10. Other Classifiers STA3142 Statistical Machine Learning

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Applied Statistics / Statistics and Data Science
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Assignment 1

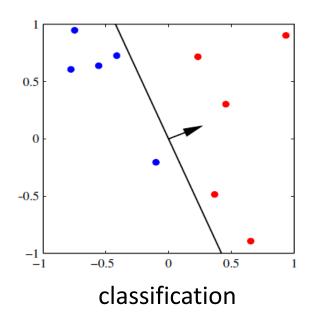
- Due Friday 3/29 Saturday 3/30, 11:59pm
 - LearnUs was under maintenance around midnight.
- Topics
 - (Programming) NumPy basics
 - (Programming) Linear regression on a polynomial
 - (Math) Derivation and proof for linear regression
- Please read the instruction carefully!
 - Submit one <u>pdf</u> and one <u>zip</u> file separately
 - Write your code only in the designated spaces
 - Do not import additional libraries
 - ...
- If you feel difficult, consider to take option 2.

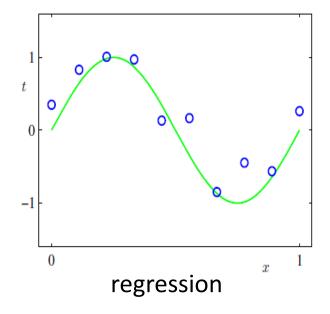
Assignment 2

- Due Friday 4/12, 11:59pm
- Topics
 - (Math/Programming) Logistic Regression
 - (Math/Programming) Softmax Regression
 - (Math) Gaussian Discriminant Analysis
 - (Programming) Naïve Bayes for Spam Classification
- Please read the instruction carefully!
 - Submit one <u>pdf</u> and one <u>zip</u> file separately
 - Write your code only in the designated spaces
 - Do not import additional libraries
 - ...
- If you feel difficult, consider to take option 2.

Recap: Supervised Learning

- Learning a function $h: \mathcal{X} \to \mathcal{Y}$
- Labels could be discrete or continuous
 - Discrete labels: classification
 - Continuous labels: regression





Recap: Discriminative vs. Generative

Probabilistic discriminative models:

- Logistic regression: $p(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T \phi(\mathbf{x}))$
- Softmax regression: $p(C_k|\mathbf{x}) = \frac{\exp(\mathbf{w}_k^T \mathbf{x})}{\sum_j \exp(\mathbf{w}_j^T \mathbf{x})}$

Probabilistic generative models:

- Gaussian discriminant analysis:
 - Prior $p(C_k)$: Bernoulli
 - Likelihood $p(\mathbf{x}|C_k)$: Gaussian
- Naïve Bayes:
 - Prior $p(C_k)$: Bernoulli
 - Likelihood $p(\mathbf{x}|C_k) = \prod_{j=1}^{M} p(x_j|C_k)$
 - For spam mail classification, Multinomial

Classification Strategies

- Learning the distributions $p(C_k|x)$
 - Discriminative models: Directly model $p(C_k|x)$ and learn parameters from the training set.
 - Generative models: Learn class densities $p(x|C_k)$ and priors $p(C_k)$ to obtain $p(x, C_k) = p(x|C_k)p(C_k)$
- Nearest neighbor classification
 - Given query data x, find the closest training points and do majority vote.
- Discriminant functions
 - Learn a function h(x) that maps x onto some C_k .

Outline

- Nearest neighbor classification
 - K-Nearest Neighbors

- Discriminant functions
 - Fisher's Linear Discriminant
 - Perceptron

• Training: Memorize all training data and labels $D_{\text{train}} = \{ (\mathbf{x}^{(1)}, y^{(1)}), ..., (\mathbf{x}^{(N)}, y^{(N)}) \}$

 Test: Given a test data (or query) x*, find K training data that are closest to x*, and then majority vote.

$$D_{KNN}(\mathbf{x}^*) = \{ (\mathbf{x}^{(1)'}, y^{(1)'}), \dots, (\mathbf{x}^{(K)'}, y^{(K)'}) \}$$

$$\subset D_{\text{train}}$$

$$\hat{y}^* = \underset{t}{\operatorname{argmax}} \qquad 1[y' = t]$$

Note: K-NN can also be used for regression.

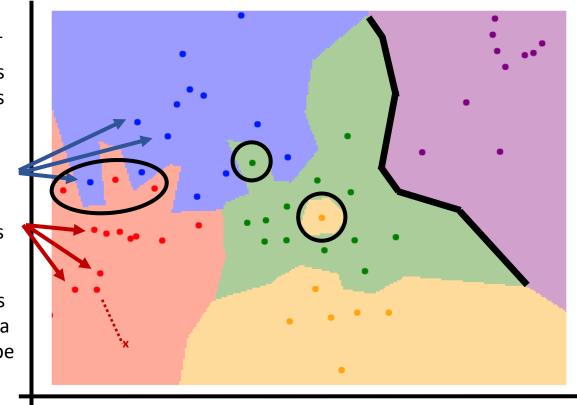
NN Decision Boundaries

 X_1

Nearest neighbors in two dimensions

Points are training examples; colors give training labels

Background colors give the category a test point would be assigned



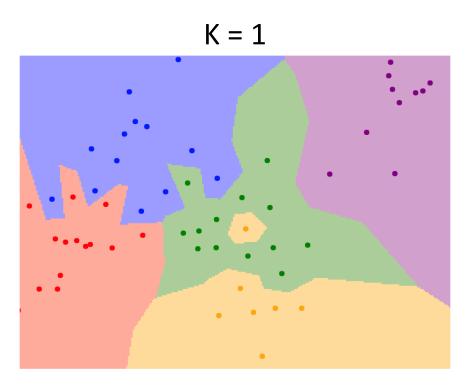
Decision boundary is the boundary between two classification regions

