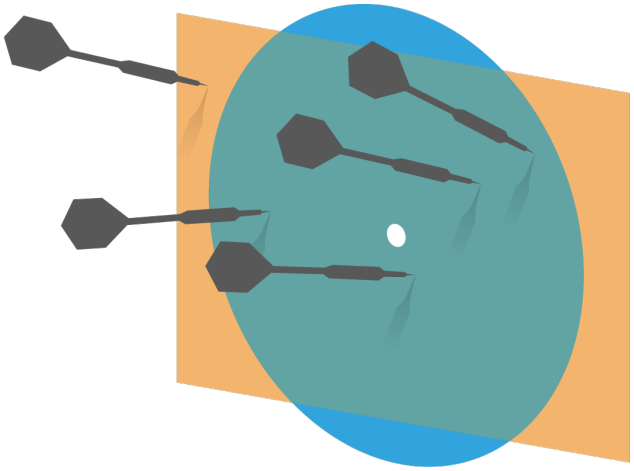
Probability and Statistics for Computer Science



Credit: wikipedia

"…many problems are naturally classification problems"---Prof. Forsyth

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 10.29.2021

Last time

- Review of Covariance matrix
- Dimension Reduction
- Principal Component Analysis
- Examples of PCA

Objectives

- Principal Component Analysis (II)
- Introduction to classification

The Mean square error of the projection

- The mean square error is the sum of the smallest d-s eigenvalues in $\mathbf{\Lambda}$

$$\frac{1}{N-1}\sum_i \|r_i - p_i\|^2 = \frac{1}{N-1}\sum_i \sum_{j=s+1}^{d} (r_i^{(j)})^2$$

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$$= \sum_{j=s+1}^{d} var(r_i^{(j)})$$

The Mean square error of the projection

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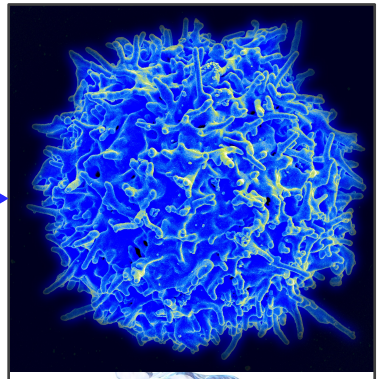
$$= \sum_{j=s+1}^{d} var(r_i^{(j)})$$

$$= \sum_{j=s+1}^{d} \lambda_j$$

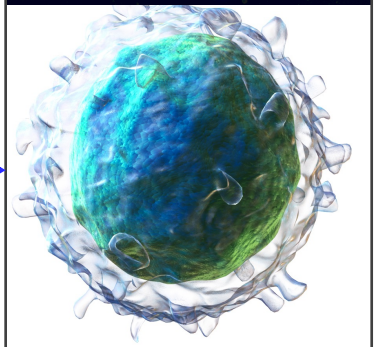
Examples: Immune Cell Data

- There are 38816 white blood immune cells from a mouse sample
- Each immune cell has 40+ features/components
- Four features are used as illustration.
- There are at least 3 cell types involved

