Model

- Loss Function

  need to be non-negative

  0 = perfect prediction

- No Free Lunch Theorem

  > No single model that works best!
  >
  > Model makes assumptions!

- Model Selection
  - Cross-validation
  - Bayesian model selection

    $P(m|D) = \frac{P(D|m_0)}{P(D|m_1)} * \frac{P(m_0)}{P(m_1)}$ (Usually same prior)

- Bias-Variance Tradeoff
  - Bias: error from mean
  - Variance: spread around center

- Bayesian Information Criterion (BIC)

  $BIC = DOF(\theta)logN - 2logP(D|\theta)$: penalise high DOF model, mitigated by its likelyhood

Linear Regression

- Assumptions:
  1. Linearity: data is linear
  2. Independence of error: data is IDD sampled
  3. Residue(error) is Gaussian
  4. Equal variance of errors
- Loss Function:
  - Based on Gaussian Error
  - MSE
- Optimization (Solution):
  - Derivation of close form solution $(X^T X)^{-1} X^T y$
- Gaussian MLE always biased: $E[\sigma^2] = \frac{n-1}{n}\sigma^2$ Smaller than the true error. Because we measure from sample
- Expectation of Error = bias * bias + variance
- Regularization
  - More regularization -> high bias term -> more bias

    - Less regularization -> more overfitting -> more variance

KNN

- Idea: choose class based on K nearst neighbor
- Caveats:
    - Need to normalise vector
- Model Complexity:
    - K too small: overfitting
    - K too high: underfit

Logistic Regression

- Idea: $p(y=1|x) = \frac{1}{1+e^{-w^T x}} y \in \{0, 1\}$
- Why not use Linear Regression for Classification?
    - Ans: Classification does not care about the magnitude of loss, outlier will hur linear regression for classification badly.
- Derivation
    - odds of two class $\frac{P(y=1|x)}{P(y=0|x)} = e^{w^T x}$
    - then we have $\frac{p}{1-p} = e^{w^T x}$
    - solve for p
- Loss function:
    - LIkelyhood function: MLE of every data
      $\sum log[y_i P(y=1|x_i) + (1-y_i)P(y_i=0|x_i)]$
- Optimization:
    - Gradient: $-\sum(y_i - p(y_i|x_i, w_i))x_i$
    - Gradient Ascent
        - SGD or Batch or Whole Data