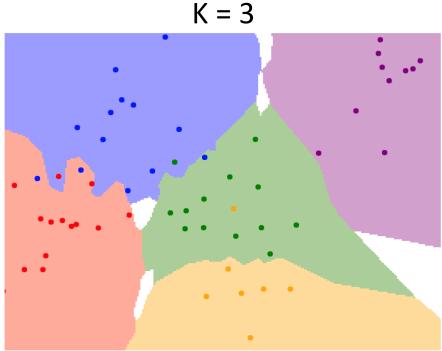
Decision boundaries can be noisy; affected by outliers

How to smooth out decision boundaries? Use more neighbors!

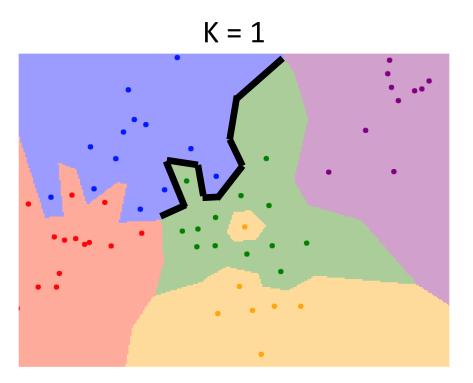
 \mathbf{X}_{0}

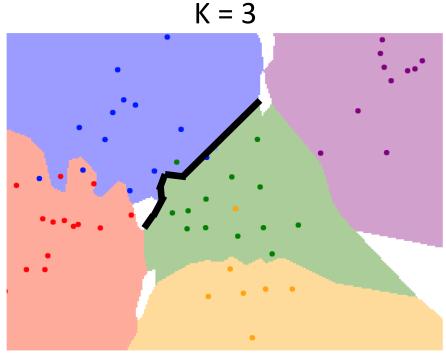
Instead of copying label from nearest neighbor, take **majority vote** from K closest points



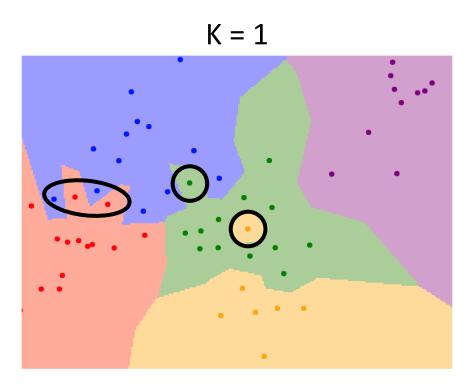


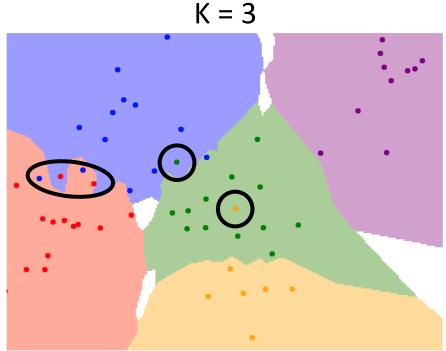
Using more neighbors helps smooth out rough decision boundaries



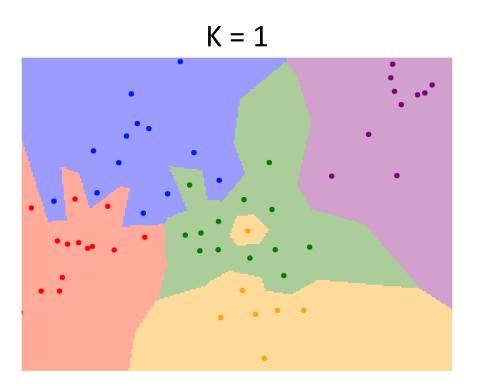


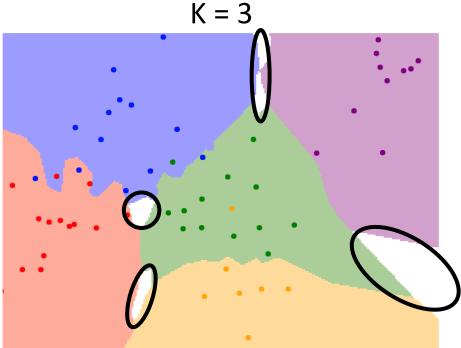
Using more neighbors helps reduce the effect of outliers





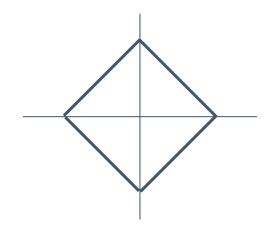
When K > 1 there can be ties between classes. Need to break somehow!





