9 The Anisotropic Multivariate Normal Distribution, QDA, and LDA

ANISOTROPIC GAUSSIANS

[Recall from our last lecture the probability density function of the multivariate normal distribution in its full generality.]

$$\text{Normal PDF: } P(x) = \frac{1}{(\sqrt{2\pi})^d \sqrt{|\Sigma|}} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1} (x-\mu)\right) \qquad [x, \mu \text{ are } d\text{-vectors}]$$

$\uparrow$ determinant of Σ

Σ is the $d \times d$ SPD covariance matrix.
Σ^{-1} is the SPD precision matrix (metric).

covariance: Let R, S be random variables—vectors or scalars
$\mathrm{Cov}(R, S) = \mathrm{E}[(R - \mathrm{E}[R])\,(S - \mathrm{E}[S])^\top] = \mathrm{E}[RS^\top] - \mu_R \mu_S^\top$
$\mathrm{Var}(R) = \mathrm{Cov}(R, R)$
If R is a vector, covariance matrix for R is

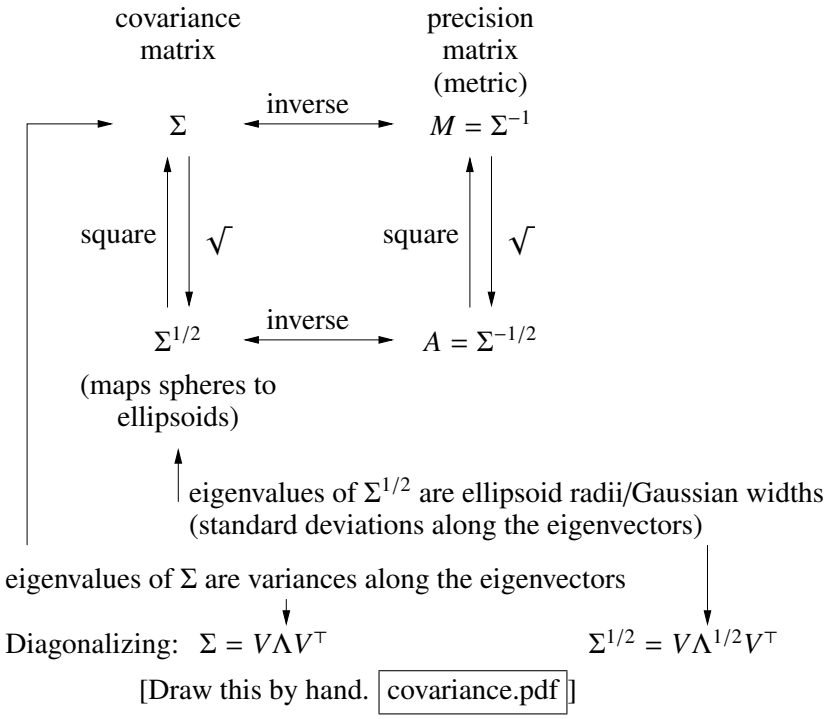
$$\mathrm{Var}(R) = \begin{bmatrix} \mathrm{Var}(R_1) & \mathrm{Cov}(R_1, R_2) & \dots & \mathrm{Cov}(R_1, R_d) \\ \mathrm{Cov}(R_2, R_1) & \mathrm{Var}(R_2) & & \mathrm{Cov}(R_2, R_d) \\ \vdots & & \ddots & \vdots \\ \mathrm{Cov}(R_d, R_1) & \mathrm{Cov}(R_d, R_2) & \dots & \mathrm{Var}(R_d) \end{bmatrix} \qquad [\text{symmetric; each } R_i \text{ is scalar}]$$

For a Gaussian $R \sim \mathcal{N}(\mu, \Sigma)$, one can show $\mathrm{Var}(R) = \Sigma$.
[. . . by integrating the expectation in anisotropic spherical coordinates. It's a painful integral.]
[An important point is that statisticians didn't just arbitrarily decide to call Σ a covariance matrix. Rather, statisticians discovered that if you find the covariance of the normal distribution by integration, it turns out that the covariance happens to be the inverse of the metric tensor. This is a happy discovery; it's rather elegant.]

