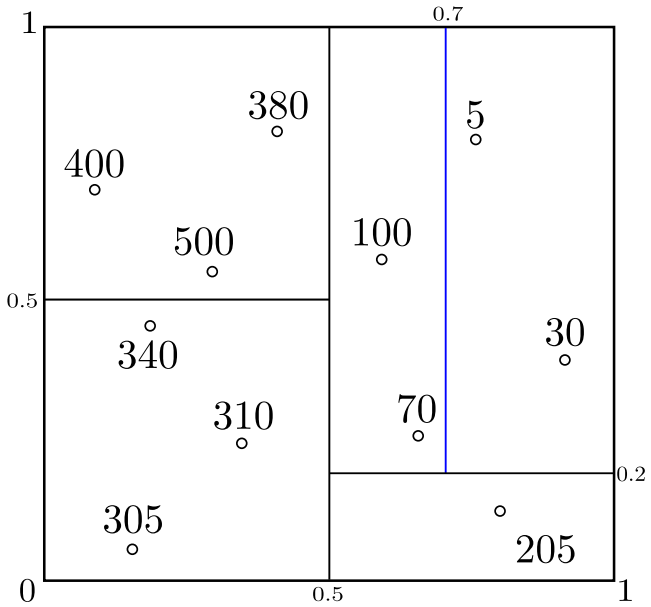

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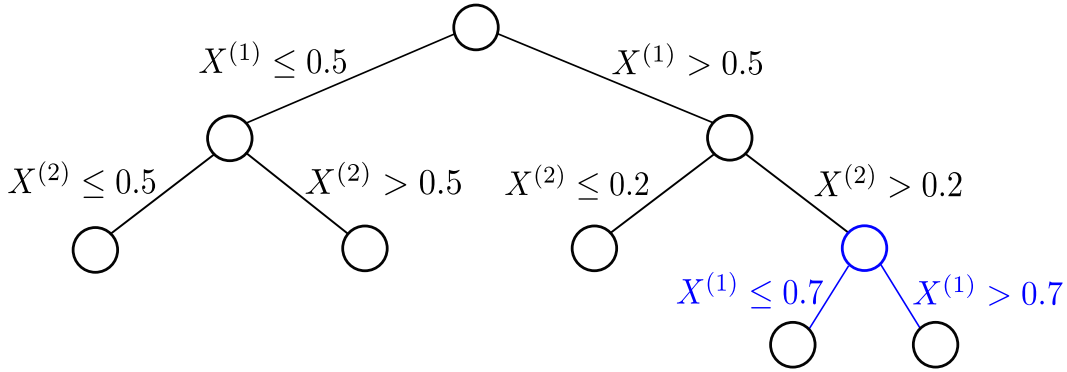

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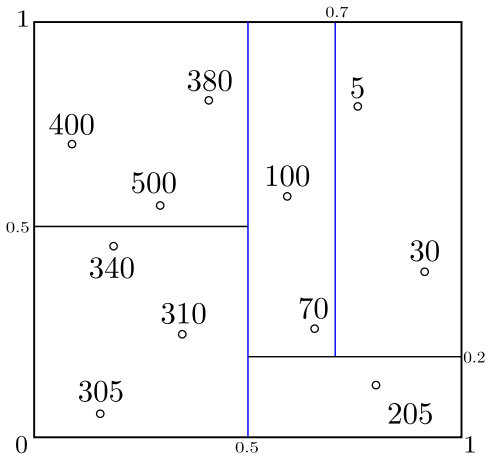

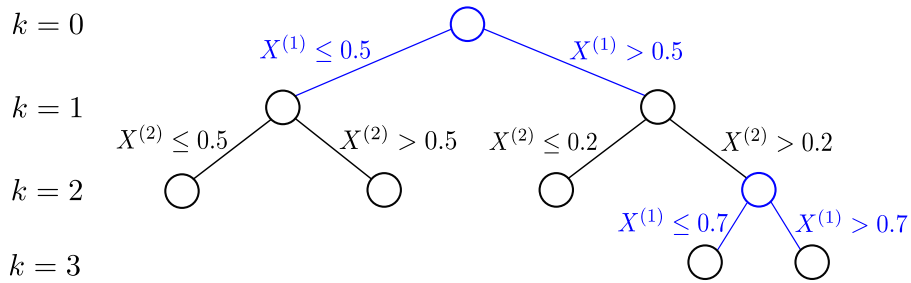

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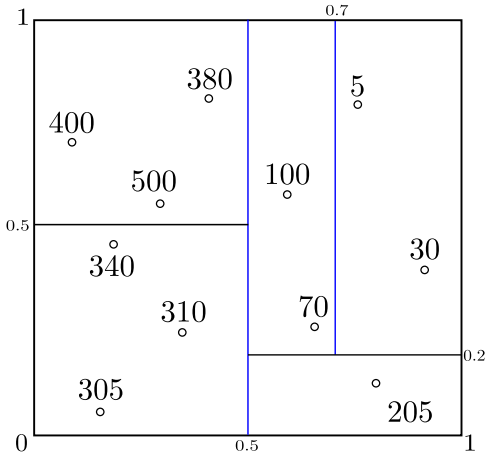
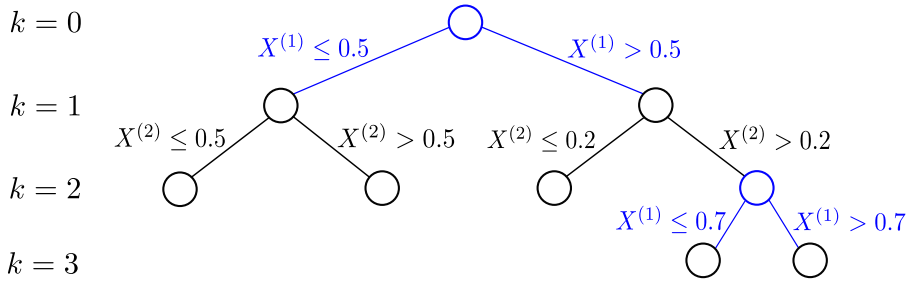
$$\widehat{\mathrm{MDI}}_{\mathcal{T}}(X^{(j)}) = \sum_{\substack{A \in \mathcal{T} \\ j_{n,A}=1}} p_{n,A}\ \Delta Imp_n(A), \tag{1}$$

where the sum ranges over all cells A in $\mathcal{T}$ that are split along variable j and $p_{A,n}$ is the fraction of observations falling into A

Mean Decrease in impurity





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- The MDI of $X^{(1)}$ output by a forest is the average of the MDI of $X^{(1)}$ of each tree.

Mean Decrease in Impurity

Pros

- Easily accessible via scikit-learn as the attribute `feature_importances_` of a RandomForest object
- No extra computations needed
- Adapted to the tree building process / the predictor

Mean Decrease in Impurity

Cons

- biased towards variables with many categories (see, e.g., Strobl et al., 2007; Nicodemus, 2011), variables that possess high-category frequency (Nicodemus, 2011; Boulesteix et al., 2011), biased in presence of correlated features (Nicodemus and Malley, 2009)
- Bias related to in-sample estimation (Li et al., 2019; Zhou and Hooker, 2021) - Same observations are used to build the tree and estimate the MDI
- Bias related to fully-grown tree
- No information about the quantity it is supposed to estimate!

MDA illustration

MDA principle: decrease of accuracy of the forest when a variable is noised up

$X^{(1)}$	$X^{(2)}$	$\dots$	$X^{(j)}$	$\dots$	$X^{(p)}$	Y
2.1	4.3	$\dots$	0.1	$\dots$	2.6	2.3
1.7	4.1	$\dots$	9.2	$\dots$	3.8	0.4
3.4	9.2	$\dots$	3.2	$\dots$	3.6	10.2
5.6	1.2	$\dots$	8.2	$\dots$	4.2	9.1
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Table: Example of the permutation of a dataset $\mathcal{D}_n$ for $n = 5$.

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quadratic error $= 13.7$
quadratic error $= 16.4$

$$\mathrm{MDA}(X^{(j)}) = 16.4 - 13.7 = 2.7$$

MDA versions

The explained variance estimate of MDA algorithms differ across implementations

Train-Test MDA: train data to fit the forest, and test data for accuracy

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Selected samples: $\Theta_\ell^{(s)} = \{1, 3, 4\}$

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OOB samples: $\{1, \ldots, n\} \setminus \Theta_\ell^{(S)} = \{2, 5\}$

Mean Decrease in Accuracy

Pros

- Can be applied to any machine learning algorithm via the function `permutation-importance` in scikit-learn
- Fast to compute (no need to retrain a forest)

Cons

- Biased in presence of correlation
- The quantity to which it converges is not the correct for either of the two objectives (designing a small model with high predictivity or finding a large set of variables linked to the output)

Take-home message on variable importance

Do not use MDI or MDA!

We do not know what quantity they are targeting

Take-home message on variable importance

Some alternatives:

- MDI
  - Out-of-sample estimation (Li et al., 2019; Zhou and Hooker, 2021; Loecher, 2022) with code in python:

    `https://github.com/ZhengzeZhou/unbiased-feature-importance`

- MDA
  - Rerun the model without a given covariate (expensive). Work for any predictive model (Williamson et al., 2021)
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Anyway, remember to check the predictive performance of a model: it it is low, the model is useless and variable importances are misleading.