L1 (Manhattan) distance

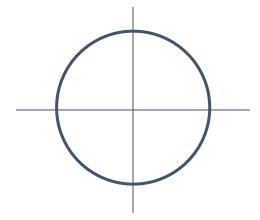
$$d_1(I_1, I_2) = \sum_{p} |I_1^p - I_2^p|$$



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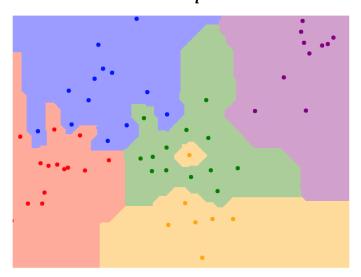
L2 (Euclidean) distance

$$d_1(I_1, I_2) = \left(\sum_{p} (I_1^p - I_2^p)^2\right)^{\frac{1}{2}}$$



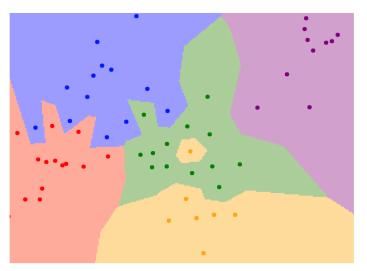
L1 (Manhattan) distance

$$d_1(I_1, I_2) = \sum_{p} |I_1^p - I_2^p|$$



L2 (Euclidean) distance

$$d_1(I_1, I_2) = \left(\sum_{p} (I_1^p - I_2^p)^2\right)^{\frac{1}{2}}$$



K = 1

With the right choice of distance metric, we can apply K-Nearest Neighbors to any type of data!

Mesh R-CNN

Georgia Gkioxari, Jitendra Malik, Justin Johnson 6/6/2019 cs.CV



Example:
Compare
research
papers using
tf-idf similarity



Rapid advances in 2D perception have led to systems that accurately detect objects in real-world images. However, these systems make predictions in 2D, ignoring the 3D structure of the world. Concurrently, advances in 3D shape prediction have mostly focused on synthetic benchmarks and isolated objects. We unify advances in these two areas. We propose a system that detects objects in real-world images and produces a triangle mesh giving the full 3D shape of each detected object. Our system, called Mesh R-CNN, augments Mask R-CNN with a mesh prediction branch that outputs meshes with varying topological structure by first predicting coarse voxel representations which are converted to meshes and refined with a graph convolution network operating over the mesh's vertices and edges. We validate our mesh prediction branch on ShapeNet, where we outperform prior work on single-image shape prediction. We then deploy our full Mesh R-CNN system on Pix3D, where we jointly detect objects and predict their 3D shapes.

http://www.arxiv-sanity.com/search?q=mesh+r-cnn



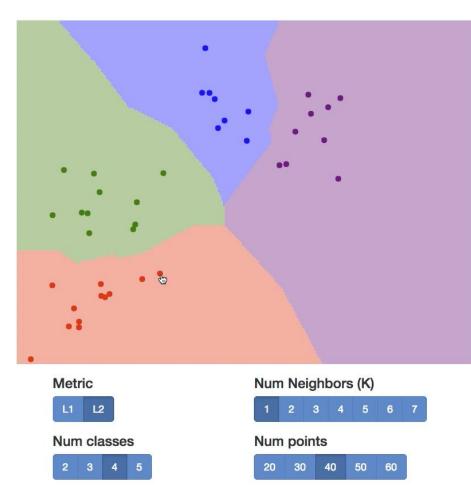
http://www.arxiv-sanity.com/1906.02739v1

K-Nearest Neighbors: Web Demo

Interactively move points around and see decision boundaries change

Play with L1 vs L2 metrics

Play with changing number of training points, value of K



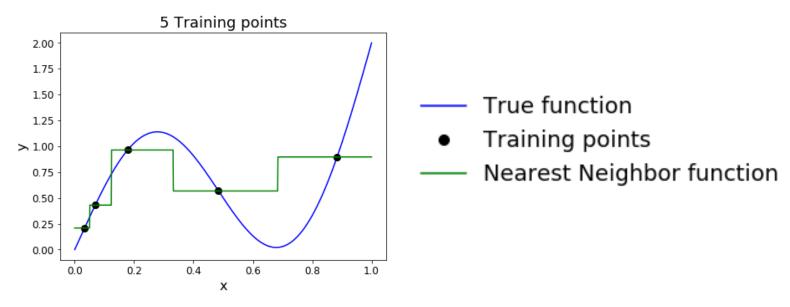
http://vision.stanford.edu/teaching/cs231n-demos/knn/