R_i, R_j independent $\Rightarrow$ $\mathrm{Cov}(R_i, R_j) = 0$ [the reverse implication is not generally true, but . . .]
$\mathrm{Cov}(R_i, R_j) = 0$ AND multivariate normal dist. $\Rightarrow$ R_i, R_j independent
all features pairwise independent $\Rightarrow$ $\mathrm{Var}(R)$ is diagonal
$\mathrm{Var}(R)$ is diagonal AND normal
$\Leftrightarrow$ axis-aligned Gaussian; squared radii on diagonal of $\Sigma = \mathrm{Var}(R)$
$\Leftrightarrow$ $\underbrace{P(x)}_{\text{multivariate}} = \underbrace{P(x_1)\,P(x_2)\cdots P(x_d)}_{\text{univariate Gaussians}}$

[So when the features are independent, you can write the multivariate Gaussian as a product of univariate Gaussians. When they aren't, you can do a change of coordinates to the eigenvector coordinate system, and write it as a product of univariate Gaussians in eigenvector coordinates.]

[It's tricky to keep track of the relationships between the matrices, so here's a handy chart.]



[Draw this by hand. covariance.pdf]

[Remember that all four of these matrices have the same eigenvectors, the columns of V. Remember that when you take the inverse or square or square root of an SPD matrix, you do the same to its eigenvalues. So the ellipsoid radii, being the eigenvalues of $\Sigma^{1/2}$, are the square roots of the eigenvalues of the covariance matrix Σ, and they are the inverse square roots of the eigenvalues of the precision matrix (metric).]

[You should also think of the ellipsoid radii as being the "widths" of the Gaussian along each of the eigenvector directions. These appear on the diagonal of $\Lambda^{1/2}$.]

Maximum Likelihood Estimation for Anisotropic Gaussians

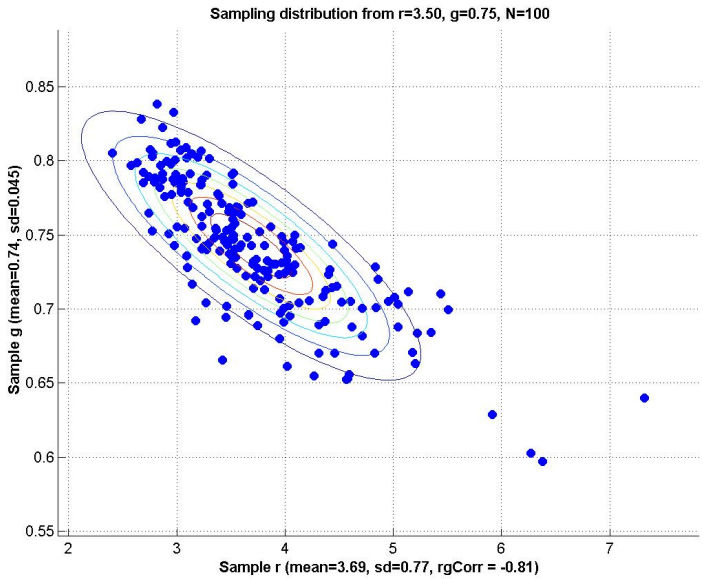
Given sample points $X_1, \ldots, X_n$ and classes $y_1, \ldots, y_n$, find best-fit Gaussians.
X_i is a column vector. [To fit our definition of the Gaussian distribution $P(x)$.]

[Once again, we want to fit the Gaussian that maximizes the likelihood of generating the sample points in a specified class. This time I won't derive the maximum-likelihood Gaussian; I'll just tell you the answer.]

For QDA:

$$\hat{\Sigma}_C = \frac{1}{n_C} \sum_{i:y_i=C} \underbrace{(X_i - \hat{\mu}_C)(X_i - \hat{\mu}_C)^T}_{\text{outer product matrix}} \qquad \Leftarrow \text{ conditional covariance for pts in class C}$$

[where n_C is the number of points in class C.]
Prior $\hat{\pi}_C$, mean $\hat{\mu}_C$: same as before
[$\hat{\pi}_C$ is number of points in class C / total sample points; $\hat{\mu}_C$ is mean of sample points in class C.]



maxlike.jpg [Maximum likelihood estimation takes these points and outputs this Gaussian].

$\hat{\Sigma}_C$ is positive semidefinite, but not always definite!
[If there are some zero eigenvalues, the standard version of QDA just doesn't work. We can try to fix it by eliminating the zero-variance dimensions (eigenvectors). But I'm not going to discuss how to do that.]

