DEFINING OBJECTIVE

- Once we have define our loss function, the ML task to solve can simply be expressed as minimizing it over some parameters:
	- ‣ E.g., for Linear Regression: *n*

Detailed way: arg min - Simplified way: arg min $L_2(f(\theta, x))$
 C Generic way: $\arg \min L_2(f(\theta, x))$ *β*0,*β*1...,*βⁿ i* $\sum (y^{i} - (\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \dots + \beta_n x_n^{(i)}))^2$ *β n* ∑ *i* $(y^{i} - f(\beta, x))^{2}$ *θ*

SOLVING MINIMIZATION

- Once we have expressed our task as a minimization problem, we just have to explore the parameter space to find a good solution
	- ‣ Exhaustive search is usually impossible
	- ‣ In the general case, no close form solution
	- ‣ One could use any optimization method
		- Genetic Algorithm
		- Simulated Annealing
		- EM…
	- ‣ Most used in general case: Gradient descent

• Greedy approach

- ‣ Start from arbitrary point
- ‣ Search for the nearest local minimum
	- If the problem is convex, find the global minimum, i.e., best possible solution
	- \Rightarrow linear regression
	- Else, find one local minimum, without guarantee.

• What is a gradient?

‣ Generalization of a derivative to multiple dimension

https://ml-cheatsheet.readthedocs.io/en/latest/gradient_descent.html

- The objective of gradient descent is to follow the gradient/ derivative in order to find a minimal point
	- ‣ Example: linear regression.
		- The "altitude" is given by the loss function
		- Each of the β is a "direction" in which we can move
		- Gradient descent answers the question: "in which direction and by how much should I change the β so as to go "down" in the loss function, optimally

- In practice:
	- Update the parameters $\mathbf a$ of function F , by subtracting its gradient ∇F at point \mathbf{a}_n , multiplied by a parameter γ to control the speed
		- $\mathbf{a}_{n+1} = \mathbf{a}_n \gamma \nabla F(\mathbf{a}_n)$
		- Subtract because we want to *descend* the gradient, i.e. minimize the function.
- The gradient has a value for each parameter
	- ‣ =>Compute the *partial derivative,* for each parameter

- Reminder: Common derivative
	- \cdot *c*^{$'=0$}
	- $x' = 1, (ax)' = a$
	- $(x^a)' = ax^{a-1} =>(x²)' = 2x$
	- \blacktriangleright . . .
- Common derivative rules
	- \rightarrow Mult by constant: $(cf)' = cf'$
	- ▶ Sum rule: $(f+g)' = f' + g'$
	- ‣ Chain rule: <=> *f*(*g*(*x*))′ = *f*′(*g*(*x*))*g*′(*x*) (*f* ∘ *g*)′ = (*f*′ ∘ *g*)*g*′
	- \mathbf{v}
- Boring? Use a solver like Wolfram alpha...

- Consider a function $f(x) = x^2 + 3$
	- $\cdot f'(x) = 2x$
	- \rightarrow $x=4$: Gradient= 8
	- \times \times = 2: Gradient=4
	- ‣ x=-1: Gradient=-2
	- \rightarrow x=-0.01: Gradient = -0.02
	- \rightarrow $\times=0$: Gradient=0
- Start at random, $x=4$, $\alpha = 0.25$
	- \times \times =4-(0.25 $*$ 8) = 2
	- $\rightarrow x=2-1=1$
	- \times = 1-0.25=0.75
	- \times \times =0.75-0.18 = 0.56…
	- \rightarrow \rightarrow Converge to $x=0$

- Of course, the choice of *α* will affect the learning
	- **► Strategies exist to adapt α dynamically**
- We stop when reaching a fix point