K-NN Hyperparameters

- What is the best value of K to use?
- What is the best distance metric $D(\mathbf{x}, \mathbf{x}')$ to use?
 - These are hyperparameters.
 - Cf. Learning rate and regularization coefficient are also hyperparameters.
 - We set them at the start of the learning process, instead of learning from the training data.
- Answer: Very problem-dependent. In general, we need to try them all and see what works best for our data/task.
 - Need validation to find the best hyperparameters
 - (We will discuss validation in the lecture on model selection)

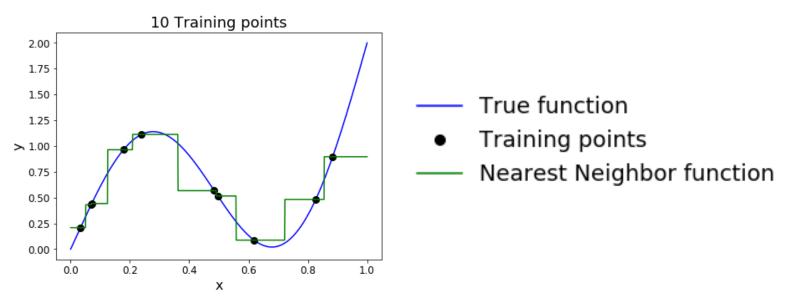
10. Other Classifiers - 20

As the number of training samples goes to infinity, nearest neighbor can represent any^(*) function!



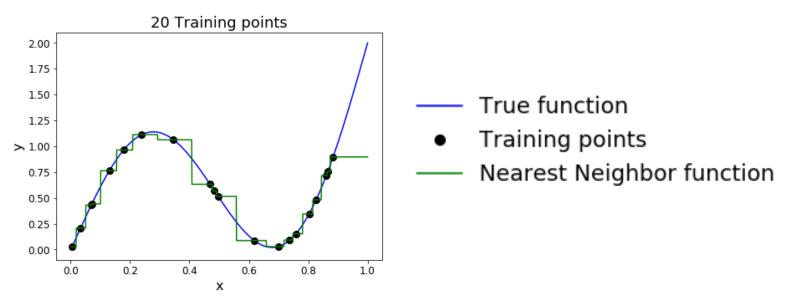
(*) Subject to many technical conditions. Only continuous functions on a compact domain; need to make assumptions about spacing of training points; etc.

As the number of training samples goes to infinity, nearest neighbor can represent any^(*) function!



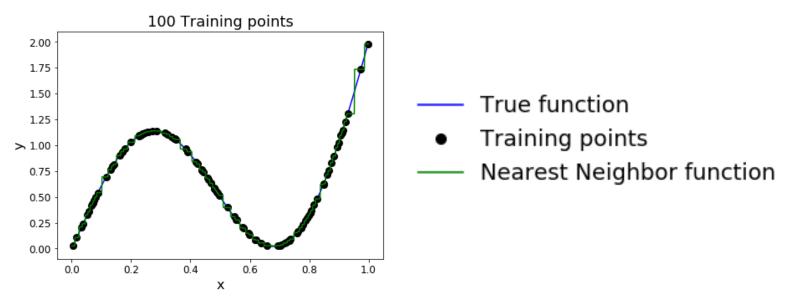
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As the number of training samples goes to infinity, nearest neighbor can represent any^(*) function!



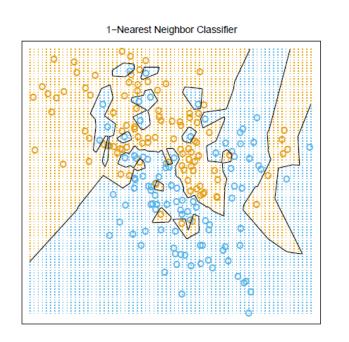
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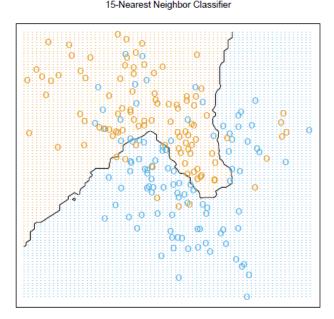
As the number of training samples goes to infinity, nearest neighbor can represent any^(*) function!



(*) Subject to many technical conditions. Only continuous functions on a compact domain; need to make assumptions about spacing of training points; etc.

K-Nearest Neighbors for Classification





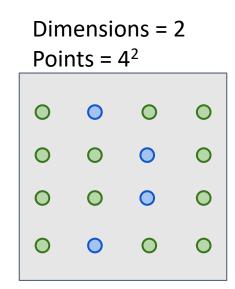
- K acts as a smother (bias-variance trade-off)
- Classification performance generally improves as N (training set size) increases.
- For $N \to \infty$, the error rate of the 1-nearest-neighbor classifier is never more than twice the optimal error (obtained from the true conditional class distributions).

