KDG Background Reading

- What are Polytopes?
  a geometric object with flat sides.

- Kernel Density Estimation (KDE)
  - a non-parametric way to estimate the PDF of a random variable.
  - Let $(x_1, x_2, \ldots, x_n)$ be i.i.d. sampled drawn from a known distribution f at a given point x. We are interested in estimating the shape of the function f.

$$\hat{f}_h(x) = \frac{1}{n}\sum_{i=1}^{n} K_h(x - x_i) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$

where $K_h \rightarrow$ Kernel (a non-negative f^n)
$h \rightarrow$ Bandwith (a smoothing parameter)

- Performance Metrics

① Expected Caliberation Error (ECE)

Measures the expected difference between accuracy and confidence by grouping all samples (size N) in to K bins & calculating

$$ECE = \sum_{i=1}^{k} \frac{|B_i|}{N} |acc_i - conf_i|$$

acc_i and $conf_i$ are accuracy & average confidence in the i-th bin & $|B_i|$ is the number of samples in bin B_i

* The pseudo-probabilities are class probabilities we get from the final layer of a NN. The pseudo-probability of the predicted class generally over-estimates the actual probability of getting a correct answer.

* If this over-estimation can be measured, it can be used to calibrate the NN such that it's pseudo-probabilities would match the actual probability of the classes.

confidence

② Cohen's Kappa

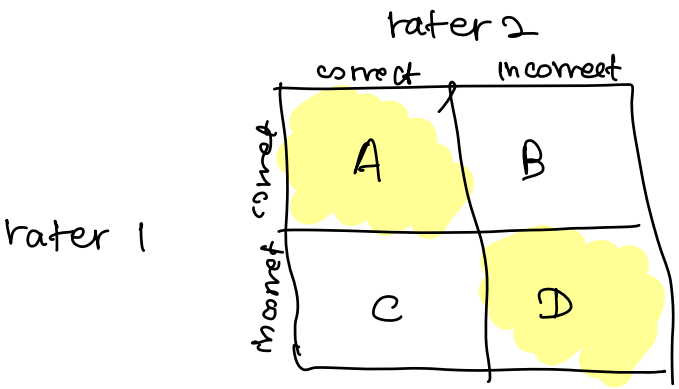
$$\kappa = \frac{P_o - P_e}{1 - P_e}$$

$P_o \rightarrow$ relative observed agreement among raters

$P_e \rightarrow$ hypothetical probability of chance agreement.

* Measures the agreement between 2 raters who each classify N times in to C mutually exclusive categories.

* It is a quantitative measure of reliability for 2 raters that are rating the same thing, corrected for how often that the raters may agree by chance.



In A & D, the two raters are in agreement.

$$P_o = P(\text{agreement}) = \frac{A+D}{A+B+C+D} = \frac{\#\text{agreements}}{\text{Total}}$$

Expected probability that both would say correct ⇒

$$P(\text{correct}) = \frac{A+B}{A+B+C+D} \times \frac{A+C}{A+B+C+D}$$

Expected probability that both would say incorrect ⇒

$$p(\text{incorrect}) = \frac{C+D}{A+B+C+D} \times \frac{B+D}{A+B+C+D}$$

P_e = overall random agreement probability that they agreed on either yes or no.

$$P_e = P(\text{correct}) + P(\text{incorrect})$$

Then $$K = \frac{P_o - P_e}{1 - P_e}$$

Understanding KDN

* Understanding polytopes formed by MLPs

- Partition & vote
- representation space learnt by DNNs is a partitioning of feature space in to a union of convex polytopes.

classical statistical formulation of classification problem ⇒

$(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n) \overset{iid}{\sim} F_{XY}$

$T_n = \{(X_i, Y_i)\}_{i \in \{1,\ldots,n\}}$: training data

(X, Y) : to-be classified test observation & its true label

$X \in \mathbb{R}^d$, $Y \in \{0, 1\}$

Learn a classification rule $g_n = g(\cdot; \tau_n)$ that maps feature vectors to class labels s.t. probability of misclassification $L(g_n) = P[g(X; \tau_n) \neq Y \mid \tau_n]$ is small.

Stone's Thm for universally consistent classification:

a successful classifier can be constructed by

1) partitioning the input space in to cells depending on n, such that the # training points in each cell goes to infinity but slowly in n
2) Estimating the posterior $\eta(x) = P[Y=1 \mid X=x]$ locally by voting based on the training class labels associated with the training feature vectors in cell $C(x) \subset \mathbb{R}^d$ in which the test observation falls.