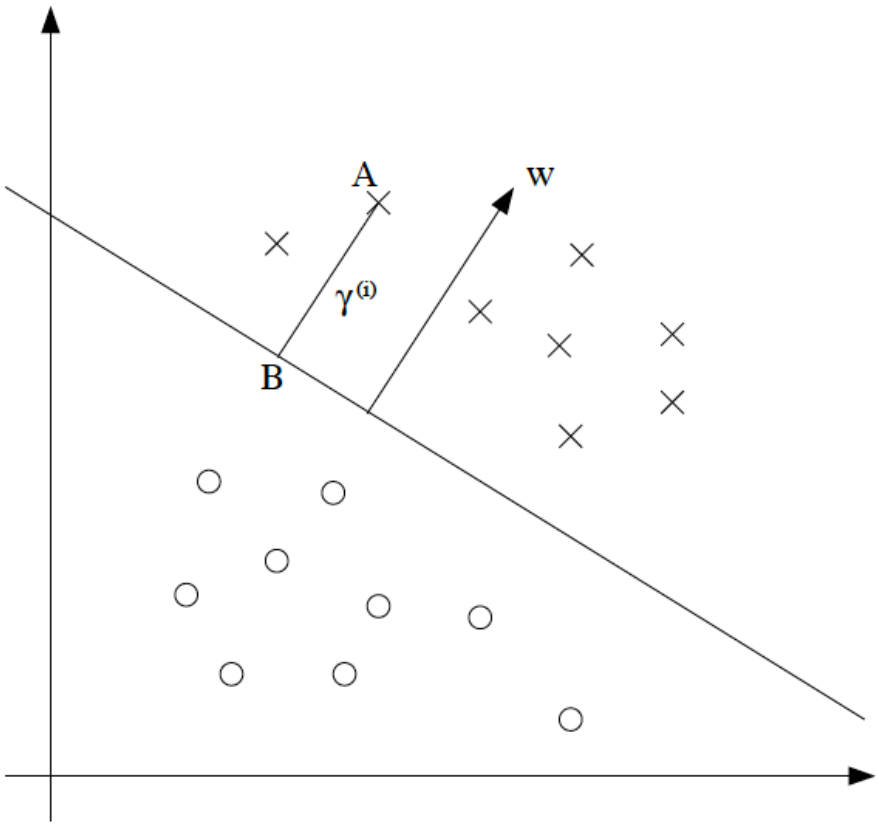
Perceptron

- Idea: $y = sign(w^T x) y \in \{-1, 1\}$
- Loss function:
    - 1 loss if incorrect, 0 otherwise
    - or $L = max(0, -y_i w^T x_i)$
- Optimization:

    - Gradient:
        - $\nabla L = 0$ if $y_i w^T x_i > 0$, else $-y_i x_i$
    - Weight Update:
        - $w^{i+1} = w^i + \eta(y_i - \hat{y}_i)x_i$
- Online-Learning vs. Batch Learning
    - Assumptions behind `batch learning`:
        - **one optimal hypothesis fits all of the data**
        - data are IID
        - Advantage:
            - Guarentee convergency
    - Online Learning:
        - No train-test data split. Infinite data steam
        - **No consistency in hypothesis**
        - Advantage
            - Handle large data
            - Faster for lots of data

SVM

- Idea: find the best plane that separate data by maximise the margin to each of example
- Derivation (highly recommend reading: Stanford CS229 Notes)
    - Functional Margin: $\hat{\gamma}_i = y_i(w^T x_i + b)$
    - Geometric Margin (norm of vector AB), and it satisfy following function $\gamma\frac{\dot{W}}{||w||} = A - B$. Also since B is on the decision boundary, $w^T B = 0$, we can derive geo margin $\gamma_i = y_i[(\frac{w}{||w|}) ^T x_i + \frac{b}{||w||}]$ We can see that if $||w|| = 1$, then $\gamma = \hat{\gamma}$, which implies $\frac{\hat{\gamma}}{\gamma} = ||w||$
    -



- Therefore, our objective is to:

  > max γ, s.t. $y_i(w^T x_i + b) \geq \gamma, \forall i$ and $||w|| = 1$

  Then, since $\frac{\hat{\gamma}}{\gamma} = ||w||$, we can rewrite objective function to:

  > max $\frac{\hat{\gamma}}{||w||}$, s.t. $y_i(w^T x_i + b) \geq \hat{\gamma}, \forall i$

  Finally, since maximise max $\frac{\hat{\gamma}}{||w||}$ is equivalent to min $\frac{1}{2}||w||^2$, and $\hat{\gamma}$ can be arbitrarily scaled, we set $\hat{\gamma} = 1$, then we have

  > max $\frac{1}{2}||w||^2$, s.t. $y_i(w^T x_i + b) \geq 1, \forall i$

- Loss function
  - Hinge Loss: $max(0, 1 - y \cdot wx)$

SVM Duality

- Dual vs Primal max (Please refer to Andrew Ng CS299 notes)

$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j (\mathbf{x}_i^T \mathbf{x}_j)$$

such that $\alpha_i \geq 0$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$

- Predictions for new examples:

$$\mathbf{x}^T \cdot \mathbf{w} = \mathbf{x}^T \cdot \sum_{i=1}^{N} [\alpha_i y_i \mathbf{x}_i] = \sum_{i=1}^{N} \alpha_i y_i (\mathbf{x}^T \mathbf{x}_i)$$

  - Note $w = \sum [a_i y_i x_i]$ and only some of a_i are non-zero, which are the support vector
- Slack Variable
  - Add regulariser term $min_w 1/2||w||^2 + C \sum \epsilon_i$ s.t $(w^T x_i) y_i + \epsilon_i \geq 1$
  - Larger C means more penalty on slack the maring
    - Better fit to data. More overfitting.
- New Prediction for test data x_j is given by $x_j^T \cdot w = x_j^T \sum [a_i y_i x_i] = \sum a_i y_i (x_j^T x_i)$

Kernel

- How to use kernel?
  1. Feature mapping: $\phi(x)$ to higher dimension to make data linearly separable. e.g $\phi(x) = [x_{(1)}^2, \sqrt{2} x_{(1)} x_{(2)}, x_{(2)}^2]$

     In primal form, we need to learn w for each feature, which could be very large

     While in dual form, we don't have w
  2. We can use $\phi(x)$ instead of x in our computation in order to learn non-linear boundary.