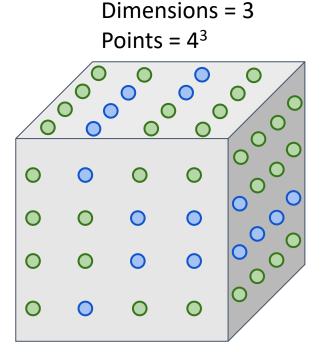
Slide credit: Ben Kuipers

Problem: Curse of Dimensionality

Curse of dimensionality: For uniform coverage of space, number of training points needed grows exponentially with dimension

Dimensions = 1 Points = 4





Problem: Curse of Dimensionality

Curse of dimensionality: For uniform coverage of space, number of training points needed grows exponentially with dimension

Number of possible 32x32 binary images:

 $2^{32\times32} \approx 10^{308}$

Number of elementary particles in the visible universe: (source)

$$\approx 10^{97}$$

K-NN Classification vs. Regression

• Classification: Given a test data (or query) \mathbf{x}^* , find K training data that are closest to \mathbf{x}^* , and then majority vote.

$$D_{KNN}(\mathbf{x}^*) = \{ (\mathbf{x}^{(1)'}, y^{(1)'}), \dots, (\mathbf{x}^{(K)'}, y^{(K)'}) \}$$

$$\subset D_{train}$$

$$\hat{y}^* = \underset{t}{\operatorname{argmax}} \qquad 1[y' = t]$$

• Regression: Take average over y' values.

$$\widehat{y}^* = \frac{1}{K} \sum_{(\mathbf{x}', \mathbf{y}') \in D_{KNN}(\mathbf{x}^*)} y'$$

Pros and Cons of K-NN

Advantages:

- Simple and flexible (no assumption on distribution)
- Effective for low dimensional inputs

Disadvantages:

- Expensive: need to remember (store) and search through all the training data for every prediction
- Curse of dimensionality: the number of data must grow exponentially to keep the same density
- Not robust to irrelevant features: If data has irrelevant/noisy features, then distance function does not reflect similarity between examples

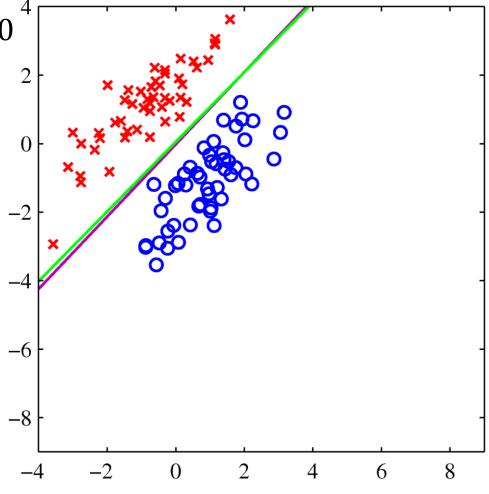
Discriminant functions

Two-Class Linear Discriminant

Classification rule:

$$C_1$$
 if $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0 \ge 0$
 C_0 otherwise.

- Suppose we do not have any probabilistic model assumption.
 - Magenta: Linear regression to one-hot encoded labels
 - Cf. Green: Logistic regression



Multi-Class Linear Discriminant

• Each class C_k gets its own function

$$h_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$

• Assign \mathbf{x} to C_k if

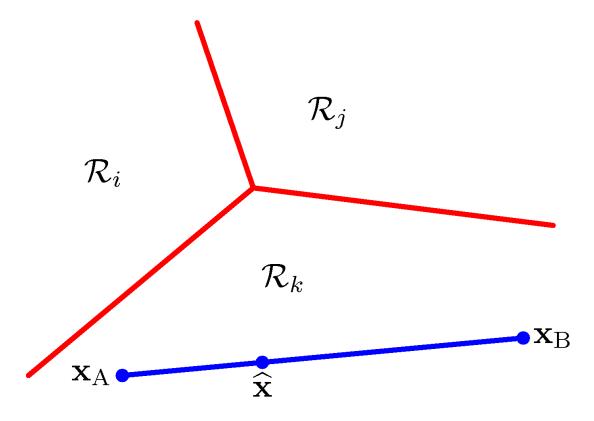
$$h_k(\mathbf{x}) > h_k(\mathbf{x})$$
 for all $j \neq k$

The decision regions are convex polyhedra.

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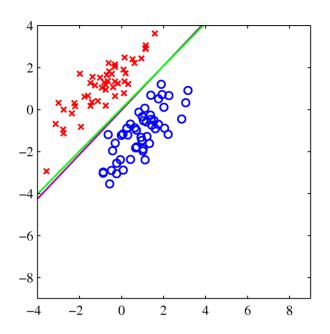
Decision Regions

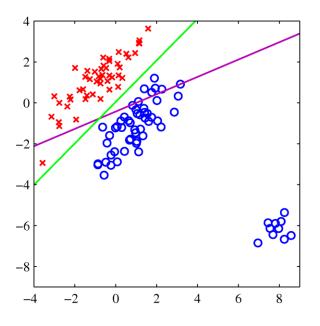
 Decision regions are convex, with piecewise linear boundaries.



Linear Discriminant Functions

- How about w that minimizes squared error?
 - Label y versus linear prediction $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$.
 - Least squares is too sensitive to outliers.
 - Logistic regression is robust to outliers, but requires an assumption (probabilistic discriminative model).