Outline

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What is Boosting?

Boosting:

- Combining weak predictors (classification/regression) in a sequential manner to obtain an aggregated predictor better than each individual predictor
- The predictor resulting from boosting is a weighted average of some weak predictors, resulting from a learning algorithm applied to a modified dataset.

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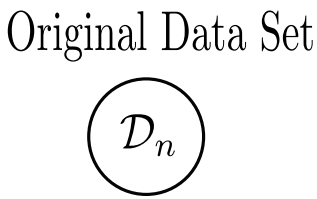
- The predictor resulting from boosting is a weighted average of some weak predictors, resulting from a learning algorithm applied to a modified dataset.

What do we need?

- A data set
  $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$
- A weak learning procedure
  - Decision tree (CART) $\rightarrow$ Tree Boosting
  - Linear models
  - ...
- A loss

Boosting in a scheme



Boosting in a scheme

Iterations	Original Data Set
$t = 0$	$\mathcal{D}_n$

Boosting in a scheme

Boosting in a scheme

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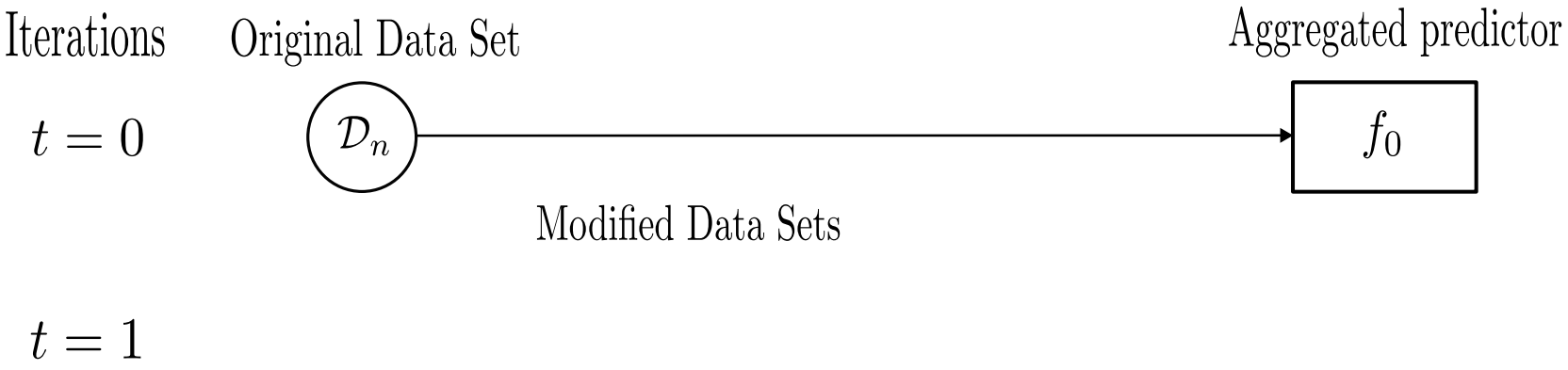

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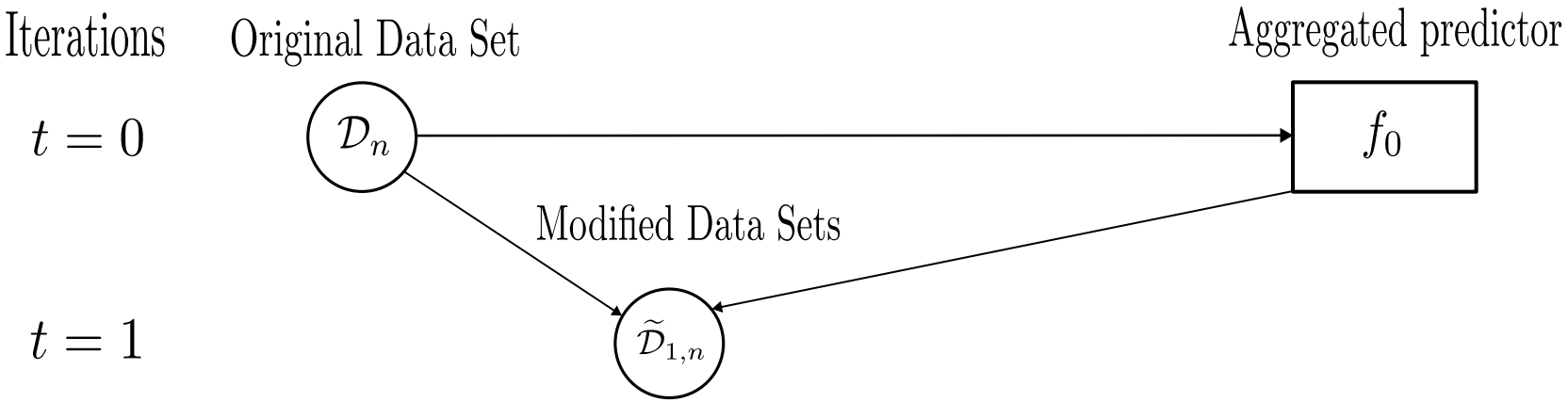
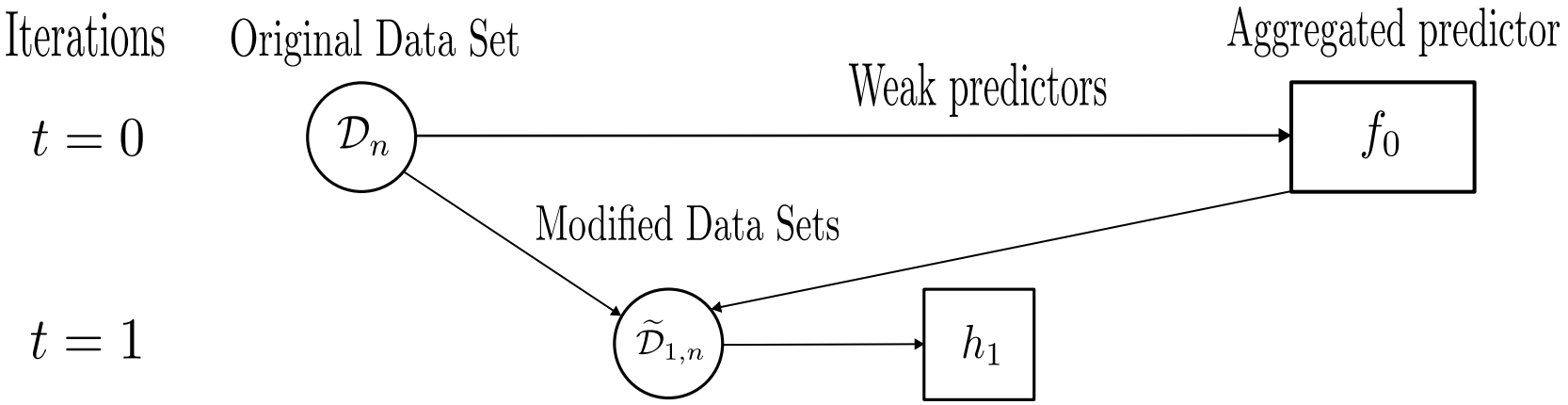
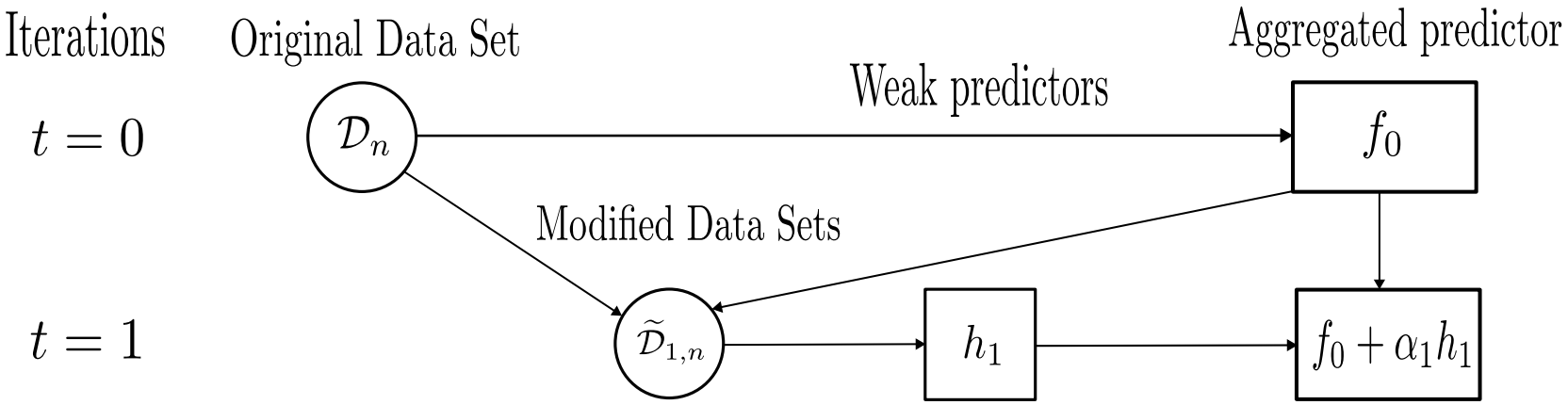