For LDA:

$$\hat{\Sigma} = \frac{1}{n} \sum_{C} \sum_{i:y_i=C} (X_i - \hat{\mu}_C)(X_i - \hat{\mu}_C)^T \qquad \Leftarrow \text{ pooled within-class covariance matrix}$$

[Let's revisit QDA and LDA and see what has changed now that we know anisotropic Gaussians. The short answer is "not much has changed, but the graphs look cooler." By the way, capital X once again represents a random variable.]

QDA

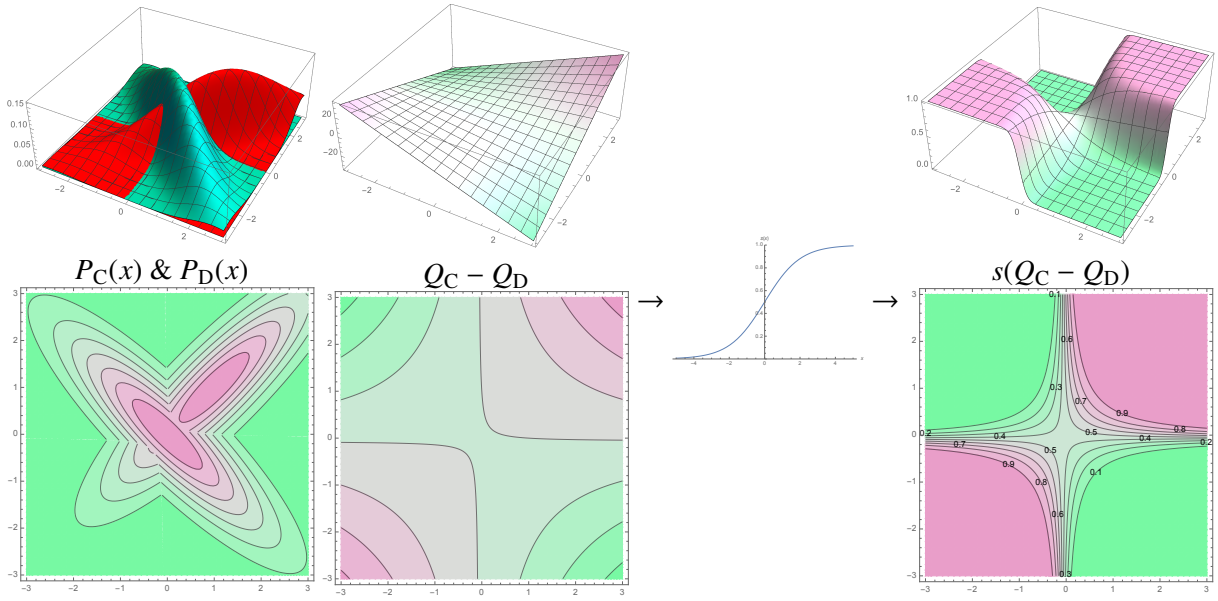
Choosing C that maximizes $P(X = x|Y = \mathrm{C})\,\pi_\mathrm{C}$ is equivalent to maximizing the quadratic discriminant fn

$$Q_\mathrm{C}(x) = \ln((\sqrt{2\pi})^d\, P_\mathrm{C}(x)\,\pi_\mathrm{C}) = -\frac{1}{2}(x-\mu_\mathrm{C})^\top \Sigma_\mathrm{C}^{-1}\,(x-\mu_\mathrm{C}) - \frac{1}{2}\ln|\Sigma_\mathrm{C}| + \ln\pi_\mathrm{C}$$

↑
Gaussian for C

[This works for any number of classes. In a multi-class problem, you just pick the class with the greatest quadratic discriminant for x.]

2 classes: Prediction fn $Q_\mathrm{C}(x) - Q_\mathrm{D}(x)$ is quadratic, but may be indefinite
⇒ Bayes decision boundary is a quadric.
Posterior is $P(Y = \mathrm{C}|X = x) = s(Q_\mathrm{C}(x) - Q_\mathrm{D}(x))$ where $s(\cdot)$ is logistic fn