Classification Strategies

- Discriminant functions: Learn a function h(x) that maps x onto some \mathcal{C}_k .
 - Fisher's linear discriminant
 - Perceptron learning

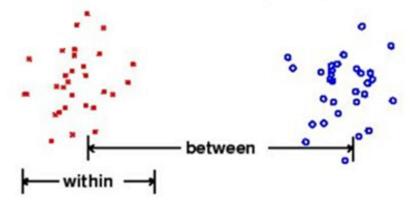
Fisher's Linear Discriminant

Fisher's Linear Discriminant

• Use **w** to project **x** onto one dimension, and then threshold the value by $-w_0$.

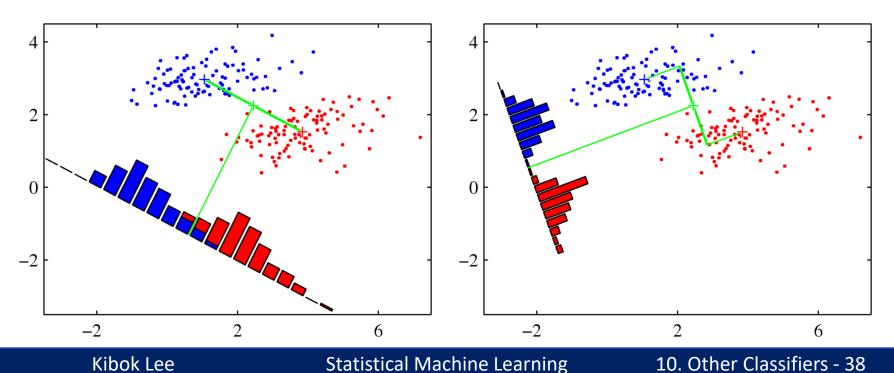
$$C_1$$
 if $h(\mathbf{x}) = \mathbf{w}^T \mathbf{x} \ge -w_0$
 C_0 otherwise.

- Select w that best separates the classes.
- The learning objective should simultaneously
 - Maximize between-class variances
 - Minimize within-class variances



Fisher's Linear Discriminant

- The learning objective should simultaneously
 - Maximize between-class variances
 - Minimize within-class variances
- Because maximizing separation alone doesn't work.
 - Minimizing class variance is a big help.



FLD: Formulation

We want to maximize the distance between classes

$$\underline{m}_2-m_1\equiv \mathbf{w}^T(\underline{\mathbf{m}}_2-\mathbf{m}_1)$$
 where $\mathbf{m}_k=\frac{1}{N_k}\sum_{n\in C_k}\mathbf{x}_n$ Projected mean

While minimizing the distance within each class

$$s_1^2 + s_2^2 \equiv \sum_{n \in C_1} (\mathbf{w}^T \mathbf{x}_n - m_1)^2 + \sum_{n \in C_2} (\mathbf{w}^T \mathbf{x}_n - m_2)^2$$

- Objective function: $J(\mathbf{w}) = \frac{(m_2 m_1)^2}{s_1^2 + s_2^2}$
 - The bias w_0 is not in the learning objective; it should be determined separately after finding \mathbf{w} .

FLD: Derivation

- Numerator: $m_2 m_1 = \mathbf{w}^T (\mathbf{m}_2 \mathbf{m}_1)$ $\Rightarrow ||m_2 - m_1||^2 = \mathbf{w}^T (\mathbf{m}_2 - \mathbf{m}_1) (\mathbf{m}_2 - \mathbf{m}_1)^T \mathbf{w}$
- Denominator:

$$S_B$$
: Between-class scatter

$$s_k^2 = \sum_{n \in C_k} (\mathbf{w}^T \mathbf{x}_n - \mathbf{w}^T \mathbf{m}_k)^2 = \sum_{n \in C_k} \mathbf{w}^T (\mathbf{x}_n - \mathbf{m}_k) (\mathbf{x}_n - \mathbf{m}_k)^T \mathbf{w}$$

$$\Rightarrow s_1^2 + s_2^2 = \mathbf{w}^T \left[\sum_{k=1}^2 \sum_{n \in C_k} (\mathbf{x}_n - \mathbf{m}_k) (\mathbf{x}_n - \mathbf{m}_k)^T \right] \mathbf{w}$$

Objective function:

 S_W : Within-class scatter

$$J(\mathbf{w}) = \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}$$

• Solution: $\mathbf{w} \propto S_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$

- Two-class
 - Learning objective: $J(\mathbf{w}) = \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}$
 - Solution: $\mathbf{w} \propto S_W^{-1}(\mathbf{m}_2 \mathbf{m}_1)$
- Multi-class
 - Learning objective: $J(W) = \operatorname{tr}(W^T S_W W)^{-1} (W^T S_B W)$
 - Solution: $S_BW = S_WW\Lambda$
 - where $S_W = \sum_k \sum_{y^{(i)}=k} (\mathbf{x}^{(i)} \mathbf{m}_k) (\mathbf{x}^{(i)} \mathbf{m}_k)^T$ $S_B = \sum_k N_k (\mathbf{m}_k \mathbf{m}) (\mathbf{m}_k \mathbf{m})^T$ $\mathbf{m} = \frac{1}{N} \sum_i x^{(i)} = \frac{1}{N} \sum_k N_k \mathbf{m}_k$

