Review

Expected cost, P(z=k|x), LDA & QDA Generative versus discriminative Generative

- ML or Bayesian
- Density-based
- PNN, kNN

Discriminative

- Logistic (binary) or softmax (multi-class), IRLS
- Perceptrons
- Decision Trees

Decision Trees:

- Tests: single attribute tests; hyperplane tests
- Continuous tests: Ranges
- Select t such that mutual information IG(z,t) is maximum

$$IG(z,t) = H(z) - H(z|t) = H(t) - H(t|z)$$

- You could consider pairs of tests at a time (JMI): IG(z,t_i, t_j). There is nothing prevents you form considering triples, quadruples, etc., but computing mutual information becomes complex!
- Other criteria: Gini index, MAP error,...
- Decision Trees have Low Bias and High Variance
- Ways to address it: Cost-complexity pruning and Error pruning, Bagging and Random Forests, Boosting: AdaBoost and Gradient Boosting ... do 10-fold cross-validation
- Bagging: Construct lots of decision trees using Bootstrap samples and average the classification decisions/regression estimates. Does not work well.
- Random Forests: Similar to bagging, but now sample features as well. Works well in practice.
- Boosting: Weak learners in series. Downstream learners use data on which upstream learners made errors for training. You can do this using weighted bootstrap sampling.... AdaBoost

• Idea:
$$\hat{z}_{M}^{n} = \operatorname{sgn}\left[\sum_{m=1}^{M} \alpha_{m} f_{m}(\underline{x}^{n})\right]; M \approx 10 - 20; n = 1, 2, ..., N; f \text{ is a weak classifier}$$

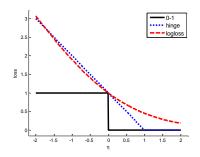
In a binary classifier, it makes correct decisions at least 50% or more.

- AdaBoost has a nice way of computing the weights $\{\alpha_m\}$
- We need some preliminaries. Suppose at step *m* have

$$\hat{z}_{m-1}^{n} = \operatorname{sgn}\left[\sum_{i=1}^{m-1} \alpha_{j} f_{j}(\underline{x}^{n})\right]; M \approx 10 - 20; n = 1, 2, ..., N$$

want
$$\hat{z}_{m}^{n} = \operatorname{sgn}[\sum_{j=1}^{m-1} \alpha_{j} f_{j}(\underline{x}^{n}) + \alpha_{m} f_{m}(\underline{x}^{n})]; M \approx 10 - 20; n = 1, 2, ..., N$$

But this is non-differentiable. Loss function: $L(z, \hat{z}) = 1 - \text{sgn}(z\hat{z})$. Plot the function versus $z\hat{z}$. Discuss Bounds: Exponential loss, log loss, hinge loss



$$L(z,\hat{z}) \le L_h(z,\hat{z}) = [1-z\hat{z}]_+ = \max(0,1-z\hat{z})$$
 hinge loss used in SVM

 $L(z,\hat{z}) \le L_e(z,\hat{z}) = e^{-z\hat{z}}$ Exponential loss used in AdaBoost

$$L(z,\hat{z}) \le L_{t}(z,y) = \ln(1 + e^{-zy}) / \ln 2$$

$$y = \hat{z} = \underline{w}^{T} \underline{x} \text{ or } y = \hat{z} = \underline{w}^{T} \phi(\underline{x})$$
Log loss

$$L_m(f_m) = \sum_{n=1}^{N} \exp\{-z^n [\hat{z}_{m-1}(\underline{x}^n) + \alpha_m f_m(\underline{x}^n)]\} = \sum_{n=1}^{N} w_n^{(m)} e^{-\alpha_m z^n f_m(\underline{x}^n)}$$

 $w_n^{(m)} = \exp\{-z^n \hat{z}_{m-1}(\underline{x}^n)\}\$ = weight on data item *n....know these*!