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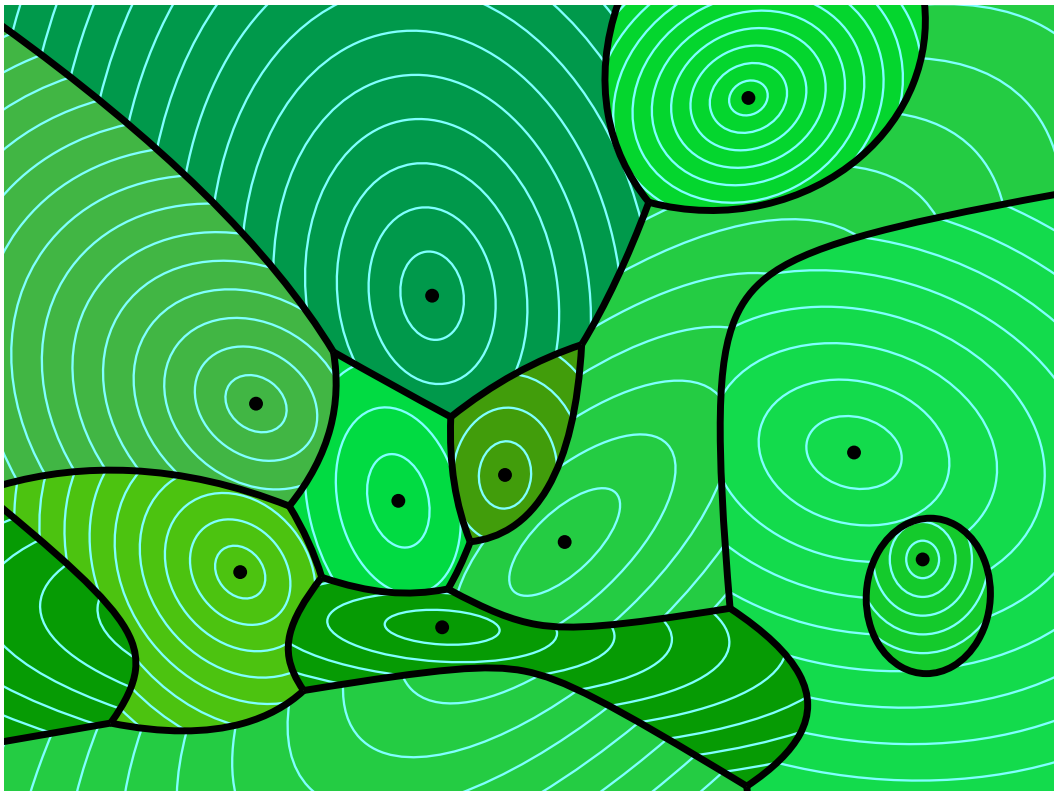
[(Show this figure on a separate "whiteboard.") An example where the decision boundary is a hyperbola—which is not possible with isotropic Gaussians. At left, two anisotropic Gaussians. Center left, the difference $Q_\mathrm{C} - Q_\mathrm{D}$. After applying the logistic function to this difference we obtain the posterior probabilities at right. However, observe that we can see the decision boundary in both the contour plot for $Q_\mathrm{C} - Q_\mathrm{D}$ and the contour plot for $s(Q_\mathrm{C} - Q_\mathrm{D})$. We don't need to apply the logistic function to find the decision boundary, but we do need to apply it if we want the posterior probabilities.]



aniso.pdf [When you have many classes, their QDA decision boundaries form an anisotropic Voronoi diagram. Interestingly, a cell of this diagram might not be connected.]