- Multi-class
 - Learning objective: $J(W) = \operatorname{tr}(W^T S_W W)^{-1} (W^T S_B W)$
 - Solution: $S_BW = S_WW\Lambda$
 - where $S_W = \sum_k \sum_{y^{(i)}=k} (\mathbf{x}^{(i)} \mathbf{m}_k) (\mathbf{x}^{(i)} \mathbf{m}_k)^T$ $S_B = \sum_k N_k (\mathbf{m}_k \mathbf{m}) (\mathbf{m}_k \mathbf{m})^T$ $\mathbf{m} = \frac{1}{N} \sum_i x^{(i)} = \frac{1}{N} \sum_k N_k \mathbf{m}_k$
 - Derived by generalized eigenvalue decomposition
 - Not directly usable for classification, as each \mathcal{C}_k does not get its own function; need to build another classifier
 - Up to (K-1) linearly independent \mathbf{w}_k 's $(\operatorname{rank}(W) \leq K-1)$
 - Not unique: WZ is also a solution for nonsingular Z

- Multi-class
 - Learning objective: $J(W) = \operatorname{tr}(W^T S_T W)^{-1} (W^T S_B W)$
 - Solution: $S_BW = S_TW\Lambda$
 - where $S_T = \sum_i (\mathbf{x}^{(i)} \mathbf{m}) (\mathbf{x}^{(i)} \mathbf{m})^T = S_W + S_B$ $S_B = \sum_i N_k (\mathbf{m}_k \mathbf{m}) (\mathbf{m}_k \mathbf{m})^T$ $\mathbf{m} = \frac{1}{N} \sum_i x^{(i)} = \frac{1}{N} \sum_k N_k \mathbf{m}_k$
 - This is equivalent to the within-scatter version.
 - Proof sketch: Intuitively,

$$\operatorname{argmax}_{W} \frac{f(W)}{g(W)} = \operatorname{argmax}_{W} \frac{f(W)}{f(W) + g(W)}$$

- Often called linear discriminant analysis (LDA)
 - Or Fisher's LDA (FLDA)
 - Cf. For two-class classification, GDA with shared covariance gives us the same weight vector w, and is also often called LDA.

- Mainly used for dimensionality reduction
 - From an arbitrary D to D' ($\leq K-1$)
 - Choose D' eigenvectors with largest eigenvalues
 - This is supervised dimensionality reduction; we will cover other (un)supervised dimensionality reduction methods later.

Recap: GDA with shared covariance

Maximum likelihood estimation (MLE):

$$\phi = \frac{1}{N} \sum_{i=1}^{N} \mathbf{1} \{ y^{(i)} = 1 \}$$

$$\mu_0 = \frac{\sum_{i=1}^{N} \mathbf{1} \{ y^{(i)} = 0 \} \mathbf{x}^{(i)}}{\sum_{i=1}^{N} \mathbf{1} \{ y^{(i)} = 0 \}}$$

 \boldsymbol{m}_2 in FLD formulation

$$\mu_1 = \frac{\sum_{i=1}^{N} \mathbf{1} \{ y^{(i)} = 1 \} \mathbf{x}^{(i)}}{\sum_{i=1}^{N} \mathbf{1} \{ y^{(i)} = 1 \}}$$

 \boldsymbol{m}_1 in FLD formulation

$$\sum_{i=1}^{N} \sum_{i=1}^{N} (\mathbf{x}^{(i)} - \mu_{y^{(i)}}) (\mathbf{x}^{(i)} - \mu_{y^{(i)}})^{T}$$

 $N \cdot S_W$ in FLD formulation

Generalized FLD (Out of Scope)

- Variations of LDA
 - Regularized LDA: $S_T \leftarrow S_T + \lambda I$
 - Uncorrelated LDA: $W^T S_T W = I$
 - Orthogonal LDA: $W \leftarrow U$ where $W = U\Sigma V^T$ is SVD
 - Kernel LDA: $\mathbf{x} \leftarrow \phi(\mathbf{x})$ and use kernel trick
 - (We will discuss the kernel method later)
 - Combination of some of the above

Generalized FLD (Out of Scope)

- Equivalent to least squares from centered data to a family of targets [Lee et al., 2015]
 - if and only if $rank(S_B) = K 1$
 - i.e., their solutions map data to the same latent space

•
$$W^T(X - \mathbf{m}\mathbf{1}^T) \approx Y \Leftrightarrow \underset{W}{\operatorname{argmax}} \operatorname{tr}(W^T S_T W)^{-1}(W^T S_B W)$$

- A possible $Y = [I_{K-1} \ \mathbf{0}_K] L \in \mathbb{R}^{(K-1) \times N}$
 - $L \in \mathbb{R}^{K \times N}$ is a one-hot encoded label matrix
 - A collection of (K-1) one-hot vectors and a zero vector
- A possible $Y = B \in \mathbb{R}^{(K-1) \times N}$ where $S_B = XB^TBX^T$
 - $X \in \mathbb{R}^{D \times N}$ is the data matrix and B is a full rank factorization

[Lee et al.] On the Equivalence of Linear Discriminant Analysis and Least Squares. In AAAI, 2015.