- Consider a function $f(x, y) = x^2 + 0.5y^2$
	- $\frac{y}{2}$ = $\frac{dy}{dx} =$ ∂*f* ∂*x* $2x + 0$ ∂*f* ∂*y* $0.5(2y) = y$
- $\cdot x=4, y=-2, \alpha = 0.25$ \times \times =4-2=2, \times \times =-2-(-0.5) =-1.5 \times \times = 2-1 = 1, \times \times = -1.5-(-0.375) = -1.125 ‣

- Practical example for parameter exploration
	- ‣ Apartments defined by surface
	- \rightarrow Price $=$

prices = 100+surface*8+np.random.normal(0, 50, len(surface))

‣ Define linear regression:

$$
y^{i} = \beta_{0} + \beta_{1}x_{i}
$$

arg min $\frac{1}{\beta_{0}, \beta_{1}} \sum_{i}^{N} (y_{i} - (\beta_{0} + \beta_{1}x_{i}))^{2}$

• Plotting the solution space:

$$
x : \beta_0, y : \beta_1, z = \frac{1}{N} \sum_{i}^{N} (y_i - (\beta_0 + \beta_1 x_i))^2
$$

‣ (Here, exhaustive search: very costly)

- Computing gradients for linear regression with 2 parameters $\ell(\beta_0, \beta_1) =$ ‣ ‣ ‣ 1 *N N* ∑ *i* $(y_i - (\beta_0 + \beta_1 x_i))^2$ ∂*ℓ* ∂*β*⁰ = 1 *N N* $\sum 2(y_i - (\beta_0 + \beta_1 x_i))(-1)$ *i* ∂*ℓ* ∂*β*⁰ = 1 *N N* ∑ *i* $-2(y_i - (\beta_0 + \beta_1 x_i))$ ∂*ℓ* ∂*β*⁰ $=\frac{-2}{\sqrt{2}}$ *N N* ∑ *i* $(y_i - \hat{y}_i)$ ̂
	- Prediction is too low=> Increase β_0 (proportionally to error).
	- Too high=> Decrease β_0 if, decrease if too high

• Computing gradients for linear regression with 2 parameters

$$
\ell(\beta_0, \beta_1) = \frac{1}{N} \sum_{i}^{N} (y_i - (\beta_0 + \beta_1 x_i))^2
$$

$$
\frac{\partial \ell}{\partial \beta_1} = \frac{1}{N} \sum_{i}^{N} 2(y_i - (\beta_0 + \beta_1 x_i))(-x_i)
$$

$$
\frac{\partial \ell}{\partial \beta_1} = \frac{1}{N} \sum_{i}^{N} -2x_i(y_i - (\beta_0 + \beta_1 x_i))
$$

$$
\frac{\partial \ell}{\partial \beta_1} = \frac{-2}{N} \sum_{i}^{N} x_i(y_i - \hat{y}_i)
$$

- x_i positive=>Lower if too high, increase if too low.
- x_i negative=>Increase if too high, decrease if too low.
- If two items with equal absolute error of opposite sign, different $|x_i| = >$ gradient correct largest $|x_i|$ (increase the slope)
- \cdot If $x_i = 0$, the coefficient have no effect anyway

• Generic case: more than a single variable

$$
\ell(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - (b + wx_i))^2
$$

- Vecteur form: w: vector of weights, x_i : vector of features
- ‣ Same derivation:

-

$$
\frac{\partial \mathcal{E}}{\partial w} = \frac{-2}{N} \sum_{i}^{N} x_i (y_i - \hat{y}_i)
$$

- Partial gradient for each feature (for each observation) is proportional to the feature value for this observation
	- ‣ A same error for an observation can contribute differently for each coefficient:
		- Increase or decrease (sign of the feature)
		- Strong or weak effect (magnitude of the feature)

- We have seen that a drawback of ML methods is that they can overfit
- When the ML objective can be clearly expressed, there is a generic way to limit overfitting: regularization
	- ‣ Two types of regularization:
		- L1 or Lasso regularization
		- L2 or Ridge regularization

L2 REGULARIZATIO

• Expressed as a general principle ‣ $\ell(b,w) =$ 1 *N N* ∑ *i* $f(y_i, \hat{y}_i, b, w) + \lambda$ ̂ *p* ∑ *j* w_j^2

- Some parameters are regularized, and some others might not be (intercept...)