$$L_{m}(f_{m}) = e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} \delta_{z^{n} f_{m}(\underline{x}^{n})} + e^{\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) = \underbrace{\left(e^{\alpha_{m}} - e^{-\alpha_{m}}\right) \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}_{\text{depends on classifier } f_{m}} + e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) = \underbrace{\left(e^{\alpha_{m}} - e^{-\alpha_{m}}\right) \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}_{\text{depends on classifier } f_{m}} + e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) = \underbrace{\left(e^{\alpha_{m}} - e^{-\alpha_{m}}\right) \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}_{\text{depends on classifier } f_{m}} + e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) = \underbrace{\left(e^{\alpha_{m}} - e^{-\alpha_{m}}\right) \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}_{\text{depends on classifier } f_{m}} + e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) = \underbrace{\left(e^{\alpha_{m}} - e^{-\alpha_{m}}\right) \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}_{\text{depends on classifier } f_{m}} + e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) = \underbrace{\left(e^{\alpha_{m}} - e^{-\alpha_{m}}\right) \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}_{\text{depends on classifier } f_{m}} + e^{-\alpha_{m}} \sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})$$

 $\Rightarrow \text{Fit weak classifier } f_m \text{ by minimizing error function } J_m = \sum_{n=1}^N w_n^{(m)} (1 - \delta_{z^n f_m(\underline{x}^n)})$

....Bootstrap sampling with weights $w_n^{(m)}$

Optimal
$$\alpha_{m}$$
 from $e^{2\alpha_{m}} = \frac{\sum_{n=1}^{N} w_{n}^{(m)} \delta_{z^{n} f_{m}(\underline{x}^{n})}}{\sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})})}$

$$= \frac{\sum_{n=1}^{N} w_{n}^{(m)} \delta_{z^{n} f_{m}(\underline{x}^{n})} / \sum_{n=1}^{N} w_{n}^{(m)}}{\sum_{n=1}^{N} w_{n}^{(m)} (1 - \delta_{z^{n} f_{m}(\underline{x}^{n})}) / \sum_{n=1}^{N} w_{n}^{(m)}} = \frac{1 - e_{m}}{e_{m}} \Rightarrow \alpha_{m} = \frac{1}{2} \ln \left(\frac{1 - e_{m}}{e_{m}} \right)$$

$$\Rightarrow w_{n}^{(m+1)} = w_{n}^{(m)} e^{-\alpha_{m} z^{n} f_{m}(\underline{x}^{n})} = \begin{cases} w_{n}^{(m)} e^{-\alpha_{m}} & \text{if } f_{m}(\underline{x}^{n}) = z^{n} \\ w_{n}^{(m)} e^{\alpha_{m}} & \text{if } f_{m}(\underline{x}^{n}) \neq z^{n} \end{cases}$$

$$\hat{z} = \text{sgn}[\sum_{m=1}^{M} \alpha_{m} f_{m}(\underline{x}^{n})]; M \approx 10 - 20$$

Show via example

 Gradient Boosting: Idea originated from iterative solution of linear equations and least squares problems

$$\underline{y} = A\underline{x} \to \underline{x}_{1} \to r_{1} = \underline{y} - A\underline{x}_{1} \to \underline{e}_{1} \to \underline{x}_{2} = \underline{x}_{1} + \underline{e}_{1} \to r_{2} = \underline{y} - A\underline{x}_{2} \to \underline{e}_{2} \to \underline{x}_{3} = \underline{x}_{2} + \underline{e}_{2}, etc.$$

$$L_{m}(f_{m}) = \sum_{n=1}^{N} L(z^{n}, \hat{z}_{m-1}(\underline{x}^{n}) + f_{m}(\underline{x}^{n})) + \Omega(f_{m})...\Omega(.) \text{ regularization term}$$

$$\approx \sum_{n=1}^{N} \{L(z^{n}, \hat{z}_{m-1}(\underline{x}^{n})) + g_{n}f_{m}(\underline{x}^{n}) + \frac{1}{2}h_{n}[f_{m}(\underline{x}^{n})]^{2}\} + \Omega(f_{m});$$

$$g_{n} = \frac{\partial L(z^{n}, \hat{z})}{\partial \hat{z}} \mid \hat{z} = \hat{z}_{m-1}(\underline{x}^{n}); h_{n} = \frac{\partial^{2} L(z^{n}, \hat{z})}{\partial \hat{z}^{2}} \mid \hat{z} = \hat{z}_{m-1}(\underline{x}^{n})$$

$$\Omega(f_m) = \gamma T + \frac{\lambda}{2} \sum_{j=1}^{T} w_j^2; T = \# \text{ of leaves}$$

 w_i = weight of leaf j (e.g., expected cost of path in the tree leading to leaf j)