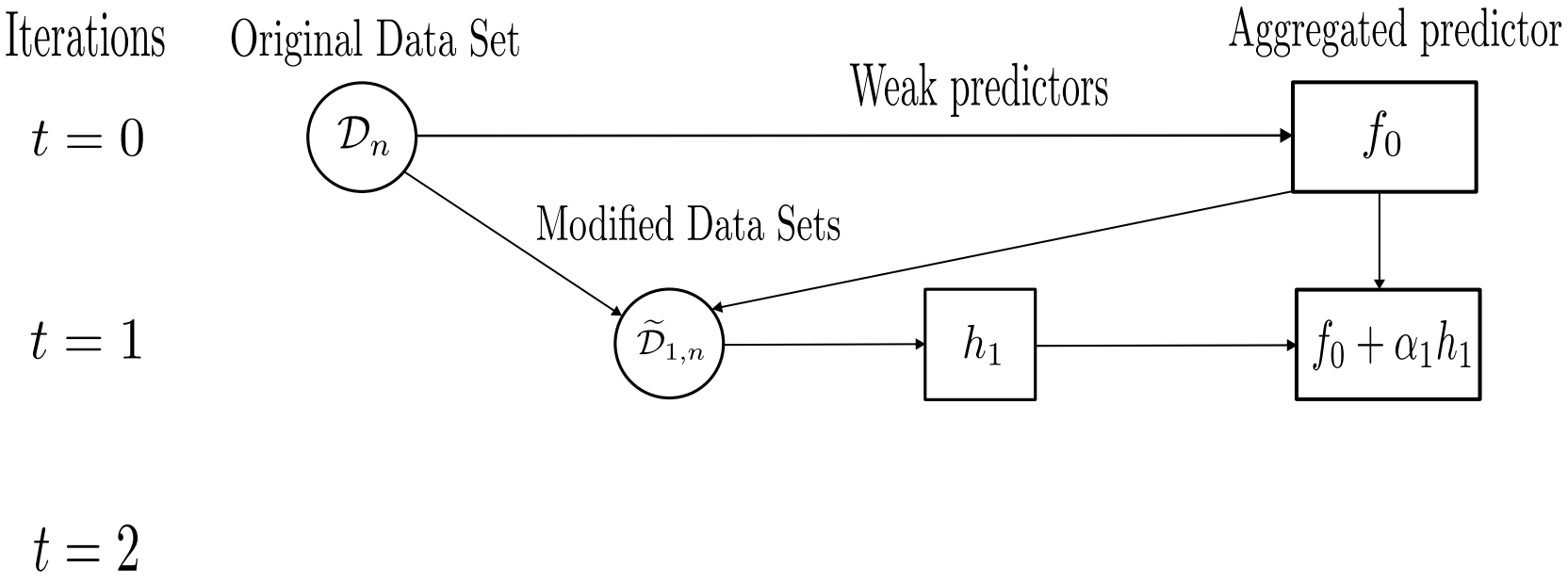
Boosting in a scheme



Boosting in a scheme



Boosting in a scheme



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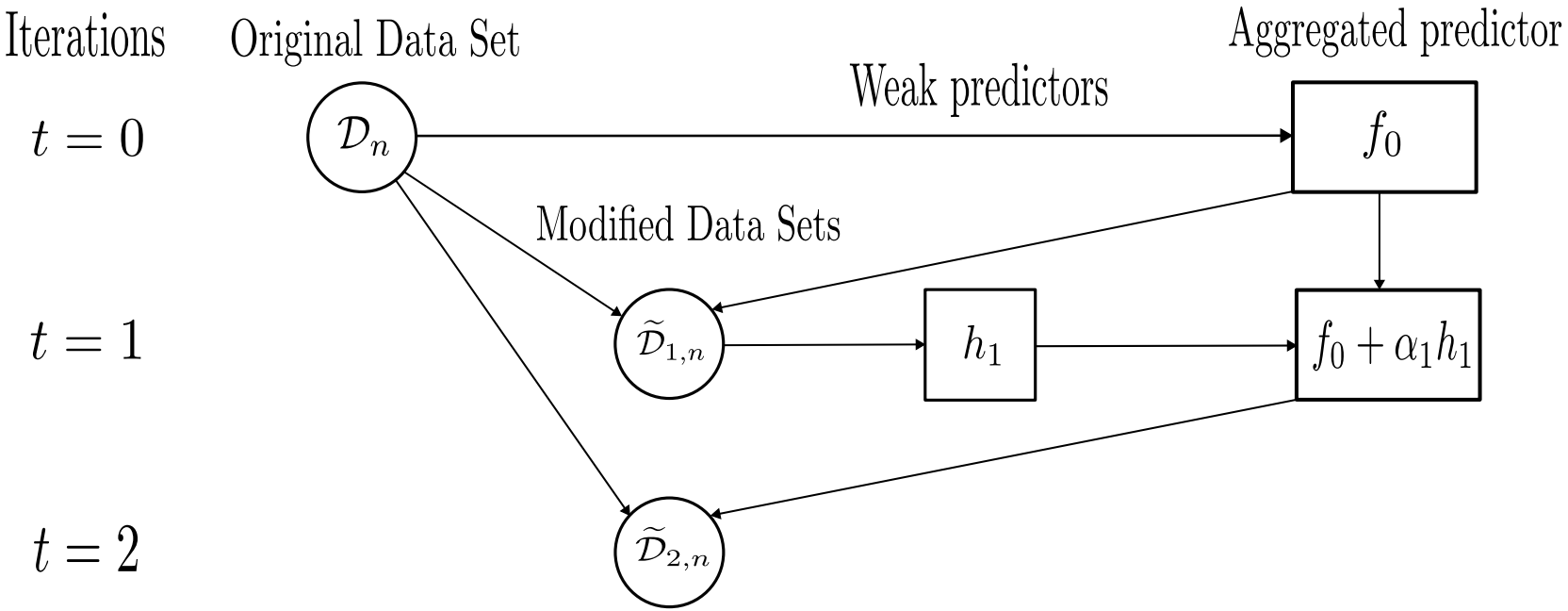

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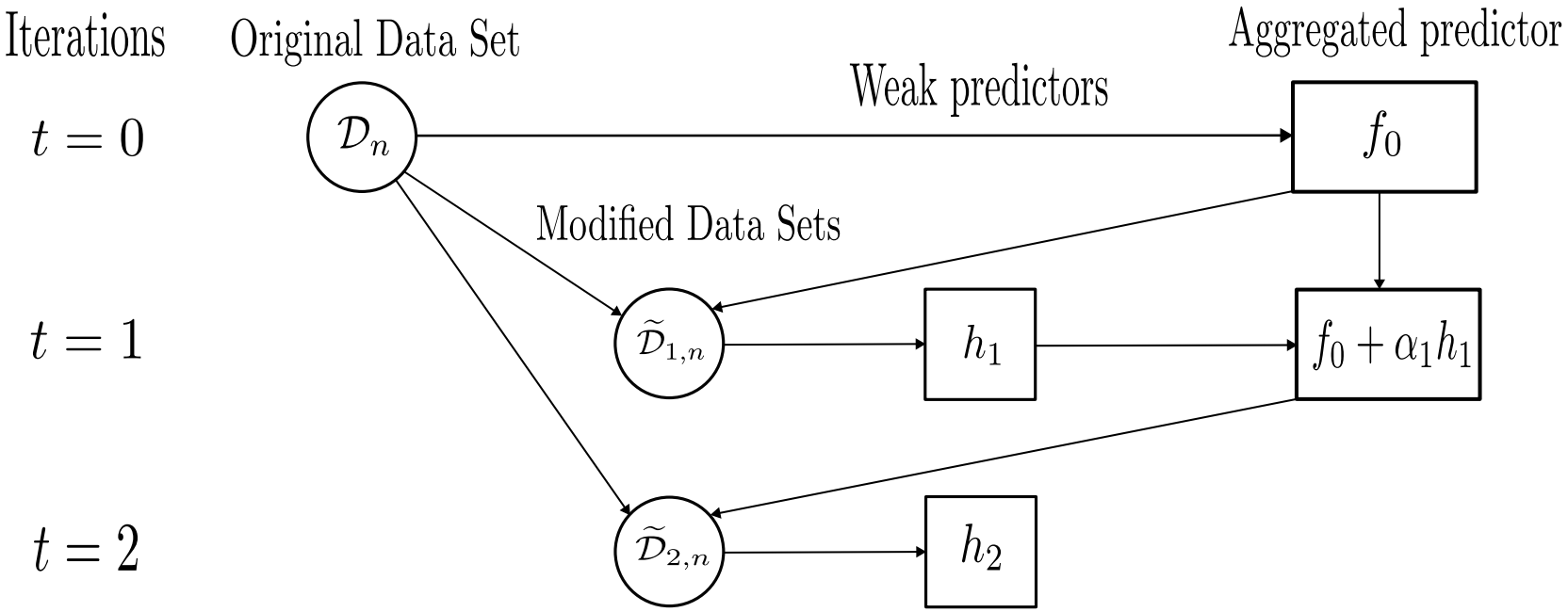