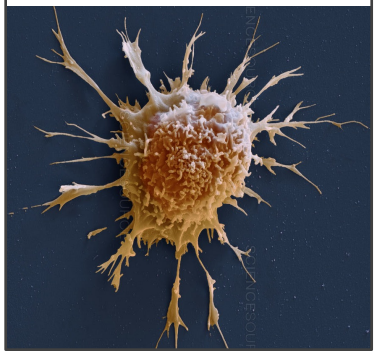
T cells



B cells



Natural killer cells



Scatter matrix of Immune Cells

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- Each immune cell has 40+ features/components
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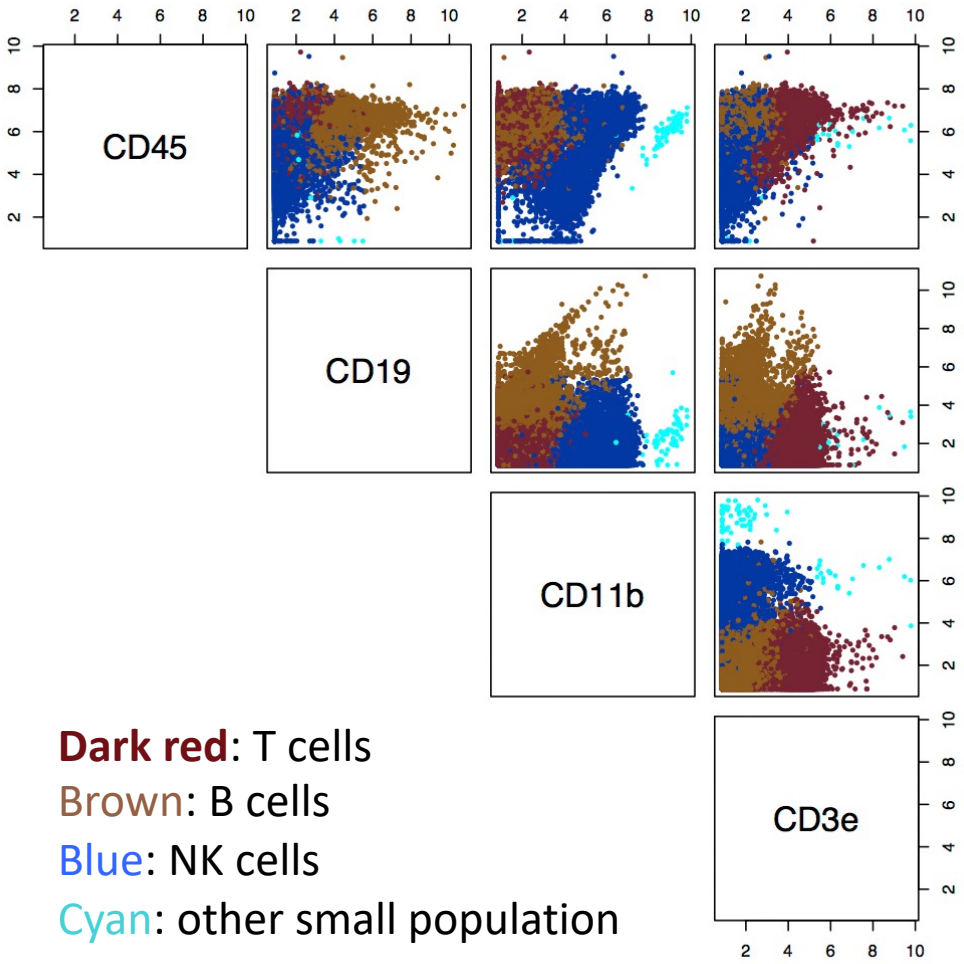
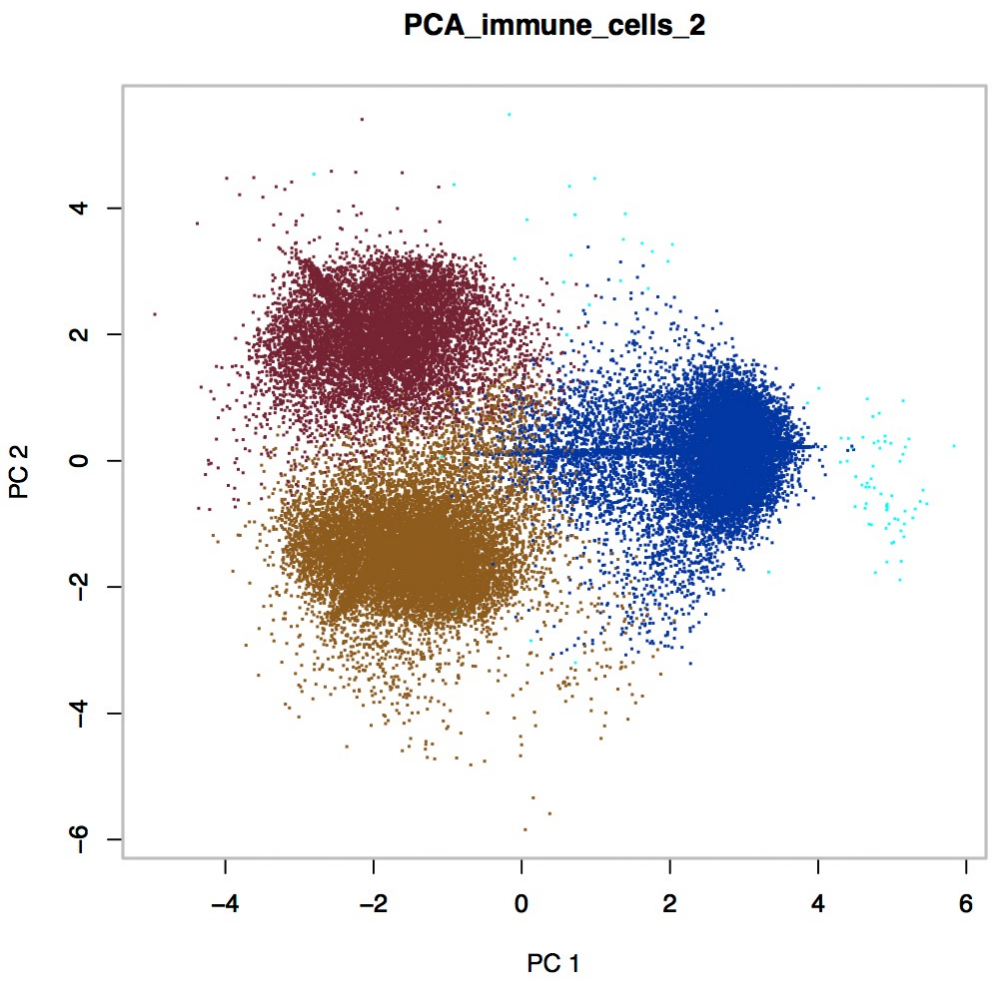