- Intuition: we force coefficients to be small.
	- **▶** If $λ=0$, normal regression
	- **λ** If λ ->∞, all coefficients tends towards 0
	- ‣ /!\ The magnitude of coefficients depends on the magnitude of variables!
		- Important to normalize the variables, else you will constraint more the variables of lower amplitude

LI REGULARIZATIO

- L1 or Lasso Regularization
	- ‣ Lasso: Least Absolute Shrinkage and Selection Operator ‣ ‣ ‣ Notation: $\ell(b,w) =$ 1 *N N* ∑ *i* $(y_i - (b +$ *p* ∑ *j* $(w_j x_{ij}))^2 + \lambda$ *p* ∑ *j* $|w_j|$ $\ell(b,w) =$ 1 *N N* ∑ *i* $(y_i - \hat{y}_i)^2 + \lambda$ ̂ *p* ∑ *j* $|w_j|$ *p* $\sum |w_j| = ||w||_1$ *j*

- Similar methods, different results:
	- ‣ L1 regularization tends to force some values to be 0
	- ‣ L2 regularization tends not to attribute 0
- L1 regularization thus performs **variable selection**
	- ‣ Variables for which the coefficient is 0 can be discarded

- Why different behaviors ?
	- ‣ We minimize the sum of error+constraints
	- ‣ Red lines represent error (every point of a circle have same error)
	- ‣ Similarly for blue.
	- ‣ Intersection is the optimal solution (for that error, minimize constraint)
- \cdot => For a same error, L1 favors 0

https://online.stat.psu.edu/stat508/book/export/html/749

- Bayesian interpretation
	- ‣ Different priors on the coefficients

FIGURE 6.11. Left: Ridge regression is the posterior mode for β under a Gaussian prior. Right: The lasso is the posterior mode for β under a double-exponential prior.

https://ekamperi.github.io/mathematics/2020/08/02/bayesian-connection-to-lasso-and-ridge-regression.html

ELASTIC NET

• Best of both worlds :)

$$
\mathcal{L}(b, w) = \frac{1}{N} \sum_{i}^{N} (y_i - \hat{y}_i) + \lambda_1 \sum_{j}^{P} |w_j| + \lambda_2 \sum_{j}^{P} w_j^2
$$

ENSEMBLE LEARNING

ENSEMBLE LEARNING

- Ensemble learning is a general principle:
	- ‣ All models have strengths and weaknesses
		- e.g., linear models struggle with non-linearities but are good at extrapolation
		- Decision trees are good at capturing non-linearities, but struggle with extrapolation
	- ‣ Could we combine the strengths of various models?
		- Direct application: **Stacking**
		- Using multiple times the same model: **Bagging**
		- Training models specifically to solve other weaknesses: **Boosting**

ENSEMBLE LEARNING

STACKING

- In the simplest approach, various models (different approaches, same approach with different parameters) are trained on the same dataset
- Their predictions are then combined:
	- Regression: averaging. Average values of the classifiers (possibly weighted)
	- ‣ Classification:
		- Voting: class with the most vote
		- Soft / Averaging: average of probabilities yielded by the classifier
- Weaknesses:
	- ‣ What if several models make the same mistake? (Correlation of errors…)
	- ‣ What if we merge good models and poor models?