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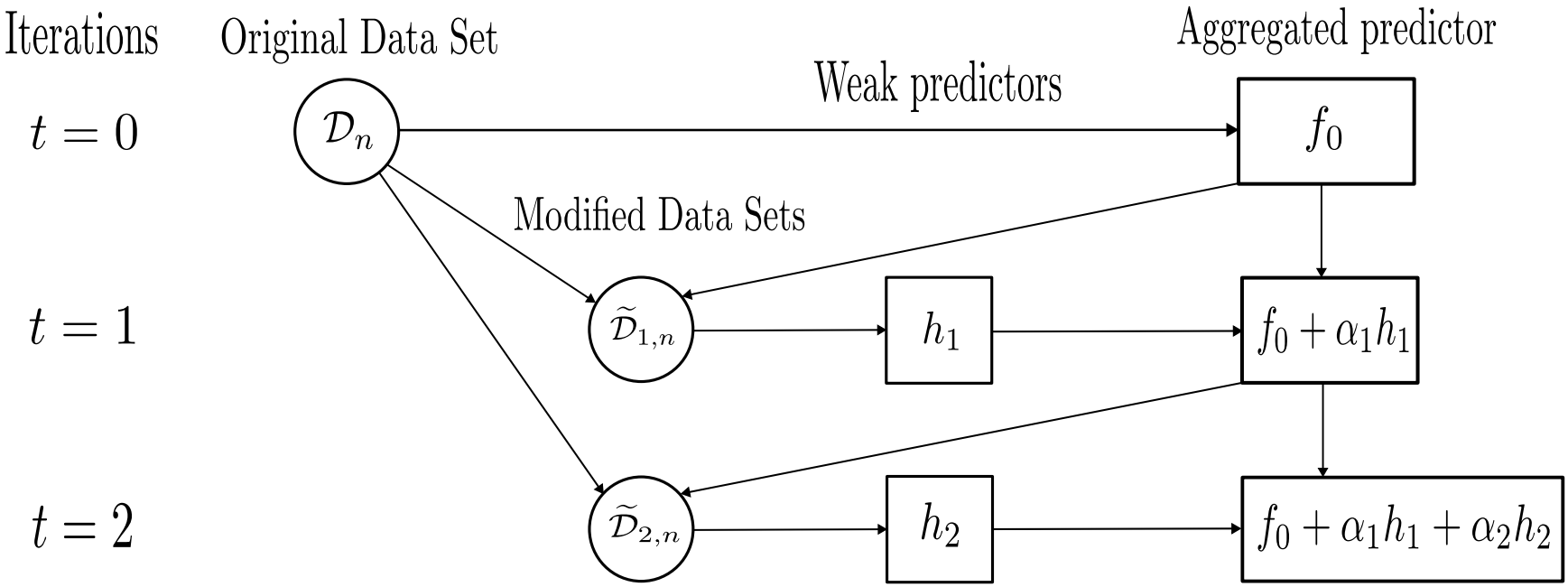

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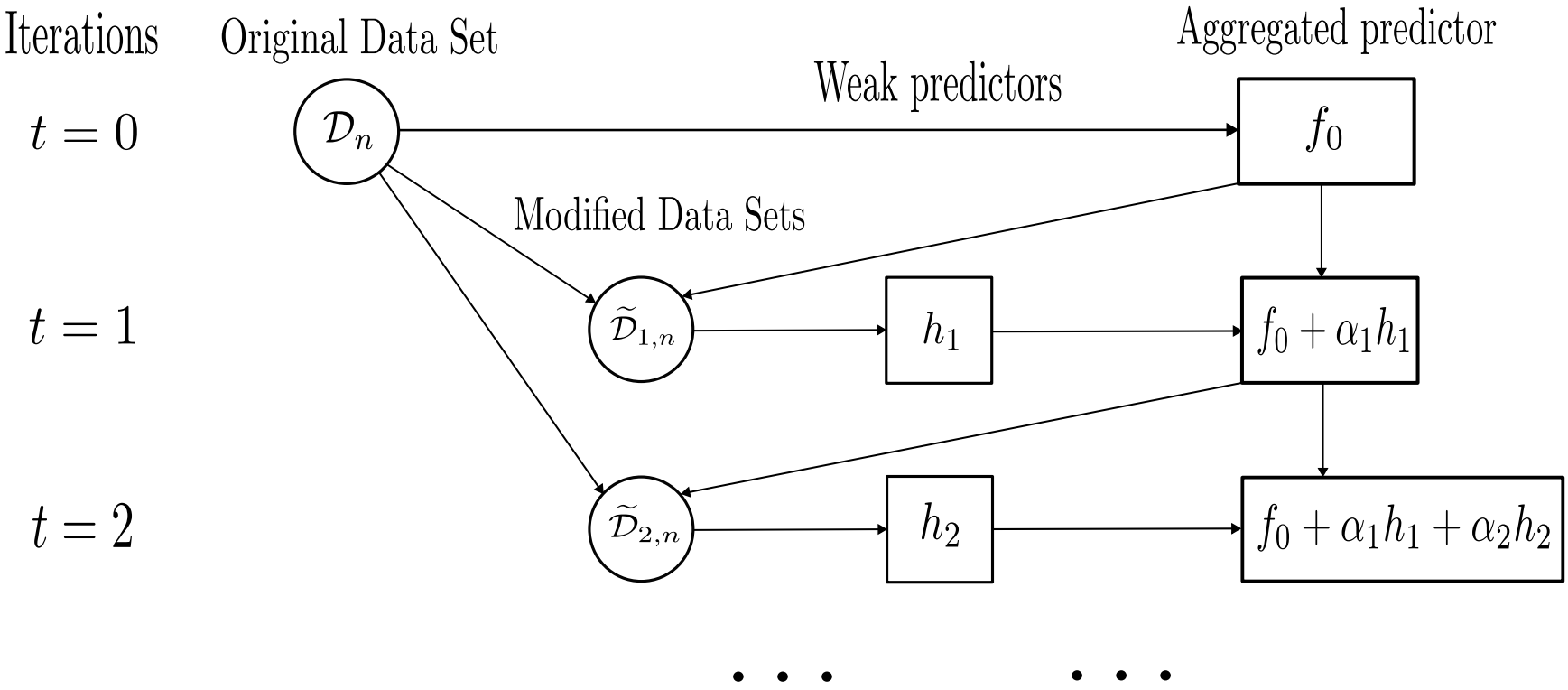

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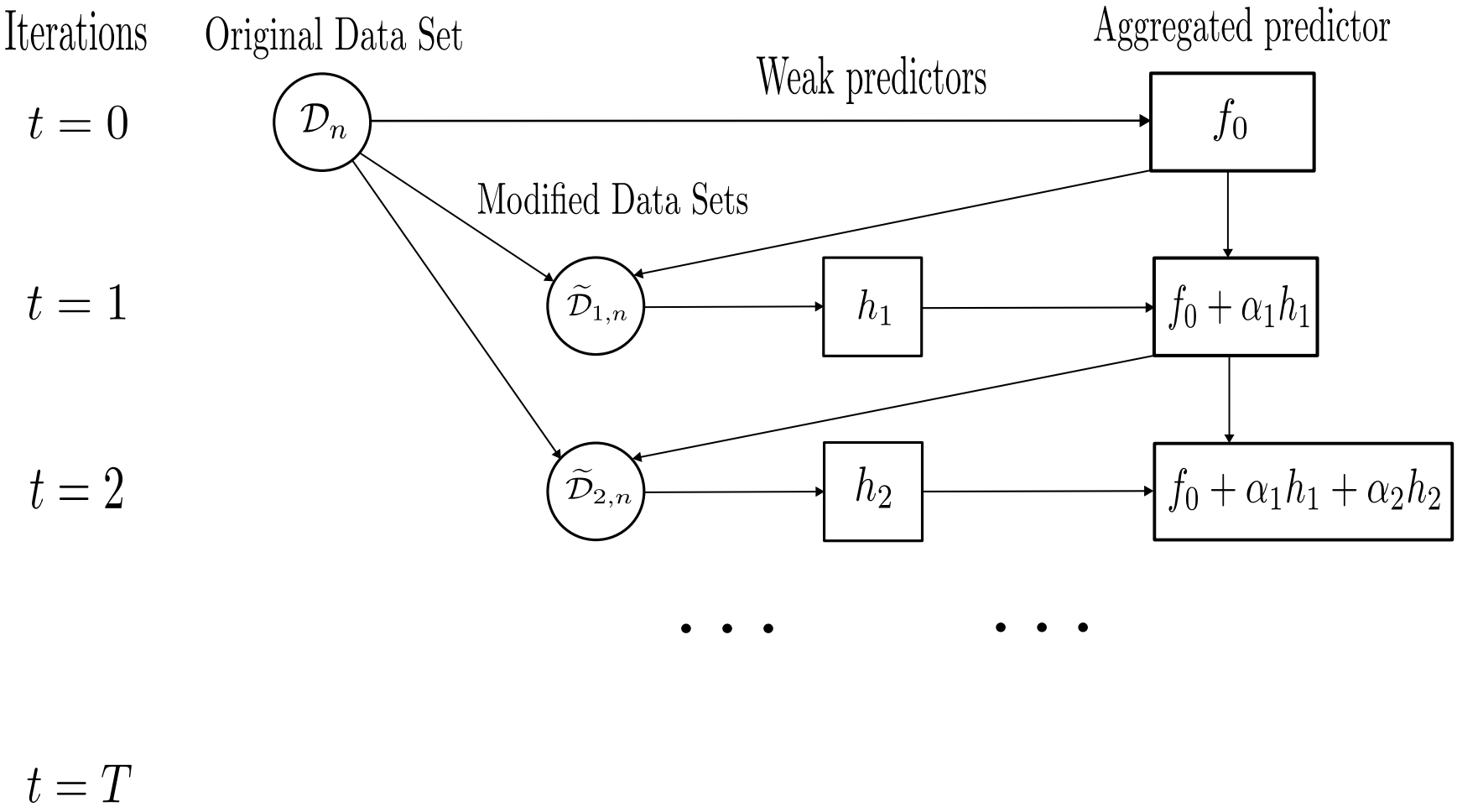