Dark red: T cells
Brown: B cells
Blue: NK cells
Cyan: other small population

PCA of Immune Cells

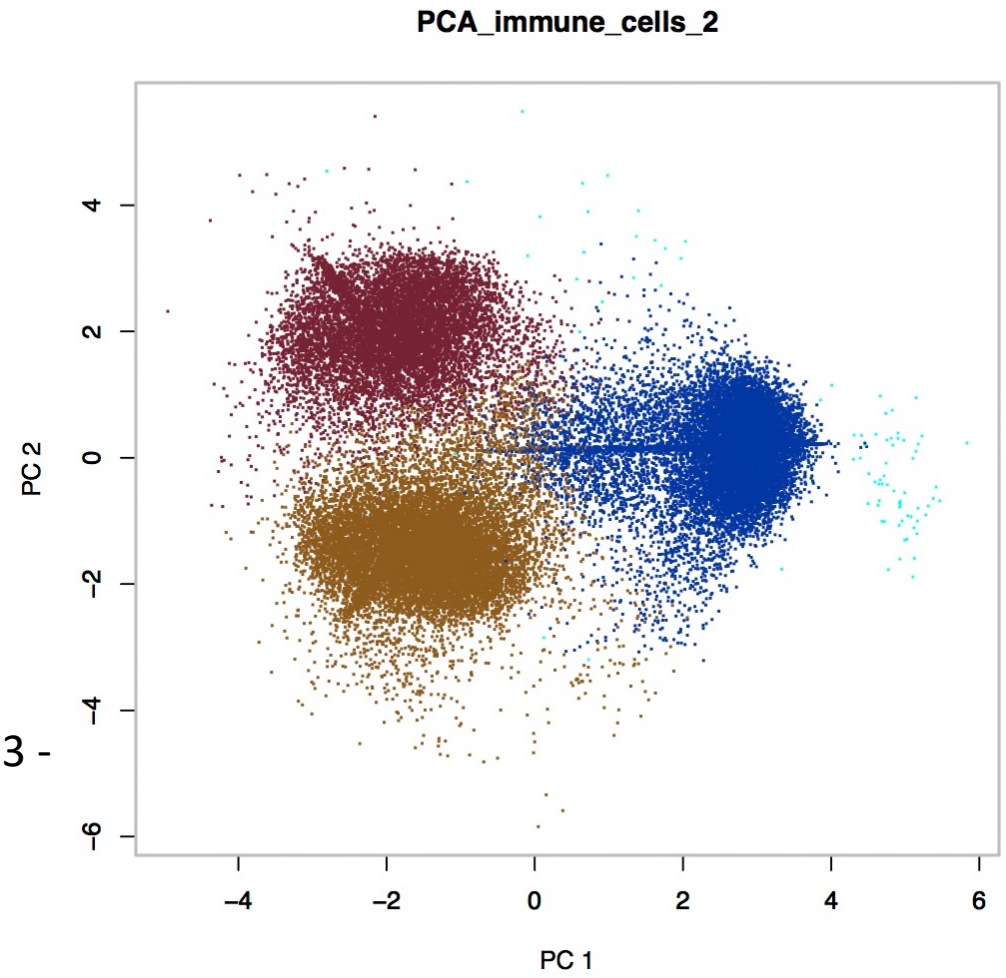
> res1
$values Eigenvalues
[1] 4.7642829 2.1486896 1.3730662
0.4968255