STACKING

- A possible solution to stacking is to use a meta-model:
	- ‣ The prediction made by each individual model is considered as a feature for the meta-model
	- ‣ The meta-model is trained as any ML model with the original target, but using sub-models outputs as features.
- Any model can be used as meta-model
- Famous for winning the \$1M prize of the 2009 Netflix prize.
	- ‣ 100+ individual predictors

BAGGING

- Bagging is an ensemble methods, but differ from stacking in two main ways:
	- ‣ The various individual predictors are made of the same algorithm
	- ‣ Each algorithm is trained on a subset of the original data
		- Different subsets on all variables
		- And/Or trained only on some variables
		- = > Various strategies exist.
- Advantages over stacking:
	- ‣ All models are comparable, less chances to average "good" and "bad" models
	- ‣ Can be understood as "lower the Variance", i.e., prevent overfit.
		- Remember the Bias/Variance tradeoff? Expressive models overfits => high variance.
		- The definition of variance is high variation over the "average" of multiple models...

 \widehat{B} ias_{*D*} $[\hat{f}(x; D)] = E_D[\hat{f}(x; D)] - f(x)$ $Var_D[\hat{f}(x; D)] = E_D[(E_D[\hat{f}(x; D)] - \hat{f}(x; D)]^2].$ D: subsets. X: all elements in all subsets

BAGGING: RANDOM FOREST

- Random forest is the most famous bagging algorithm
	- ‣ It is based on decision trees (thus the name *forest*…)
	- ‣ A direct application of bagging
		- innovations to bagging came from random forests
- Trees are good candidates for bagging because overfit is their main problem
	- ‣ What is similar between trees will stay, and when they disagree, taking the average of all the errors should get close to right answer.
		- Similar to "Wisdom of the crowds"

RANDOM FOREST

- Set
	- ‣ Parameters of individual trees (not too simple, not too large…)
	- ‣ Averaging function
	- ‣ #trees
- What is specific is the subsamble strategy
	- ‣ What is key is to avoid correlation between trees, i.e., train on different data
	- ‣ Subsample observations: With replacement. Sample n at random among n items
		- Variants: m among n. Or without replacement: random samples, or "folds" (each observation used in a single tree, but requires lot of data)…
	- ‣ Specific to trees: subsample of variables at each node: to chose the best split, restrain to a random fraction of variables.
		- Impose diversity in the trees

BOOSTING

BOOSTING

- Again, a general principle
- We train various models in sequence
	- ‣ First, train a normal, first model
		- Usually, this model will be tuned to be relatively simple, and thus underfit=>Weak learners
	- Then, extract the errors of the model (incorrect classes/residuals).
	- ‣ Train a second model, focusing on predicting the errors missed by the first model
	- Update the main model and recompute the errors
	- Repeat until we cannot improve anymore
- Final prediction is the sum of all weak learners (not average: each method *corrects, complement* previous ones)

$$
F_T(x) = \sum_{t=1}^T f_t(x)
$$

- First boosting method to reach wide recognition
- Method for classification
- Weak learners are *decision stumps*
	- ‣ Choose only one variable. Split it only once

$$
ADABOOST
$$

Error to minimize at each step m: $\epsilon_m = \frac{\sum_i^N w_i^m I(f_m(x_i) \neq y_i)}{\sum_i^N w_i^m}$

- I (true)=1, I (false)=0
- $-w_i^m$: weight of element *i* at step *m*
- Interpretation: fraction of weights w_i^m for misclassified elements
- Weights are initialized at 1: first, minimize fraction of errors

•
$$
w_i^{m+1} = w_i^m e^{\alpha_m I(fm(x_i) \neq y_i)}
$$

• Updates weights of <u>misclassified</u> items($e^0 = 1$) by a coefficient proportional to the error

$$
\text{With } \alpha_m = \ln\left(\frac{1 - \epsilon_m}{\epsilon_m}\right)
$$

- ‣ : correct / incorrect => *eαm*
	- Sum of Weights of correct pts: correct *(w=1)=correct
	- Sum of Weigths of incorrect pts: incorrect *(w=correct/incorrect) =correct
	- Incorrectly classified now weights equal to correctly classified.