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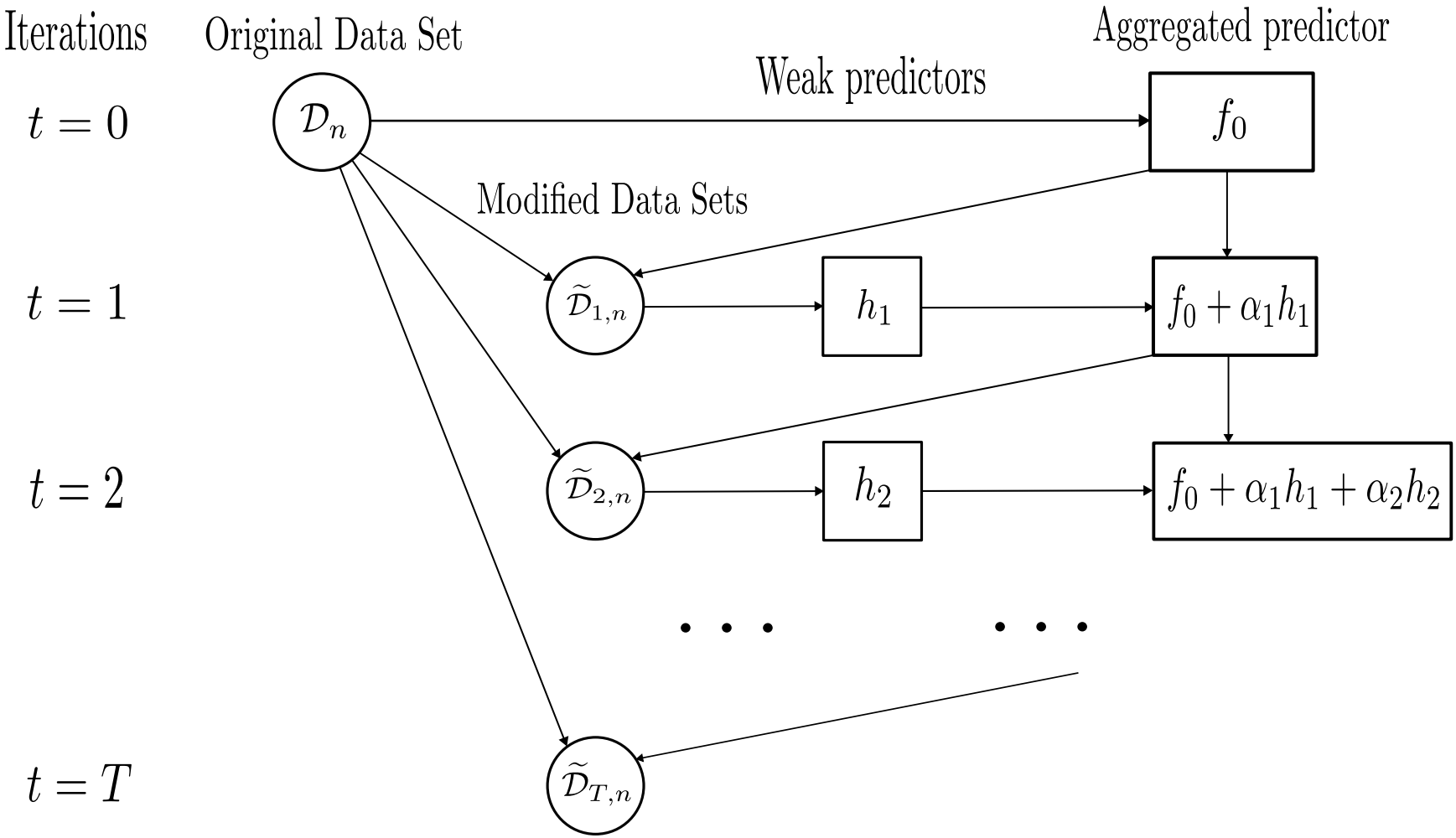

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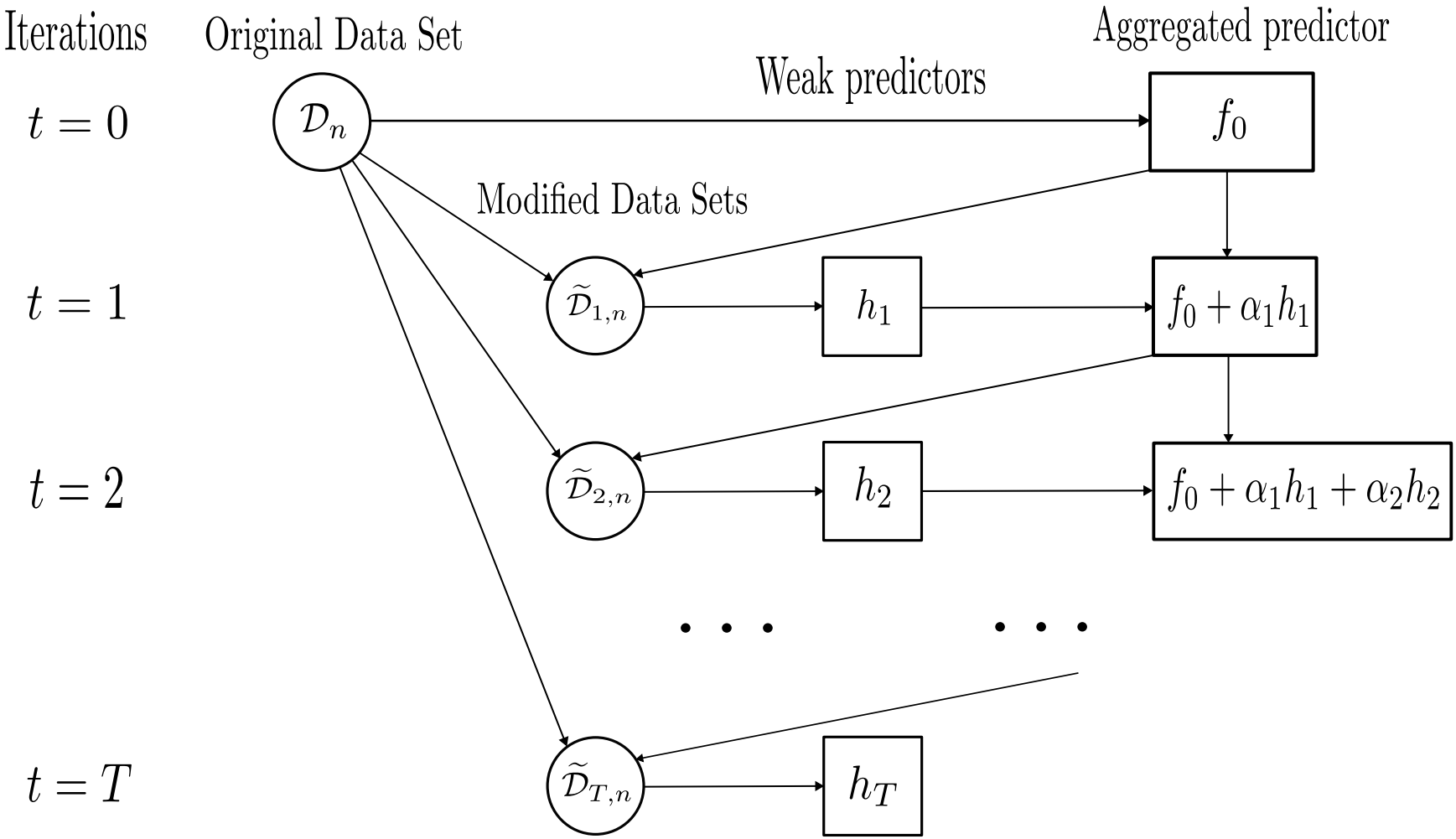