Eigenvectors
$vectors
[,1] [,2] [,3] [,4]
[1,] 0.2476698 0.00801294 -0.6822740
0.6878210
[2,] 0.3389872 -0.72010997 -0.3691532 -
0.4798492
[3,] -0.8298232 0.01550840 -0.5156117 -
0.2128324
[4,] 0.3676152 0.69364033 -0.3638306 -
0.5013477



New coordinates in PCA

```
> head(new_coord_t)
        PC1        PC2        PC3        PC4
1  3.6739228  0.1127233 -1.32744266
0.61005994
2 -0.9255199 -2.1016573 -0.80762548 -
0.29104900
3  3.1150230  0.3526459 -0.83994064
0.46074556
4  3.1801414  0.5679807 -0.07097689
0.01539266
5  2.7972723 -0.1073053 -0.39168826 -
0.03981390
6  3.3012610  0.1979659  0.17965423
0.45373049CD3e  -0.3676152  0.69364033 -
0.3638306 -0.5013477 [4,]  0.3676152
0.69364033 -0.3638306 -0.5013477
```



What is the percentage of variance that PC1 covers?

Given the eigenvalues: 4.7642829 2.1486896 1.3730662 0.4968255, what is the percentage that PC1 covers?

A. 54%
B. 16%
C. 25%

Reconstructing the data

- Given the projected data $\boldsymbol{p}_{d\times n}$ and mean({x}), we can approximately reconstruct the original data

$$\widehat{\boldsymbol{D}} = \boldsymbol{U}\boldsymbol{p} + mean(\{\boldsymbol{x}\})$$

- Each reconstructed data item $\widehat{\boldsymbol{D}_i}$ is a linear combination of the columns of $\boldsymbol{U}$ weighted by $\boldsymbol{p}_i$

- The columns of $\boldsymbol{U}$ are the normalized eigenvectors of the Covmat({x}) and are called the **principal components** of the data {x}

End-to-end mean square error

- Each $\boldsymbol{x}_i$ becomes $\boldsymbol{r}_i$ by translation and rotation
- Each $\boldsymbol{p}_i$ becomes $\widehat{\boldsymbol{x}}_i$ by the opposite rotation and translation
- Therefore the end to end mean square error is:

$$\frac{1}{N-1}\sum_i \|\widehat{\boldsymbol{x}}_i - \boldsymbol{x}_i\|^2 = \frac{1}{N-1}\sum_i \|\boldsymbol{r}_i - \boldsymbol{p}_i\|^2 = \sum_{j=s+1}^{d} \lambda_j$$