$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j (\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j))$$

the only increase for the size of the dataset

ere is no w!

  3. Then we can define Kernel $K(x, x') = \phi(x)^T \phi(x')$.

     Why we want to define it as kernel? Because we can often have simpler solution to Kernel without actually computing the ϕ in a possibly very high dimension

$$
\begin{aligned}
K(\mathbf{x}, \mathbf{x}') &= (\mathbf{x} \cdot \mathbf{x}')^2 \\
&= (x_{(1)}x'_{(1)} + x_{(2)}x'_{(2)})^2 \\
&= (x^2_{(1)}x'^2_{(1)} + x^2_{(2)}x'^2_{(2)} + 2x_{(1)}x_{(2)}x'_{(1)}x'_{(2)}) \\
&= (x^2_{(1)}, x^2_{(2)}, \sqrt{2}x_{(1)}x_{(2)}) \cdot (x'^2_{(1)}, x'^2_{(2)}, \sqrt{2}x'_{(1)}x'_{(2)}) \\
&= \phi(\mathbf{x}) \cdot \phi(\mathbf{x}')
\end{aligned}
$$

```
 For example above, we **don't** need to actually compute the inner product
of $\phi(x)$, which is $(x^2_{1}x'^2_{(1)} + …… +
2x_{(1)}x_{(2)}x'_{(1)}x'_{(2)})$
 All we need to compute is $(x \dot{} x')^2$
```

- Kernel as similarity Function

$$
\alpha K(\mathbf{x}, \mathbf{x}') = \alpha\phi(\mathbf{x}) \cdot \phi(\mathbf{x}') = \alpha||\phi(\mathbf{x})||||\phi(\mathbf{x}')|| \cos(\theta)
$$

same for all x'

- What qualify a Kernel?
  - You can decompose it into $\phi(x)^T\phi(x')$
  - Or it satisfy Mercer's Theorem : kernel matrix is symmetric positive semi-definite
    - Kernel Matrix $\mathbf{K}_{ij} = \mathbf{K}_{ji}$
    - $\mathbf{x}^T K\mathbf{x} \geq 0, \forall \mathbf{x} \in R^m$
- Kernel formation

$$
\begin{aligned}
K(\mathbf{x}, \mathbf{x}') &= cK_1(\mathbf{x}, \mathbf{x}') \\
K(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x})K_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') \\
K(\mathbf{x}, \mathbf{x}') &= \exp\left(K_1(\mathbf{x}, \mathbf{x}')\right) \\
K(\mathbf{x}, \mathbf{x}') &= K_1(\mathbf{x}, \mathbf{x}') + K_2(\mathbf{x}, \mathbf{x}') \\
K(\mathbf{x}, \mathbf{x}') &= K_1(\mathbf{x}, \mathbf{x}')K_2(\mathbf{x}, \mathbf{x}')
\end{aligned}
$$

- Gaussian Kernel

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\sigma^2}\right)$$

Larger σ means the support vector has greater influence area

- Summary
  - Good
    - Arbitrarily high dimension
    - Extension to other data types
    - Non-linearity
  - -Bad
    - Choose kernel is not easy
    - Can not handle large data

Decision Tree

- ID3 Algorithm

```
function buildDecisionTree(data, labels):
    if all labels the same:
        return leaf node for that label
    else:
        let f be best feature for splitting (needs to be computed)
        left = buildDecisionTree(data with f=0, labels with f=0)
        right = buildDecisionTree(data with f=1, labels with f=1)
        return Tree(f, left, right)
```

Does this always terminate?