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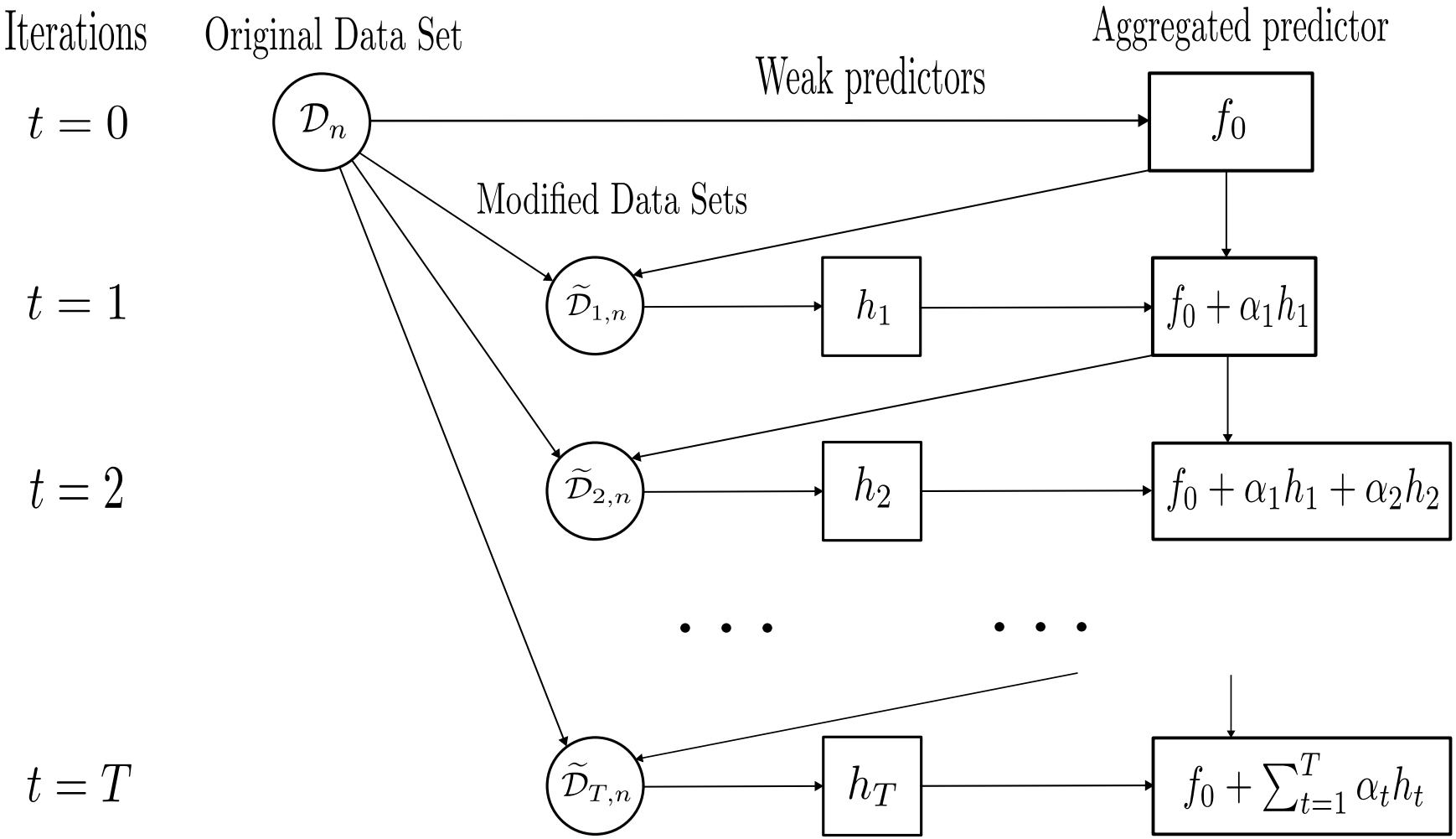
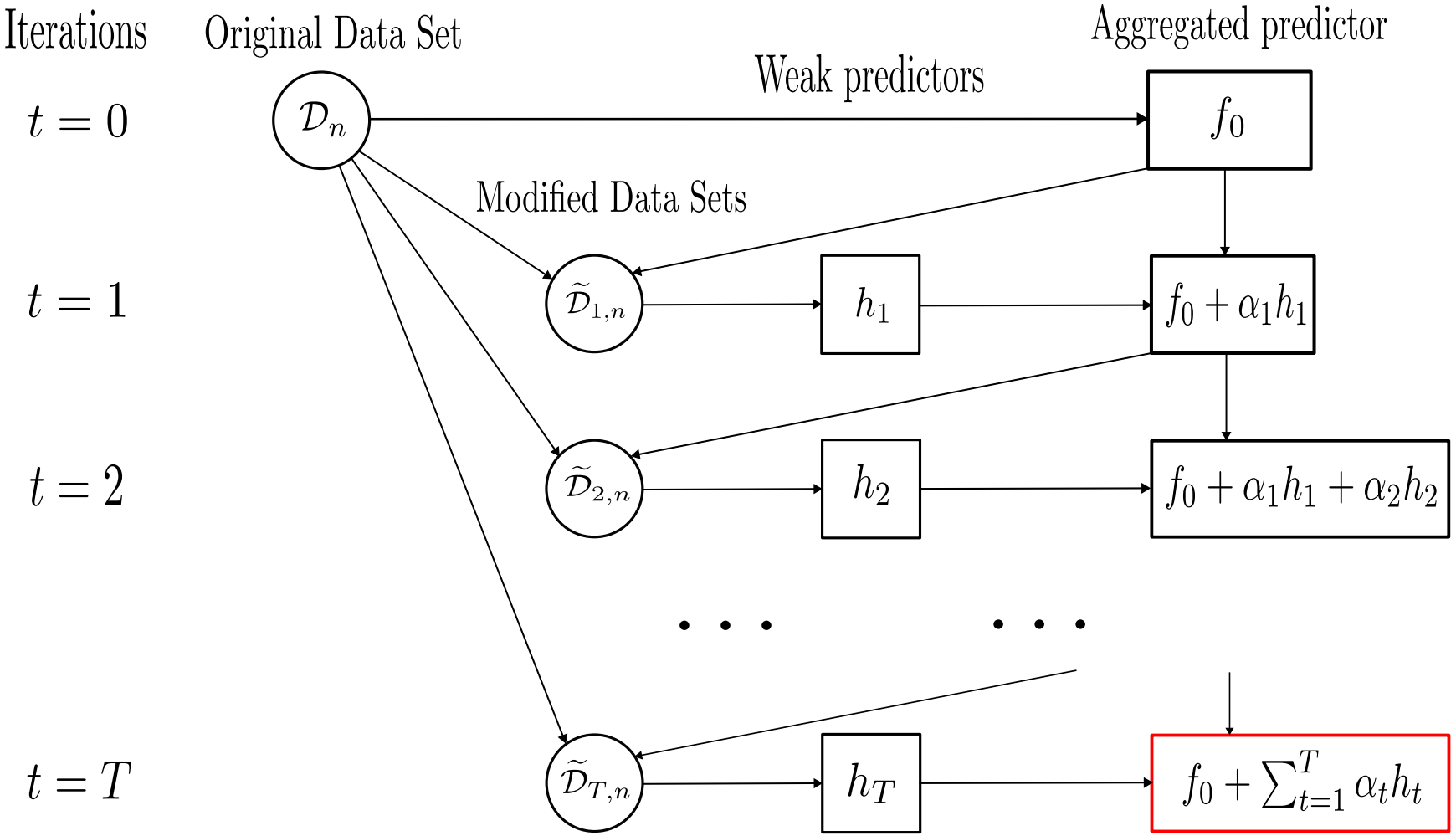


Boosting in a scheme



Outline

Generic Boosting pseudo-algorithm

Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
2. Set $f = 0$
3. For $t = 1, \ldots, T$
   1. Select
   $$(h_t, \alpha_t) \in \underset{h \in \mathcal{H}, \alpha \in \mathbb{R}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell(y_i, f(x_i) + \alpha h(x_i)) \tag{2}$$
   2. Update $f = f + \alpha_t h_t$
4. The final predictor is given by $f = \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Idea. At each iteration, we try to find the weak predictor that, when added to the current overall predictor, decreases the most the risk on the training set.

Generic Boosting pseudo-algorithm

Boosting algorithm

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Remarks. Finding minimizers in equation is difficult in general:

- Optimization on a large space - the class $\mathcal{H}$ can be infinite or very large, for example the set of all decision trees.
- Joint optimization procedure in (h, α).

Generic Boosting pseudo-algorithm

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A special case to understand better the procedure: the exponential loss (Adaboost).

AdaBoost algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ with $Y_i \in \{-1, 1\}$, a set $\mathcal{H}$ of weak learners.
2. Set $f = 0$
3. For $t = 1, \ldots, T$
   1. Select
   $$(h_t, \alpha_t) \in \operatorname*{argmin}_{h,\alpha} \sum_{i=1}^{n} \exp(-y_i(f(x_i) + \alpha h(x_i))) \tag{3}$$
   2. Update $f = f + \alpha_t h_t$
4. The final predictor is given by $f = \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

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   2. Update $f = f + \alpha_t h_t$
4. The final predictor is given by $f = \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Assumptions

Assume that, for all $h \in \mathcal{H}$,

- $-h \in \mathcal{H}$ (symmetry)
- There exist $1 \leq i \neq j \leq n$ such that $h(X_i) = Y_i$ and $h(X_j) \neq Y_j$ (no perfect classifier).

Under these assumptions, AdaBoost can be rewritten as follows.