LDA

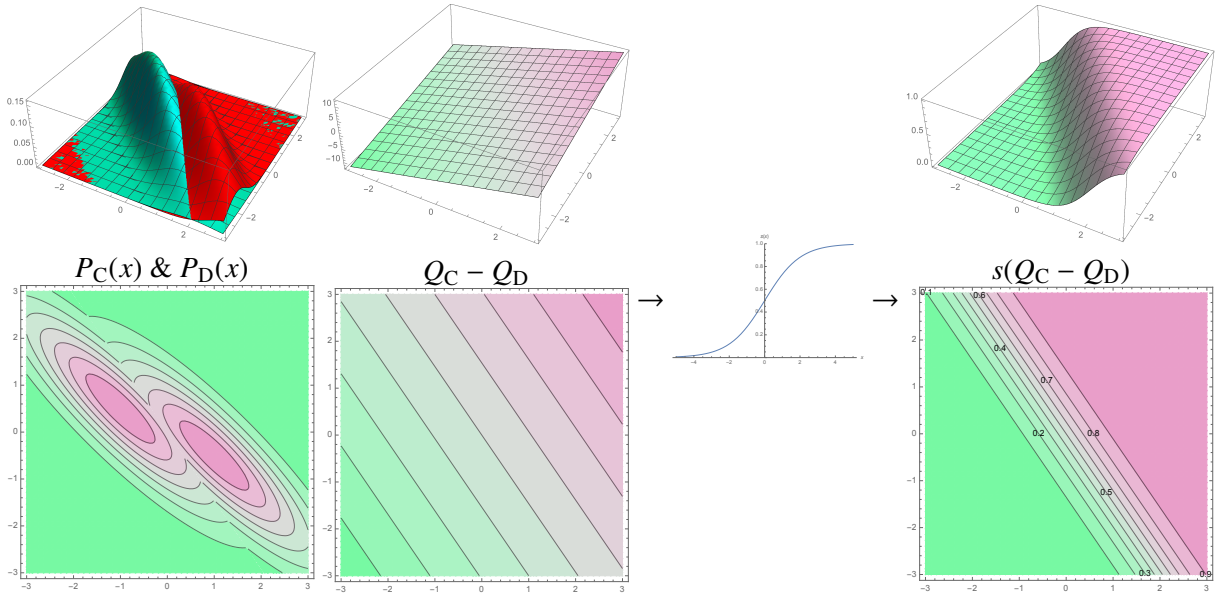
One $\hat{\Sigma}$ for all classes.
[Once again, the quadratic terms cancel each other out so the decision function is linear and the decision boundary is a hyperplane.]

$$Q_{\mathrm{C}}(x) - Q_{\mathrm{D}}(x) = \underbrace{(\mu_{\mathrm{C}} - \mu_{\mathrm{D}})^{\top} \Sigma^{-1}}_{w^{\top}} x \underbrace{- \frac{\mu_{\mathrm{C}}^{\top} \Sigma^{-1} \mu_{\mathrm{C}} - \mu_{\mathrm{D}}^{\top} \Sigma^{-1} \mu_{\mathrm{D}}}{2} + \ln \pi_{\mathrm{C}} - \ln \pi_{\mathrm{D}}}_{+\alpha}$$

Choose class C that maximizes the linear discriminant fn

$$\mu_{\mathrm{C}}^{\top} \Sigma^{-1} x - \frac{1}{2} \mu_{\mathrm{C}}^{\top} \Sigma^{-1} \mu_{\mathrm{C}} + \ln \pi_{\mathrm{C}} \qquad \text{[works for any \# of classes]}$$

2 classes: Decision boundary is $w^{\top} x + \alpha = 0$
Posterior is $P(Y = \mathrm{C} | X = x) = s(w^{\top} x + \alpha)$