Then $L(g_n) \to L^*$ almost surely for any F_{XY} where L^* is the Bayes optimal probability of misclassification.

Polytopes in Decision Forests

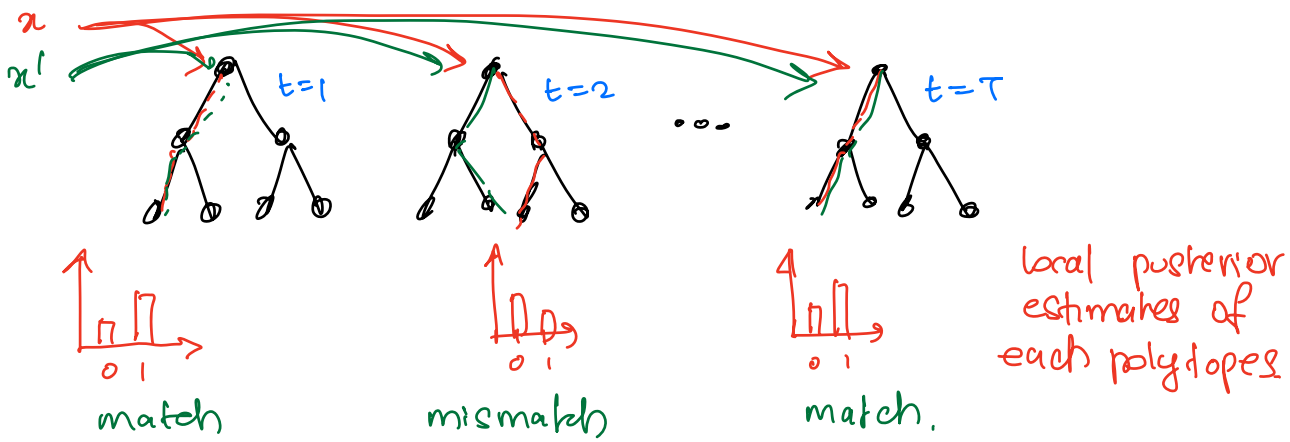
* given training data τ_n each tree t in RF constructs a partition $P_{n,t}$ by splitting the

input space.

* each tree results in a partition $P_{n,t} \in \mathbb{R}^d$ (each leaf of each tree)
* this partition admits a posterior estimate

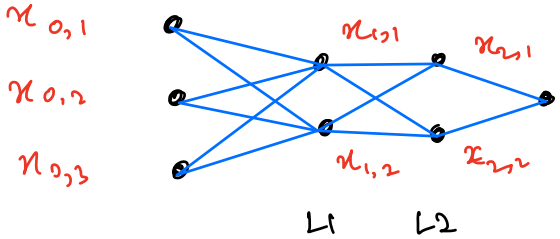
$$\hat{\eta}_{n,t,j} = \left(1/N_{n,t,j}\right) \sum_{i: x_i \in C_{n,t,j}} I\{Y_i = 1\}$$

based on the class labels of training data feature vectors in cell $C_{n,t,j}$



∴ The more the matched leaf ids are the more likely that x & x' belong in the same polytope

Polytopes in Deep Networks



$$x_{1,1} = f\left(w_{1,1,1}\, x_1 + w_{1,2,1}\, x_2 + w_{1,3,1}\, x_3 + b_{1,1}\right)$$

$$x_{1,2} = f\left(w_{1,1,2}\, x_1 + w_{1,2,2}\, x_2 + w_{1,3,2} x_3 + b_{1,2}\right)$$

$$\begin{bmatrix} x_{1,1} \\ x_{1,2} \end{bmatrix} = f\left\{ \begin{bmatrix} w_{1,1,1} & w_{1,2,1} & w_{1,3,1} \\ w_{1,1,2} & w_{1,2,2} & w_{1,3,2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_{1,1} \\ b_{1,2} \end{bmatrix} \right\}$$

$$\therefore \begin{bmatrix} x_{2,1} \\ x_{2,2} \end{bmatrix} = f\left\{ \begin{bmatrix} w_{2,1,1} & w_{2,2,1} \\ w_{2,1,2} & w_{2,2,2} \end{bmatrix} \begin{bmatrix} x_{1,1} \\ x_{1,2} \end{bmatrix} + \begin{bmatrix} b_{2,1} \\ b_{2,2} \end{bmatrix} \right\}$$

$$x_{3,1} = \sigma\left(w_{3,1,1}\, x_{2,1} + w_{3,2,1}\, x_{2,2} + b_{3,1} \right)$$

* all the samples that turn on/off the same ReLUs (nodes) ends up in the same polytope at the penultimate layer.