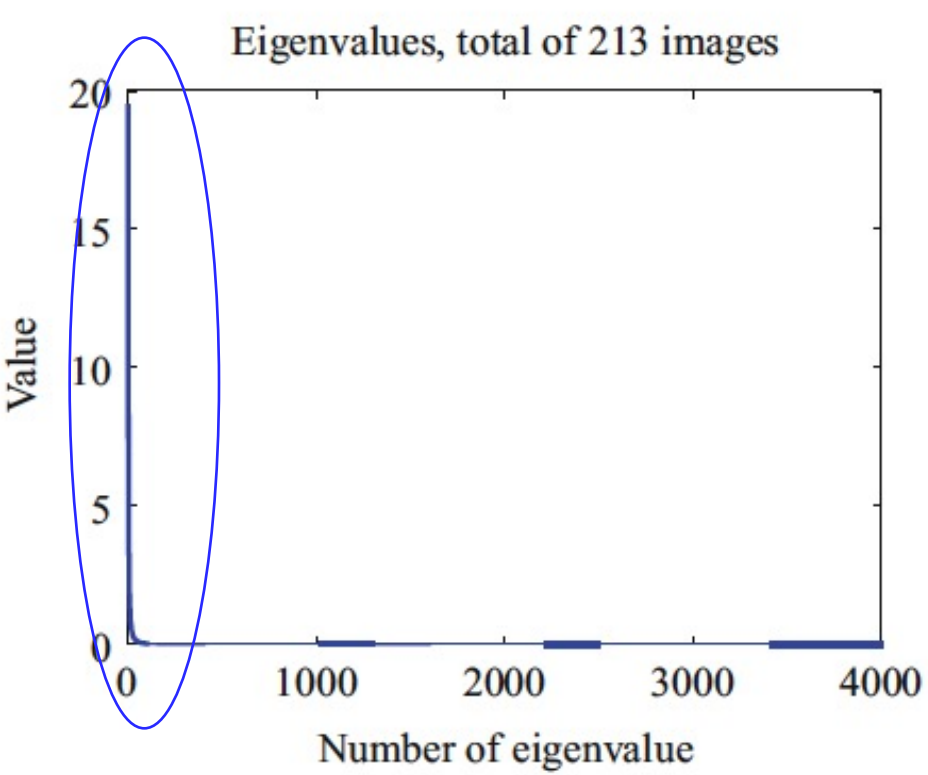
- $\lambda_{s+1}, \ldots, \lambda_d$ are the smallest d-s eigenvalues of the Covmat({x})

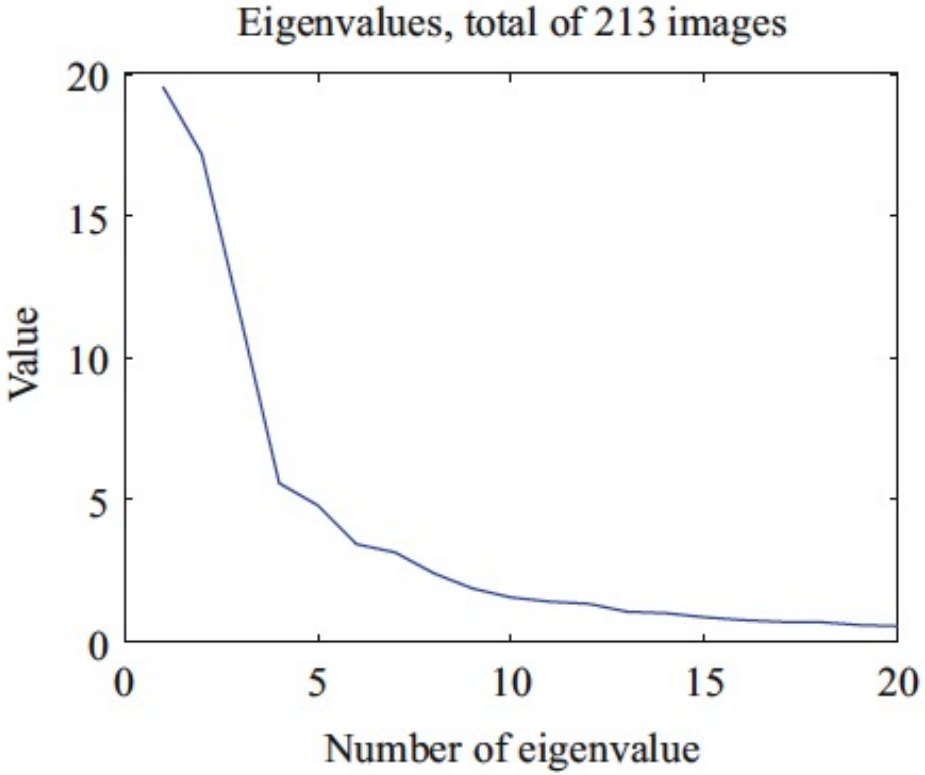
PCA: Human face data

- The dataset consists of 213 images
- Each image is grayscale and has 64 by 64 resolution
- We can treat each image as a vector with dimension d = 4096

Credit: Prof. Forsyth

How quickly the eigenvalues decrease?





Credit: Prof. Forsyth

What do the principal components of the images look like?