  - Terminating when:
    - All data has same label
    - Unseen example or feature value
    - No further splits possible (run out of splitting feature or feature value for data are the same, but somehow label are not)
- IG and Entropy

- Entropy: $H(X) = -\sum_{x \in X} p(x) \log(p(x))$
- Conditional Entropy: $H(Y|X) = \sum_{x \in X} p(x) H(Y|X = x)$

$$= -\sum_{x \in X} p(x) \sum_{y \in Y} p(y|X = x) \log(p(y|X = x))$$

- Information Gain: $IG(Y|X) = H(Y) - H(Y|X)$

- Overfitting and Underfitting
  - Overfitting: complete tree remembers every data
  - Underfitting: one level tree returns majority label
- Tree Pruning

  - Stop when too few examples in the branch
  - Stop when max depth reached
  - Stop when my classification error is not much more than the average of my children

    Build a whole tree first and then check the error rate improve a lot after adding additional layer
    - Requires first computing and then removing
  - χ^2-pruning: stop when remainder is no more likely than chance

    Stop if accuracy is no more than chance
- Summary

Pros	Cons
• Easy to interpret	• Not as accurate as other models, partly due to greedy training
• Easily handle mixed continuous and discrete data types	• Unstable
• Insensitive to monotonic transformations of inputs (no need to normalize)	• Small changes in training data can have large effects on tree structure
• Perform variable selection automatically	• Errors at the top propagate down due to hierarchical nature
• Scalable	
• Can handle missing inputs	

Ensemble Method

Random Forrest

- Data Sampling: With dataset of size N, create M different samples of size N by resampling wit replacement

    - Bootstrapping and Bagging
- Feature Sampling: random subset of feature at each node

AdaBoost

- Idea: weighted combined decision for weak learners
- Algorithm:

For each iteration $t=1$ to T

1. Train weak learner using samples weighted by D_t
2. Get weak hypothesis h_t with error

$$\varepsilon_t = \Pr\left[h_t(\mathbf{x}_i) \neq y_i\right] = \frac{\sum_{i=1}^{N} D_t(i) I(h_t(\mathbf{x}_i) \neq y_i)}{\sum_{i=1}^{N} D_t(i)}$$

3. Set $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)$

- α_t is larger for small error
- α_t is negative for error above 0.5

negative means it is worse than random

4. Update weights (where Z_t is a normalization constant)

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases}$$

$$= \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

if right, weight goes down,
if wrong, give it more weight
if a_t is 0, then no adjustment

    - Note:
        1. Loss function is different for different classifier
        2. a_m increases as error rate decreases, giving this classifier more weight in the final product
- Why AdaBoos t is not prune to over-fittting
    1. Implicit L1 regularization through stopping at a finite number of weak learners
    2. AdaBoost continues to maximize the margin, leading to better generalization (this yields the similarities with SVMs)
- AdaBoost is able to find better margin even though it training error goes down fast.
    - Other practical Advantages
        - Not prune to over-fitting
        - Fast
        - Easy to implement
        - No parameter tunning
        - Not specific to any weak learner
        - Well-motivated by learning theory
        - Can identify outliers

Diversity and Weighted Experts

- Idea: Diversity in classifiers, datasets
    - Data diversity: feature/instance bagging

Neural Net

- Two layer NN classification
    - $y_k(x, w) = \sigma(\sum_j^M w_{kj}[h(\sum_i^D w_{ji}x_i) + w_{j0}] + w_{k0})$

      Where D is number of input;

      M is number of hidden layer neurones

      K is number of classes

      σ Is sigmoid function

      h Is a non-linear activation function
- Loss function:
    - Cross Entropy for classification: Cross entropy is the number of bits we'll need if we encode symbols from yy using the *wrong* tool ŷ

$$H(y, \hat{y}) = \sum_i y_i \log \frac{1}{\hat{y}_i} = -\sum_i y_i \log \hat{y}_i$$

        - Sidenotes: KL divergence is just the difference between cross and entropy
    - OLS
- Optimisation:
    - Gradient descent
    - Back propagation: Chain rule of derivation through computation graph.

Problems with NN:

1. Required Large Labelled Data otherwise easy to overfit.
2. Non-convex objective -> easy stuck in local optima
3. "Vanishing Gradient": as gradient propagate back, gradient become even smaller

How To Solve?

- Idea1: Back-propragate + SGD -> not always work
- Idea 2: Supervised Pre-training
    - Iteratively add hidden layer. Train current hidden layer with previous hidden layer fixed
    - Then train once together
- Idea 3: Unsupervised Pre-training via Auto-Encoder
    - Auto-encoder: learn input structure by training to encoding input.

- Better than idea 2 because it is trying to perform a different task: learning the structure in the data which can resulting in a better starting point