Adaboost algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners.
2. Set $f = 0$ and $w_{1,i} = 1/n$ for all $i \in \{1, \ldots, n\}$.
3. For $t = 1, \ldots, T$
   1. Select
   $$h_t \in \operatorname*{argmin}_{h \in \mathcal{H}} \sum_{i=1}^{n} w_{t,i} \mathbb{1}_{Y_i \neq h(X_i)} \tag{3}$$
   2. Compute
   $$\alpha_t = \frac{1}{2} \log\left(\frac{\varepsilon_t(h_t)}{1 - \varepsilon_t(h_t)}\right), \quad \text{with} \quad \varepsilon_t(h_t) = \sum_{i=1}^{n} w_{t,i} \mathbb{1}_{Y_i \neq h_t(X_i)}. \tag{4}$$
   3. Set $w_{t+1,i} = w_{t,i} \exp(-y_i \alpha_t h_t(x_i))/Z_{t+1}$, where Z_{t+1} is such that $\sum_{i=1}^{n} w_{t+1,i} = 1$.
   4. Update $f = f + \alpha_t h_t$
4. The final predictor is given by $f = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t\right)$.

Adaboost algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners.
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   4. Update $f = f + \alpha_t h_t$
4. The final predictor is given by $f = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t\right)$.

- Each observation receives an initial weight $w_{1,i} = 1/n$
- The weak classifier that minimizes the $0-1$ loss on the weighted sample is selected
- Its coefficient α is computed based on its error
- The aggregated classifier is computed and weights are updated.

Adaboost algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners.
2. Set $f = 0$ and $w_{1,i} = 1/n$ for all $i \in \{1, \ldots, n\}$.
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   4. Update $f = f + \alpha_t h_t$
4. The final predictor is given by $f = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t\right)$.

In practice, finding the best weak predictor (equation (3)) might be difficult. We thus simply fit an algorithm on the weighted training sample instead.

Adaboost algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a weak learning procedure (e.g., decision trees of depth one trained with CART).
2. Set $f = 0$ and $w_{1,i} = 1/n$ for all $i \in \{1, \ldots, n\}$.
3. For $t = 1, \ldots, T$
   1. Fit a weak learning algorithm (e.g., CART trees of depth 1, stumps) to the training set with weights $w_{t,i}$. Denote by h_t the predictor.
   2. Compute
   $$\alpha_t = \frac{1}{2} \log \left(\frac{\varepsilon_t(h_t)}{1 - \varepsilon_t(h_t)} \right), \quad \text{with} \quad \varepsilon_t(h_t) = \sum_{i=1}^{n} w_{t,i} \mathbb{1}_{Y_i \neq h_t(X_i)}. \tag{3}$$
   3. Set $w_{t+1,i} = w_{t,i} \exp(-y_i \alpha_t h_t(x_i))/Z_{t+1}$, where Z_{t+1} is such that $\sum_{i=1}^{n} w_{t+1,i} = 1$.
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AdaBoost / Gradient Boosting

- Adaboost among state-of-the-art methods for binary classification (2003 Gödel Prize, see Freund and Schapire, 1995)
- Can be adapted to multiclass (Hastie et al., 2009) and regression (Drucker, 1997) via the function `AdaBoostClassifier` and `AdaBoostRegressor` in scikit-learn.
- Beware: it was claimed that AdaBoost does not overfit but this is not true! Hyperparameters need to be chosen carefully to prevent overfitting.

AdaBoost / Gradient Boosting

Pros:

- Powerful classifier
- Deterministic strategy: two runs of Adaboost leads to the same classifier.

Cons:

- Sensible to noise / outliers in the data

  $\rightarrow$ High importance is given to incorrectly classified observations due to the *exponential* loss

Going back to the general case

Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
2. Set $f_0 = 0$
3. For $t = 1, \ldots, T$
   1. Select
   $$(h_t, \alpha_t) \in \underset{h \in \mathcal{H}, \alpha \in \mathbb{R}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h(x_i)) \tag{4}$$
   2. Update $f_t = f_{t-1} + \alpha_t h_t$
4. The final predictor is $f_T = f_0 + \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Remarks. At each step, we try to find the base/weak predictor h_t that reduces the most the training set error of the aggregated predictor.

Going back to the general case

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1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
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Problem. Finding minimizers in equation (4) is difficult in general:

- Optimization on a large space - the class $\mathcal{H}$ can be infinite or very large, for example the set of all decision trees.
- Joint optimization procedure in (h, α).

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1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
2. Set $f_0 = 0$
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   2. Update $f_t = f_{t-1} + \alpha_t h_t$
4. The final predictor is $f_T = f_0 + \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Solution. Consider a first-order approximation

$$\ell(y_i, f_{t-1}(x_i) + \alpha h(x_i)) \simeq \ell(y_i, f_{t-1}(x_i)) + \alpha h(x_i) \left[\frac{\partial \ell(y_i, z)}{\partial z} \right]_{z = f_{t-1}(x_i)}. \tag{5}$$

that is, solving

$$h_t \in \underset{h \in \mathcal{H}}{\operatorname{argmin}} \sum_{i=1}^{n} h(x_i) \left[\frac{\partial \ell(y_i, z)}{\partial z} \right]_{z = f_{t-1}(x_i)}. \tag{6}$$

Going back to the general case

Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
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   2. Select
   $$\alpha_t \in \operatorname*{argmin}_{\alpha \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h_t(x_i)). \tag{5}$$
   3. Update $f_t = f_{t-1} + \alpha_t h_t$
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Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
2. Set $f_0 = 0$
3. For $t = 1, \ldots, T$
   1. Select h_t in $\mathcal{H}$ such that, for all $i \in \{1, \ldots, n\}$,
   $$h_t(x_i) \simeq -\left[\frac{\partial \ell(y_i, z)}{\partial z}\right]_{z=f_{t-1}(x_i)}. \tag{4}$$
   2. Select
   $$\alpha_t \in \underset{\alpha \in \mathbb{R}}{\operatorname{argmin}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h_t(x_i)). \tag{5}$$
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4. The final predictor is $f_T = f_0 + \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Going back to the general case

Gradient Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
2. Set $f_0 = 0$
3. For $t = 1, \ldots, T$
   1. For all $i \in \{1, \ldots, n\}$, compute the gradient
   $$r_i = -\left[\frac{\partial \ell(y_i, z)}{\partial z}\right]_{z=f_{t-1}(x_i)}. \tag{4}$$
   2. Denote by h_t the predictor, obtained by fitting the weak learning procedure to the *residual* dataset $(x_1, r_1), \ldots, (x_n, r_n)$.
   3. Select
   $$\alpha_t \in \operatorname*{argmin}_{\alpha \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h_t(x_i)). \tag{5}$$
   4. Update $f_t = f_{t-1} + \alpha_t h_t$
4. The final predictor is $f_T = f_0 + \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Going back to the general case

Gradient Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a set $\mathcal{H}$ of weak learners, a loss ℓ.
2. Set $f \in \text{argmin}_{c \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, c)$
3. For $t = 1, \ldots, T$
   1. For all $i \in \{1, \ldots, n\}$, compute the gradient
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   2. Denote by h_t the predictor, obtained by fitting the weak learning procedure to the *residual* dataset $(x_1, r_1), \ldots, (x_n, r_n)$.
   3. Via Backtracking line search, find an approximated solution
   $$\alpha_t \in \underset{\alpha \in \mathbb{R}}{\text{argmin}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h_t(x_i)). \tag{5}$$
   4. Update $f_t = f_{t-1} + \alpha_t h_t$
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   4. Update $f_t = f_{t-1} + \nu \alpha_t h_t$
4. The final predictor is $f_T = f_0 + \nu \sum_{t=1}^{T} \alpha_t h_t$ in regression (or its sign in binary classification).

Gradient boosting. Improving the performance of a base/weak learning algorithm (e.g. decision trees) by successively fitting it to a modified training set. Here, outputs of the training set are replaced by the negative gradient of the loss at each iteration.

A simple example: Gradient boosting with quadratic loss

Now, consider the Gradient Boosting algorithm with the square loss: $\ell(y, z) = (y - z)^2$.

Gradient Boosting algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a weak learning procedure.
2. Set $f \in \text{argmin}_{c \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, c)$
3. For $t = 1, \ldots, T$
   1. For all $i \in \{1, \ldots, n\}$, compute the gradient
   $$r_i = - \left[\frac{\partial \ell(y_i, z)}{\partial z} \right]_{z = f_{t-1}(x_i)}. \tag{6}$$
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Gradient Boosting with quadratic loss amounts to iteratively fitting a weak learner to the residuals of the current predictor.

Outline

Gradient Boosting Decision Tree (GBDT)

GBDT algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a weak learning procedure, a loss ℓ.
2. Set $f \in \text{argmin}_{c \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, c)$
3. For $t = 1, \ldots, T$
   1. For all $i \in \{1, \ldots, n\}$, compute the gradient
   $$r_i = - \left[\frac{\partial \ell(y_i, z)}{\partial z} \right]_{z = f_{t-1}(x_i)}. \tag{8}$$
   2. Denote by h_t the predictor, obtained by fitting a weak learning procedure to the *residual* dataset $(x_1, r_1), \ldots, (x_n, r_n)$.
   3. Via Backtracking line search, find an approximated solution
   $$\alpha_t \in \underset{\alpha \in \mathbb{R}}{\text{argmin}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h_t(x_i)). \tag{9}$$
   4. Update $f_t = f_{t-1} + \nu \alpha_t h_t$
4. The final predictor is f_T in regression (or its sign in binary classification).