Mean image

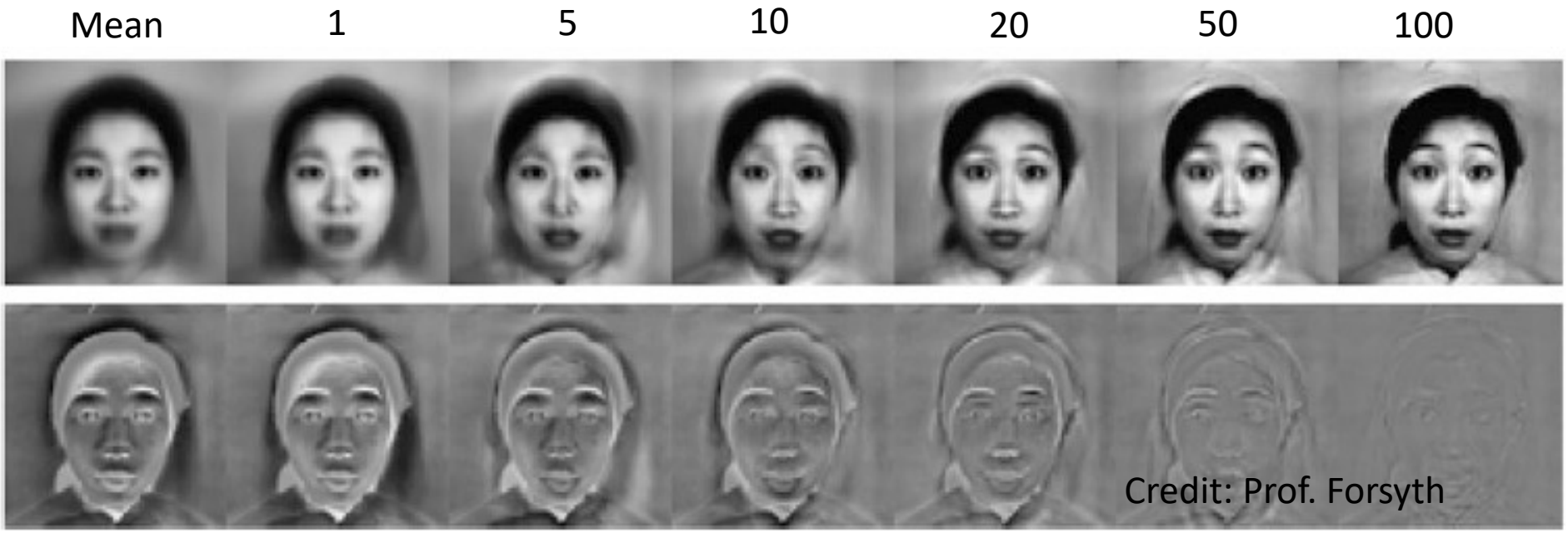
The first 16 principal components arranged into images

Credit: Prof. Forsyth

Reconstruction of the image

The original

1st row show the reconstructions using some number of principal components
2nd row show the corresponding errors



Q. Which are true?

A . PCA allows us to project data to the direction along which the data has the biggest variance

B. PCA allows us to compress data

C. PCA uses linear transformation to show patterns of data

D. PCA allows us to visualize data in lower dimensions

E. All of the above

Q. Which of these is NOT true?

A. The eigenvectors of covariance can have opposite signs and it won't affect the reconstruction

B. The PCA analysis in some statistical program returns standard deviation instead of variance

C. It doesn't matter how you store the data in matrix

Demo: PCA of Immune Cell Data

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- There are at least 3 cell types involved

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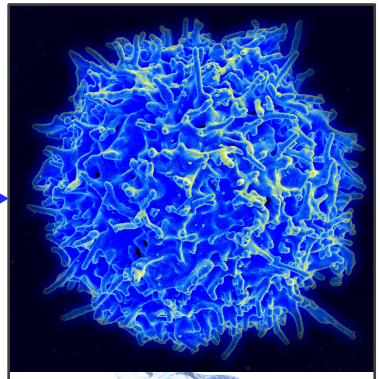