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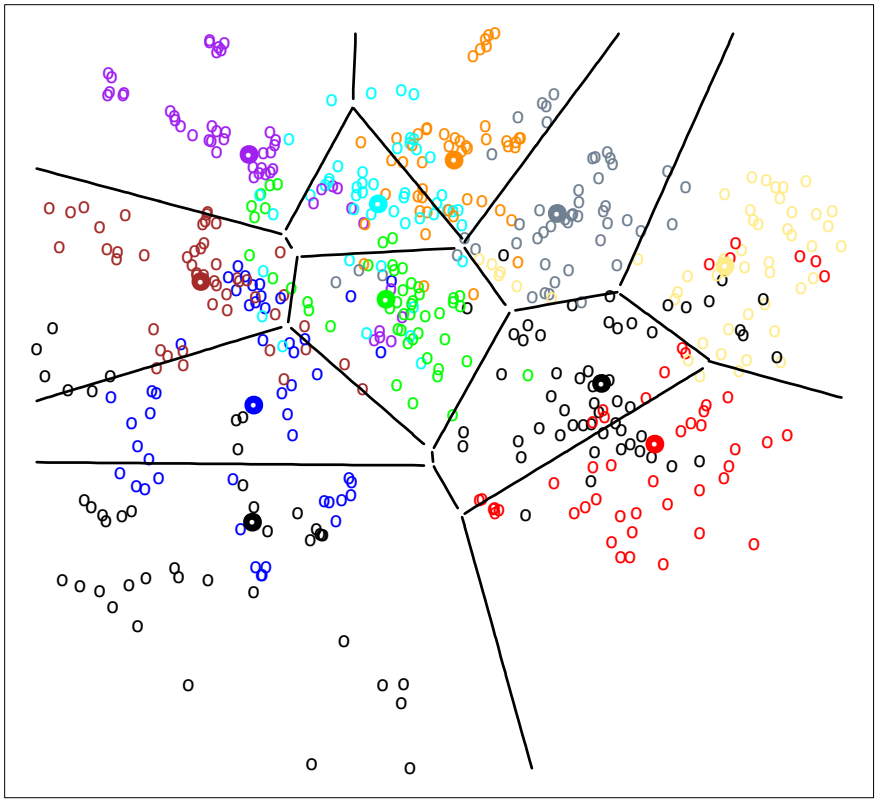
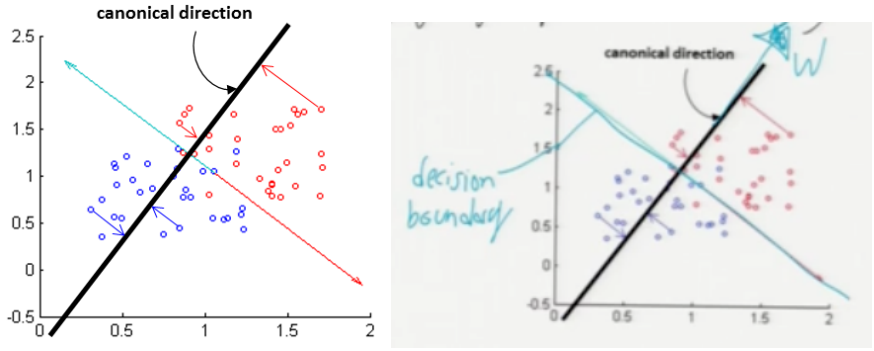
[(Show this figure on a separate "whiteboard.") In LDA, the decision boundary is always a hyperplane. Note that Mathematica messed up the top left plot a bit; there should be no red in the left corner, nor blue in the right corner.]



LDAdata.pdf (ESL, Figure 4.11) [An example of LDA with messy data. The points are not sampled from perfect Gaussians, but LDA still works reasonably well.]

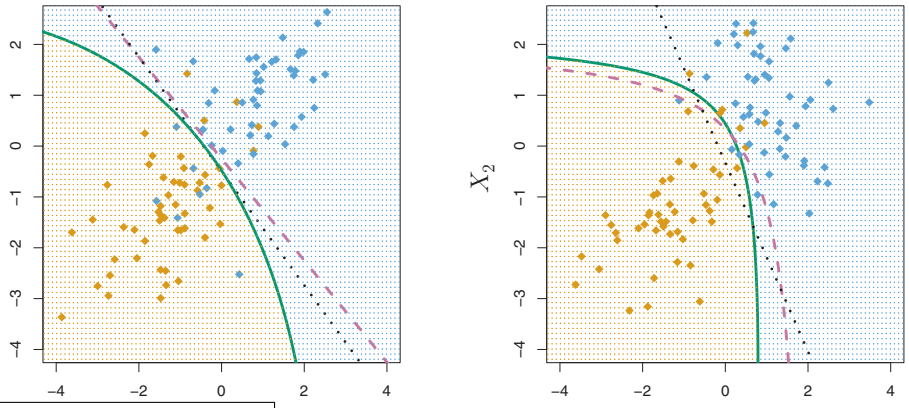
Notes:

– LDA often interpreted as projecting points onto normal w; cutting the line in half.



project.png

– For 2 classes,
  – LDA has $d + 1$ parameters (w, α);
  – QDA has $\frac{d(d+3)}{2} + 1$ params;
  – QDA more likely to overfit. [The danger is much bigger when the dimension d is large.]



ldaqda.pdf (ISL, Figure 4.9) [In these examples, the Bayes optimal decision boundary is purple (and dashed), the QDA decision boundary is green, the LDA decision boundary is black (and dotted). When the optimal boundary is linear, as at left, LDA gives a more stable fit whereas QDA may overfit. When the optimal boundary is curved, as at right, QDA better fits it.]