 $f_m(\underline{x}^n) = w_j$ if \underline{x}^n is mapped to leaf j, i.e., $q(\underline{x}^n) = j$; q is the mapping function

$$\begin{split} L_{m}(f_{m}) &\approx \sum_{n=1}^{N} \{L(z^{n}, \hat{z}_{m-1}(\underline{x}^{n}))] + g_{n}f_{m}(\underline{x}^{n}) + \frac{1}{2}h_{n}[f_{m}(\underline{x}^{n})]^{2}\} + \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_{j}^{2} \\ &= \sum_{j=1}^{T} \{\underbrace{\left(\sum_{n \in I_{j}} g_{n}\right)}_{G_{j}} w_{j} + \frac{1}{2}(\sum_{n \in I_{j}} h_{n} + \lambda)w_{j}^{2} + \gamma\} + \text{constant.....} \text{ separable in } w_{j}.... \text{ but huge possibilities for } \{I_{j}\}! \end{split}$$

For known
$$\{I_j\}$$
, optimal $w_j = -\frac{G_j}{H_j + \lambda}$; $L_m(f_m) = \frac{1}{2} \sum_{j=1}^{T} (\frac{-G_j^2}{H_j + \lambda} + 2\gamma)$

$$Gain = \frac{1}{2} \left[\frac{G_{Lj}^{2}}{H_{Lj} + \lambda} + \frac{G_{Rj}^{2}}{H_{Rj} + \lambda} - \frac{G_{j}^{2}}{H_{j} + \lambda} \right] - \gamma; G_{j} = G_{Lj} + G_{Rj}; H_{j} = H_{Lj} + H_{Rj}$$

$$\hat{z}_{m} = \hat{z}_{m-1} + \varepsilon f_{m}; \varepsilon \approx 0.1$$

Percepron is an incremental gradient (stochastic gradient descent (SGD)) algorithm:

$$\underline{w} \leftarrow \underline{w} + \eta e_n \underline{x}_n$$

Why gradient algorithms work even if step size is off?

Consider
$$\min_{x,y} f(x,y) = \frac{h_1}{2} (x-4)^2 + \frac{h_2}{2} (y-2)^2 \Rightarrow x^* = 4, y^* = 2$$

Suppose we start at (0,0)

$$\nabla f = g = \begin{bmatrix} h_1(x-4) \\ h_2(y-2) \end{bmatrix}; \nabla^2 f = \begin{bmatrix} h_1 & 0 \\ 0 & h_2 \end{bmatrix}; h_i = \text{a measure of curvature} > 0$$

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ y_k \end{bmatrix} - \eta \begin{bmatrix} h_1(x_k-4) \\ h_2(y_k-2) \end{bmatrix} \Rightarrow \begin{bmatrix} x_{k+1}-4 \\ y_{k+1}-2 \end{bmatrix} = \begin{bmatrix} (1-\eta h_1)(x_k-4) \\ (1-\eta h_2)(y_k-2) \end{bmatrix}$$

$$\Rightarrow need - 1 < 1 - \eta h_i < 1 \Rightarrow \eta > 0 & \eta < \min_i (\frac{2}{h_i}) = \frac{2}{\max(h_i)}$$

$$optimal \ \eta : \frac{h_1}{2} (1-\eta h_1)^2 (x_k-4)^2 + \frac{h_2}{2} (1-\eta h_2)^2 (y_k-2)^2$$

$$\Rightarrow -h_1^2 (1-\eta h_1)(x_k-4)^2 - h_2^2 (1-\eta h_2)(y_k-2)^2 = 0$$

$$\Rightarrow \eta = \frac{h_1^2 (x_k-4)^2 + h_2^2 (y_k-2)^2}{h_1^3 (x_k-4)^2 + h_2^3 (y_k-2)^2}$$

If $h_1 >> h_2, \eta \approx \frac{1}{h_1} \dots \eta$ can be off by a factor of 2 and still get function reduction!