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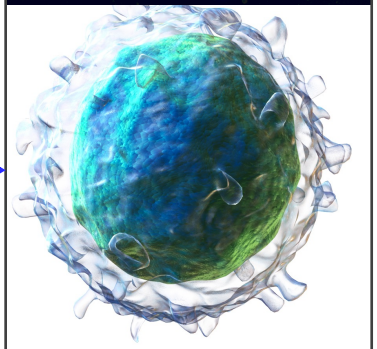
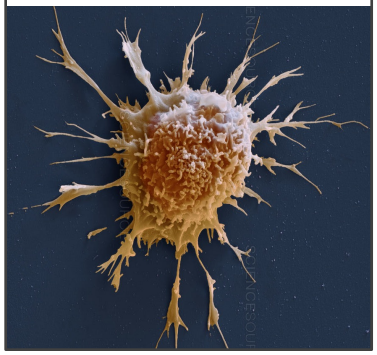


Natural killer cells



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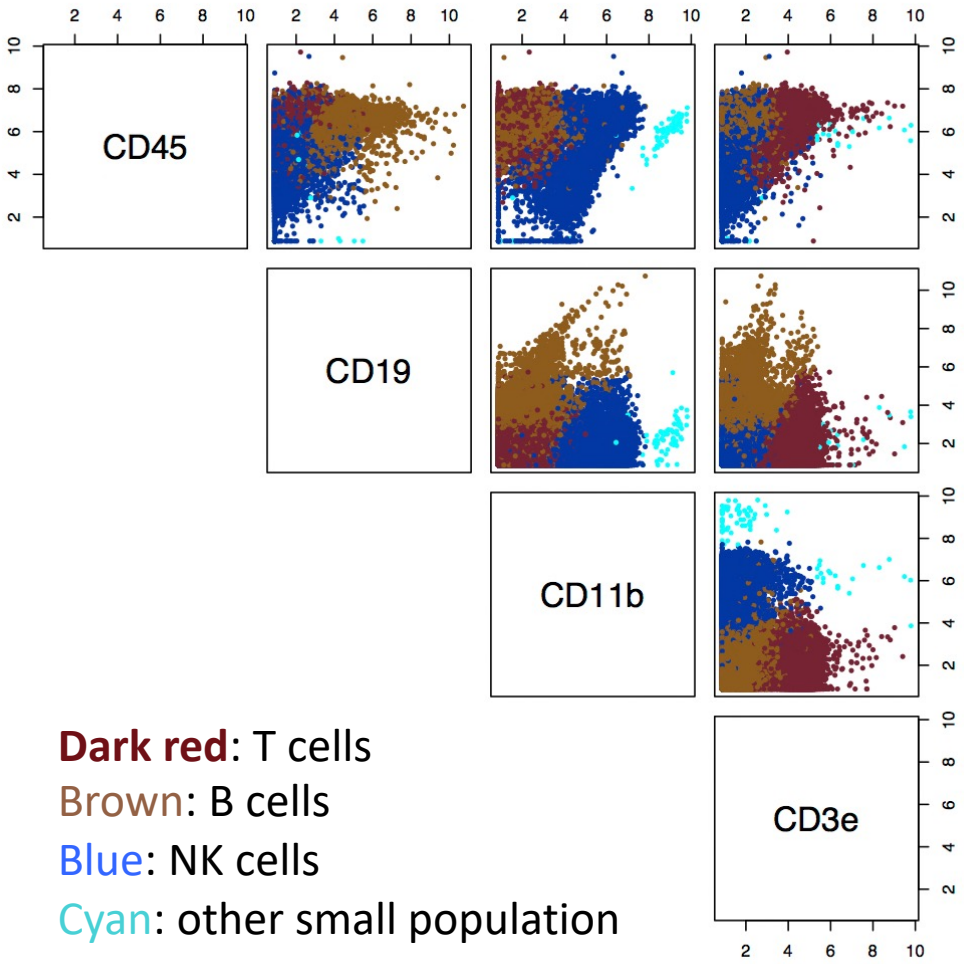