$0.7/0.3=2.33$

Weight incorrect=3*2.33=7 Weight correct=7*1=7

$0.7/0.3=2.33$

Weight incorrect=3*3.66=11 Weight correct=4*1+3*2.33=11

• Finally, we need to combine our various weak learners into a single prediction

$$
F_m(x) = F_{m-1}(x) + \alpha_m h_m(x) = \sum_m \alpha_m h_m(x)
$$

- The new set of rules at step m is the previous set of rules to which we add the new rule weighted by coefficient $\alpha_m = \ln \left(\frac{m}{\sigma_m} \right)$ $1 - \epsilon_m$ ϵ_m
- In(Correct /errors): 0 if as many correct as error (ignore if rangom...), the more we have correct results, the higher the value. (Infinite with perfect solution…)

$3OOS$

2nd iteration's weight = $ln(11/3) = 1.30$ 3rd iteration's weight= $ln(19/3) = 1.85$

• Why does it work?

- **Intuitively:**
	- We force the latest weak learner to focus on what was missed by others.
	- The weights of models are stronger when we solve errors found in many other models
	- "ADA: adaptative (weights adapt based on previous step)"
- **•** Theoretically:
	- It can be shown that Adaboost minimizes the Exponential loss, which is a way to estimate the probability of having a given class given the data

$$
\operatorname{argmin}_{f(X)} \mathbb{E}_{Y|X} e^{-Yf(X)} = \frac{1}{2} \log \frac{\mathbb{P}(Y=1 \mid X)}{\mathbb{P}(Y=-1 \mid X)},
$$

(A posteriori improvement and explanations, everything not fully clear IMO...)

XGBOOST

XGBOOST

- As of today, certainly the most popular method among those not using neural networks
- Used in winning solution in countless ML challenges
	- ‣ And at Google, Amazon, Uber…
- Both :
	- ‣ A method described in a scientific paper
	- ‣ A library developed and improved by a community
		- Changes in the ML scientific culture…

XGBOOST

• In a few words:

- ‣ A tree boosting methods
	- Can be used for classification and regression
- ‣ Weak learners not as weak as in AdaBoost
	- Default to 3 or 6 levels max
- ‣ Introduces Regularization
	- Each new leaf add some regularization cost
- ‣ Gradient Boosting method:
	- Explicitly do a gradient-descent like approach

• Gradient boosting is the application of boosting to explicit gradient descent

XGBOOST IN A NUTSHELL

• In our loss for the tree, we decompose the prediction \hat{y} as

- ‣ Prediction given by previous tree + prediction of new tree.
- **»** *ω* regularization, explained later

XGBOOST IN A NUTSHELL

$$
w_j = -\frac{G_j}{H_j + \lambda}
$$

- w_j : score of a leaf (like AdaBoost)
- Using RMSE as objective:
	- **•** G_j: Sum of errors (to residuals)
	- \rightarrow H_j : Number of items in the leaf
	- ‣ : Regularization parameter *λ*

GAIN ON A SPLIT

$$
Gain = \frac{1}{2} \left[\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right] - \gamma
$$

• L, R = > Left and Right children

• Sum of regularized averaged error of the children squared, minus that of parent, minus regularization *γ*

https://xgboost.readthedocs.io/en/stable/tutorials/model.html

XGBOOST IN A NUTSHELL

- For First tree:
	- ‣ For each leaf
		- We compute the gain to find the best possible split,
		- If regularization makes the gain negative, do nothing
		- If we reach the maximal tree depth, do nothing
		- Compute the final score of the leaf : signed error. To add to the final prediction
- Next tree: same process, but compute error relatively to previous tree (residuals)
- When finished, for each prediction, sum the (signed) prediction of each tree (weighted by learning rate *η*)

LEARNING RATE

- As in most gradient descent methods, there is a learning rate (eta) parameter, allowing to tune how fast we converge *η*
	- ‣ To avoid the "ping-pong" effect around global minimum
	- ‣ In practice, the prediction of the previous tree is shrinked by *η*
- $\hat{y} = \eta \hat{y}_i^{(t-1)} + f_t(x_i)$ ̂