LMS:

$$\underline{w}^{(n+1)} = \underline{w}^{(n)} + \eta^n e_n \underline{x}^n; \eta^n = \frac{\lambda}{\left\|\underline{x}^n\right\|^2} 0 < \lambda < 2. \ \lambda = 1 \text{ implies projection.}$$

$$\min_{\underline{w}} \frac{1}{2} \left\|\underline{w} - \underline{w}^{(n)}\right\|^2 \qquad \text{s.t. } \underline{w}^T \underline{x}^n = z^n$$

$$L(\underline{w}, \mu) = \frac{1}{2} (\underline{w} - \underline{w}^{(n)})^T (\underline{w} - \underline{w}^{(n)}) + \mu \left[z^n - \underline{w}^T \underline{x}^n\right]$$

$$\nabla_{\underline{w}} L = \underline{w} - \underline{w}^{(n)} - \mu \underline{x}^n = 0 \qquad \text{using } \underline{w}^T \underline{x}^n = z^n$$

$$\Rightarrow \mu = \frac{z^n - \underline{w}^{(n)T} \underline{x}^n}{\left(\underline{x}^n\right)^T \underline{x}^n}$$

$$\Rightarrow w^{(n+1)} = w^{(n)} + \frac{(z^n - \underline{w}^{(n)T} \underline{x}^n)}{\left\|\underline{x}^n\right\|^2} \underline{x}^n$$

Convergence of LMS: Convergence in the mean; convergence in mean square

Momentum:
$$\underline{w}^{(n+1)} = \underline{w}^{(n)} + \eta(z^n - \underline{w}^{(n)T}\underline{x}^n)\underline{x}^n + \mu(\underline{w}^{(n)} - \underline{w}^{(n-1)})$$

$$\Delta \underline{w}^{(n)} = \mu \Delta \underline{w}^{(n-1)} + \eta e_n \underline{x}^n$$

$$or \underline{d}^{(n)} = \mu \underline{d}^{(n-1)} - \eta \underline{g}^{(n)}$$
clearly need $\mu < 1$

Nesterov:
$$\underline{d}^{(n)} = \mu \underline{d}^{(n-1)} - \eta \underline{g}^{(n)} |_{w^{(n)} + \mu \underline{d}^{(n-1)}} \dots gradient evaluated at \underline{w}^{(n)} + \mu \underline{d}^{(n-1)}$$

AdaGrad:

$$w_{i}^{(n+1)} = w_{i}^{(n)} - \eta_{i}^{(n)} g_{i}^{(n)}; \eta_{i}^{(n)} = \frac{\eta}{\sqrt{\sum_{j=1}^{n} (g_{i}^{(j)})^{2} + \varepsilon}} = \frac{\eta}{\sqrt{G_{n} + \varepsilon}}; \varepsilon \approx 10^{-8}$$

$$G_n = G_{n-1} + (g_i^{(n)})^2; G_0 = 0$$

RMSprop:

$$G_{n} = \gamma G_{n-1} + (1 - \gamma) \| \underline{g}^{(n)} \|_{2}^{2}; G_{0} = 0; \gamma \approx 0.9$$

$$\underline{w}^{(n+1)} = \underline{w}^{(n)} - \frac{\eta}{\sqrt{G_{n} + \varepsilon}} \underline{g}^{n}; \eta \approx 0.001$$

Adam:

$$\overline{g}^{(n)} = \theta \ \overline{g}^{(n-1)} + (1-\theta)g^{(n)}; \overline{g}^{(0)} = 0$$

$$G_n = \gamma G_{n-1} + (1 - \gamma) \| \underline{g}^{(n)} \|_2^2$$

$$\underline{w}^{(n+1)} = \underline{w}^{(n)} - \frac{\eta^{(n)}}{\sqrt{G_n} + \varepsilon} \underline{g}^n; \eta^{(n)} = \eta \frac{\sqrt{1 - \gamma^t}}{1 - \theta^t}$$

Quick prop:
$$w_i^{(n+1)} - w_i^{(n)} = \frac{g_i^{(n)}}{g_i^{(n-1)} - g_i^{(n)}} \Big[w_i^{(n)} - w_i^{(n-1)} \Big]$$

Single layer network

Incremental Newton and RLS

Modified RLS = Gauss-Newton = EKF

Fisher's Linear Discriminant