Also called "Multiple additive regression trees" (MARS, see Friedman and Meulman, 2003).

Gradient Boosting Decision Tree (GBDT)

GBDT algorithm

1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a weak learning procedure (shallow trees), a loss ℓ.
2. Set $f \in \text{argmin}_{c \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, c)$
3. For $t = 1, \ldots, T$
   1. For all $i \in \{1, \ldots, n\}$, compute the gradient
   $$r_i = - \left[\frac{\partial \ell(y_i, z)}{\partial z} \right]_{z = f_{t-1}(x_i)}. \tag{8}$$
   2. Denote by h_t the predictor, obtained by fitting a shallow tree to the *residual* dataset $(x_1, r_1), \ldots, (x_n, r_n)$.
   3. Via Backtracking line search, find an approximated solution
   $$\alpha_t \in \underset{\alpha \in \mathbb{R}}{\text{argmin}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \alpha h_t(x_i)). \tag{9}$$
   4. Update $f_t = f_{t-1} + \nu \alpha_t h_t$
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1. Inputs: a dataset $\mathcal{D}_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$, a weak learning procedure (shallow trees), a loss ℓ.
2. Set $f \in \text{argmin}_{c \in \mathbb{R}} \sum_{i=1}^{n} \ell(y_i, c)$
3. For $t = 1, \ldots, T$
   1. For all $i \in \{1, \ldots, n\}$, compute the gradient
   $$r_i = - \left[\frac{\partial \ell(y_i, z)}{\partial z} \right]_{z = f_{t-1}(x_i)}. \tag{8}$$
   2. Denote by h_t the predictor, obtained by fitting a shallow tree to the *residual* dataset $(x_1, r_1), \ldots, (x_n, r_n)$. Let us denote by $R_1, \ldots, R_j$ the leaves of h_t.
   3. Via direct computations, select
   $$\alpha_t \in \underset{\alpha \in \mathbb{R}^J}{\text{argmin}} \sum_{i=1}^{n} \ell(y_i, f_{t-1}(x_i) + \sum_{j=1}^{J} \alpha_j \mathbb{1}_{x_i \in R_j}). \tag{9}$$
   4. Update $\quad f_t(x) = f_{t-1}(x) + \nu \sum_{j=1}^{J} \alpha_{j,t} \mathbb{1}_{x_i \in R_j}$.
4. The final predictor is f_T in regression (or its sign in binary classification).

Also called "Multiple additive regression trees" (MARS, see Friedman and Meulman, 2003).

Parameters in Gradient Boosting Decision Tree (GBDT)

Functions `GradientBoostingClassifier` and `GradientBoostingRegressor` in scikit-learn.

Parameters in Gradient Boosting Decision Tree (GBDT)

Optimization/Statistical complexity trade-off.

- Number of boosted trees T.

  $\rightarrow$ Controls both the statistical complexity of the final predictor (how many trees are aggregated) *and* the number of iterations in the optimization procedure (as adding a tree can be seen as a gradient descent step).

- The shrinkage parameter ν.

  $\rightarrow$ It helps to prevent overfitting in the early iterations. It can be seen as the learning rate of the boosting procedure. The smaller ν, the more iterations are needed to converge. Related to the optimization procedure

$\Rightarrow$ Heuristic: fix ν to a small value (typically 0.1) and $T = 100$ (or optimize T via early stopping).

Parameters in Gradient Boosting Decision Tree (GBDT)

Tree structure.

- Same parameters as in CART
- No split randomization is performed, i.e. `max-features` $= d$
- Maximal depth is set to `max-depth` $= 3$
- `square-loss` in regression / `log-loss` in classification (as in logistic/multinomial regression).

Gradient Boosting

Pros:

- State-of-the-art algorithm for supervised learning with tabular data
- Can handle regression and classification tasks for various loss functions
- Can handle continous and discrete features
- Deterministic strategy: two runs leads to the same predictor.

Cons:

- Can be computationally expensive - may require a large number of trees
- May overfit if too many trees are used (early stopping can be used to prevent overfitting)
- May be sensible to outliers / noise in the data

XGBoost

- Stands for eXtreme Gradient Boosting (Chen and Guestrin, 2016)
- State-of-the-art methods on tabular data sets (often better than random forests)

XGBoost

Differences with Gradient Boosting

- Second-order approximation of the loss with a penalty term (number of leaves + leaf values): assuming that f_{t-1} has been built, the loss at step t is

$$\underset{h}{\operatorname{argmin}} \sum_{i=1}^{n} \underbrace{\ell(y_i, f_{t-1}(x_i) + h(x_i))}_{\text{Replaced by a 2nd-order approx.}} + \Omega(h)$$

  $\rightarrow$ New objective function to build a boosted tree
- Feature discretization based on second-order statistics
- Feature subsampling can be used as in random forest (in each node) or prior to the tree construction.
- Computationally more efficient (handling sparse data, parallel and distributed computing)

XGBoost

Benefits/drawbacks

- Computationally efficient
- Can be applied to large-scale data set due to the new split finding scheme
- High predictive acuracy on most tabular data sets.

Variable importance in Gradient Boosting

The same variable importances as that in Random Forests can be computed:

- Mean Decrease in Impurity (MDI) for each tree, which is then averaged (with equal weights even with shrinkage) over trees
- Mean Decrease in Accuracy which is computed on the final boosted predictor.

Variable importance in Gradient Boosting

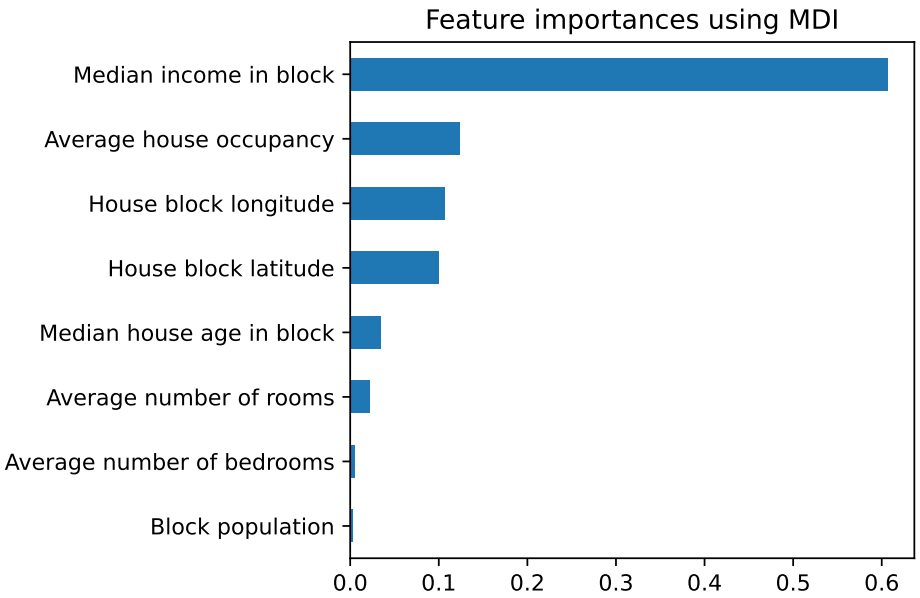

Figure: MDI computed with Gradient Boosting on the California housing data set.

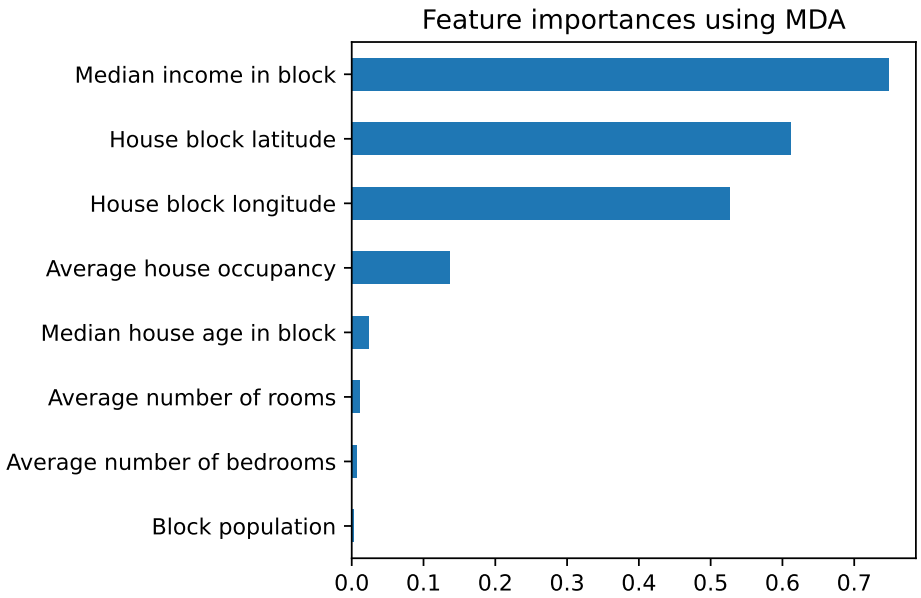

Figure: MDA computed with Gradient Boosting on the California housing data set.

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