1 single tree for prediction: Learning rate effect…

DETAILS ON WHY

https://xgboost.readthedocs.io/en/stable/tutorials/model.html

REGULARIZATION TERM

XGB: REGULARIZATION

obj =
$$
\sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{T} \omega(f_i)
$$

$$
\omega(f) = \gamma T + \frac{1}{2} \lambda \sum_{j=1}^{T} w_j^2
$$

- **P** \cdot **T**: number of leaves
- λ : parameter for the strength of the regularization
- *γ*: gain threshold below which we choose not to split a leaf
- \cdot w_j "score" of leaf *j*, next slide

=>Chosen to simplify computations

DEFINITION USING ANY LOSS FUNCTION

$$
obj^{(t)} = \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{t} \omega(f_i)
$$

$$
= \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \omega(f_t)
$$

• In our loss for the tree, we decompose the prediction \hat{y} as

- ▶ Prediction given by previous tree + prediction of new tree.
- **»** *ω* regularization, explained later

$$
\sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \omega(f_t)
$$

Instead of classic gradient descent, uses Taylor series to compute an approximation, allowing any error function

obj^(t) =
$$
\sum_{i=1}^{n} [l(y_i, \hat{y}_i^{(t-1)}) + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i)] + \omega(f_t) + \text{constant}
$$

With g_i , h_i first and second derivatives $h_i = \partial_{\hat{g}^{(t-1)}}^2 l(y_i, \hat{y}_i^{(t-1)})$

$$
g_i = \partial_{\hat{y}_i^{(t-1)}} l(y_i, \hat{y}_i^{(t-1)})
$$

$$
h_i = \partial_{\hat{y}_i^{(t-1)}}^2 l(y_i, \hat{y}_i^{(t-1)})
$$

LEAF AND TREE SCORES

After development:

 $G_j = \sum g_i$ *H_j* = \sum $i \in I_j$ $i \in I$ _i With $G_j = \sum_{i \in I} g_i$ $H_j = \sum_{i \in I} h_i$ Score of leaf I_j , sum for items inside it

FROM GENERICTO MSE

SCORES WITH MSE

$$
w_j = -\frac{G_j}{H_j + \lambda}
$$

Looks complicated… In practice, meaning for squared loss?

$$
g_i = \partial_{\hat{y}_i^{(t-1)}} l(y_i, \hat{y}_i^{(t-1)}) \qquad \qquad \partial_{\hat{y}_i^{t-1}} (y_i - \hat{y}_i^{t-1})^2 = 2(y_i - \hat{y}_i^{t-1})(-1) \in 2(\hat{y}_i^{t-1} - y_i)
$$
\n
$$
h_i = \partial_{\hat{y}_i^{(t-1)}}^2 l(y_i, \hat{y}_i^{(t-1)}) \qquad \qquad \partial_{\hat{y}_i^{t-1}}^2 (y_i - \hat{y}_i^{t-1})^2 = \partial_{\hat{y}_i^{t-1}} 2(\hat{y}_i^{t-1} - y_i) = 2
$$

 $w_j = -\frac{G_j}{H}$ $H_j + \lambda$ \approx avg (signed) error

CLASSIC ML VS DNN

- Until now, I have presented "classic" methods.
- In the news, we hear often about Neural networks methods when talking about IA. Are classic obsolete?
	- ‣ DNN are mostly "chained" classic methods. Nothing different in the theory
	- ‣ DNN are good for problems with
		- Huge quantity of data
		- Huge quantity of attributes
		- Attributes being semantically related to each other (adjacent pixels, following words…)
		- Attributes are of the same nature
		- => Currently, extremely specialized for tasks on images, text, audio, etc.
	- ‣ If limited data, set of unrelated, loosely known features: XGboost & Co. are the most used and usually most efficient methods