– With features, LDA can give nonlinear boundaries; QDA nonquadratic.
– We don't get **true** optimum Bayes classifier
  – estimate distributions from finite data
  – real-world data not perfectly Gaussian
– Changing priors or loss = adding constants to discriminant fns
  [So it's very easy. In the 2-class case, it's equivalent to changing the isovalue . . .]
– Posterior gives decision boundaries for 10% probability, 50%, 90%, etc.
  – choosing isovalue = probability p is same as choosing asymmetrical loss p for false positive, $1 - p$ for false negative; OR as choosing $\pi_C = 1 - p$, $\pi_D = p$.

[LDA & QDA are the best method in practice for many applications. In the STATLOG project, either LDA or QDA were in the top three classifiers for 10 out of 22 datasets. But it's not because all those datasets are Gaussian. LDA & QDA work well when the data can only support simple decision boundaries such as linear or quadratic, because Gaussian models provide stable estimates. See ESL, Section 4.3]

Some Terms

Let X be $n \times d$ design matrix of sample pts
Each row i of X is a sample pt $X_i^\top$.

[Now I'm using capital X as a matrix instead of a random variable vector. I'm treating X_i as a column vector to match the standard convention for multivariate distributions like the Gaussian, but $X_i^\top$ is a row of X.]

centering X: subtracting μ from each row of X. $\quad X \to \dot{X}$
[μ is the mean of all the rows of X. Now the mean of all the rows of $\dot{X}$ is zero.]

Let R be uniform distribution on sample pts. Sample covariance matrix is

$$\text{Var}(R) = \frac{1}{n}\dot{X}^\top \dot{X}$$

[This is the simplest way to remember how to compute a covariance matrix for QDA. Imagine splitting the design matrix into several smaller design matrices, one for each class C; then you have $\hat{\Sigma}_C = \frac{1}{n_C}\dot{X}_C^\top \dot{X}_C$.]

[When we have points from an anisotropic Gaussian distribution, sometimes it's useful to perform a linear transformation that maps them to an axis-aligned distribution, or maybe even to an isotropic distribution. Recall that $\Sigma^{-1/2}$ maps ellipsoids to spheres.]

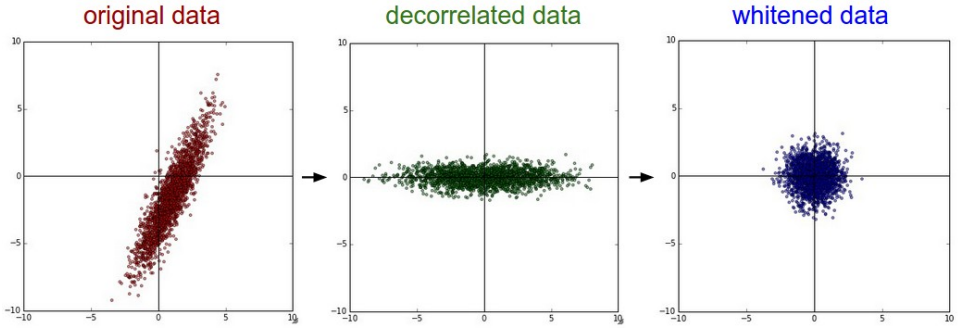
decorrelating $\dot{X}$: applying transform $Z = \dot{X}V$, where $\text{Var}(R) = V\Lambda V^\top$
[transforms the sample points to the eigenvector coordinate system]

Then $\text{Var}(Z) = \Lambda$. $\quad$ [Z has diagonal covariance. If $X_i \sim \mathcal{N}(\mu, \Sigma)$, then approximately, $Z_i \sim \mathcal{N}(0, \Lambda)$.]

sphering $\dot{X}$: applying transform $W = \dot{X}\,\text{Var}(R)^{-1/2}$

whitening X: centering + sphering, $X \to W$

Then W has covariance matrix I. $\quad$ [If $X_i \sim \mathcal{N}(\mu, \Sigma)$, then approximately, $W_i \sim \mathcal{N}(0, I)$.]



whiten.jpg

[Whitening input data is often used with other machine learning algorithms, like SVMs. The idea is that some features may be much bigger than others—for instance, because they're measured in different units. SVMs penalize violations by large features more heavily than they penalize small features. Whitening the data before you run an SVM puts the features on an equal basis. Once nice thing about discriminant analysis is that whitening is built in.]

[Incidentally, what we've done here—computing a sample covariance matrix and its eigenvectors/values—is about 75% of an important unsupervised learning method called principal components analysis, or PCA, which we'll learn later in the semester.]