Perceptron

Perceptron: Formulation

- Classification model: $h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \phi(\mathbf{x}))$
 - where $sign(a) = \begin{cases} +1 & \text{if } a \ge 0 \\ -1 & \text{if } a < 0 \end{cases}$
- Target: y = +1 for C_1 , y = -1 for C_2 .
- Then, we always want:

$$\mathbf{w}^T \phi(\mathbf{x}) y > 0$$

Perceptron: Formulation

Objective function

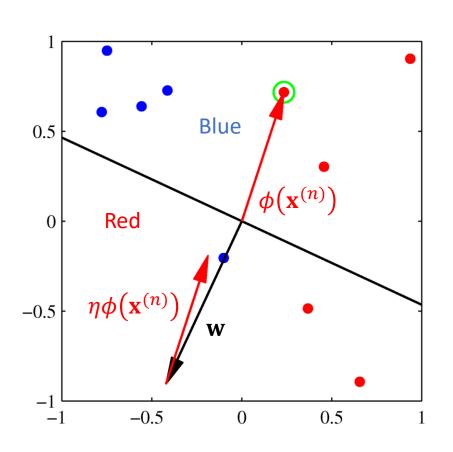
$$E_P(\mathbf{w}) = -\sum_{\mathbf{x}^{(n)} \in \mathcal{M}} \mathbf{w}^T \phi(\mathbf{x}^{(n)}) y^{(n)}$$

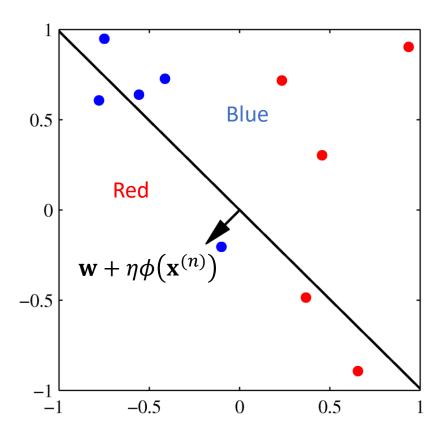
- where $\mathcal{M} = \{\mathbf{x}^{(n)}: y^{(n)} \neq \mathbf{w}^T \phi(\mathbf{x}^{(n)})\}$ is a set of misclassified points
- It counts errors from misclassified data.
- Iterative optimization
 - By stochastic gradient descent
 - Update w according to the misclassified data:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla E_P(\mathbf{w}) = \mathbf{w} + \eta \phi(\mathbf{x}^{(n)}) y^{(n)}$$

Perceptron: Learning Example

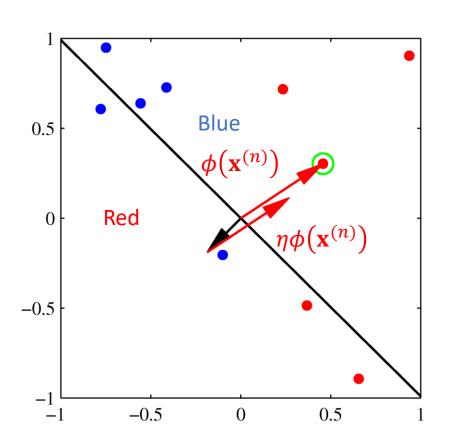
• If $\mathbf{x}^{(n)}$ is misclassified, add $\eta\phi(\mathbf{x}^{(n)})$ into \mathbf{w} .

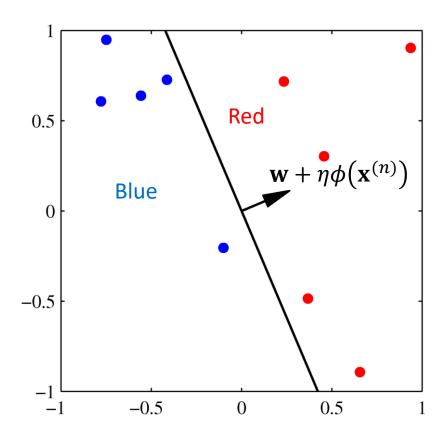




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Perceptron Learning

- Perceptron convergence theorem:
 - If there exists an exact solution (i.e., if the training data is linearly separable),
 - Then the learning algorithm will find it in a finite number of steps.

- Limitations of perceptron learning:
 - The convergence can be very slow.
 - If dataset is not linearly separable, it won't converge.
 - Does not generalize well to K > 2 classes.

Recap: Classification Strategies

- Learning the distributions $p(C_k|x)$
 - Discriminative models: Directly model $p(C_k|x)$ and learn parameters from the training set.
 - Generative models: Learn class densities $p(x|C_k)$ and priors $p(C_k)$ to obtain $p(x,C_k)=p(x|C_k)p(C_k)$
- Nearest neighbor classification
 - Given query data x, find the closest training points and do majority vote.
- Discriminant functions
 - Learn a function h(x) that maps x onto some C_k .

Next: Regularization, Validation