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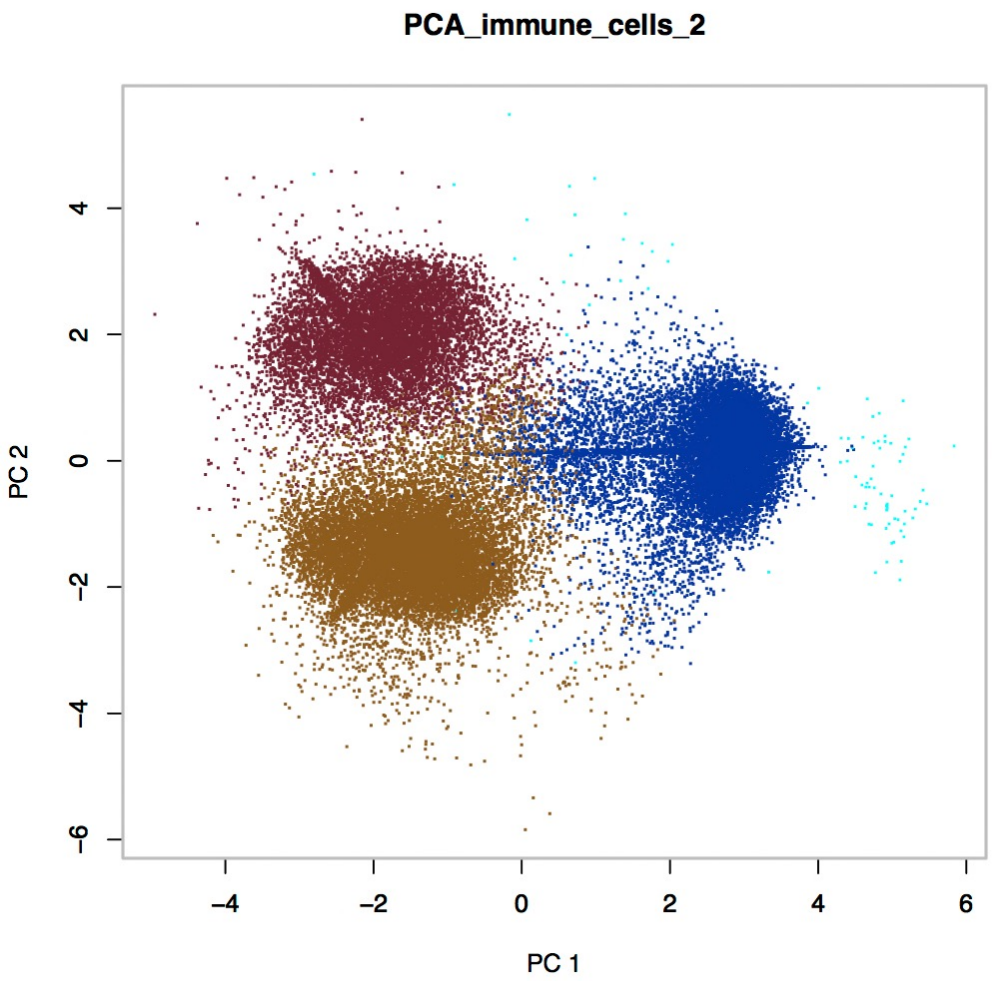
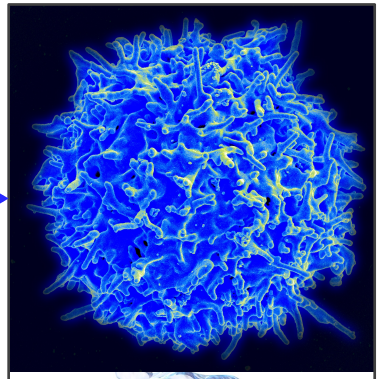


More features used

- There are 38816 white blood immune cells from a mouse sample
- Each immune cell has **42 features**/components
- There are at least 3 cell types involved

T cells



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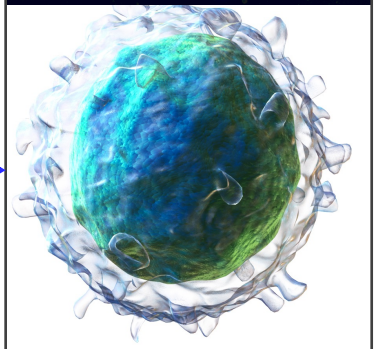

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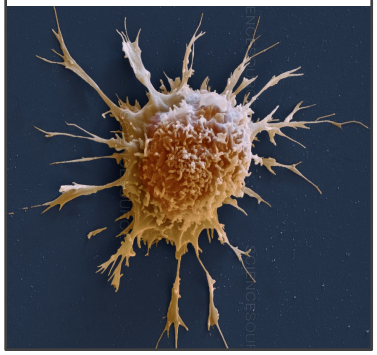
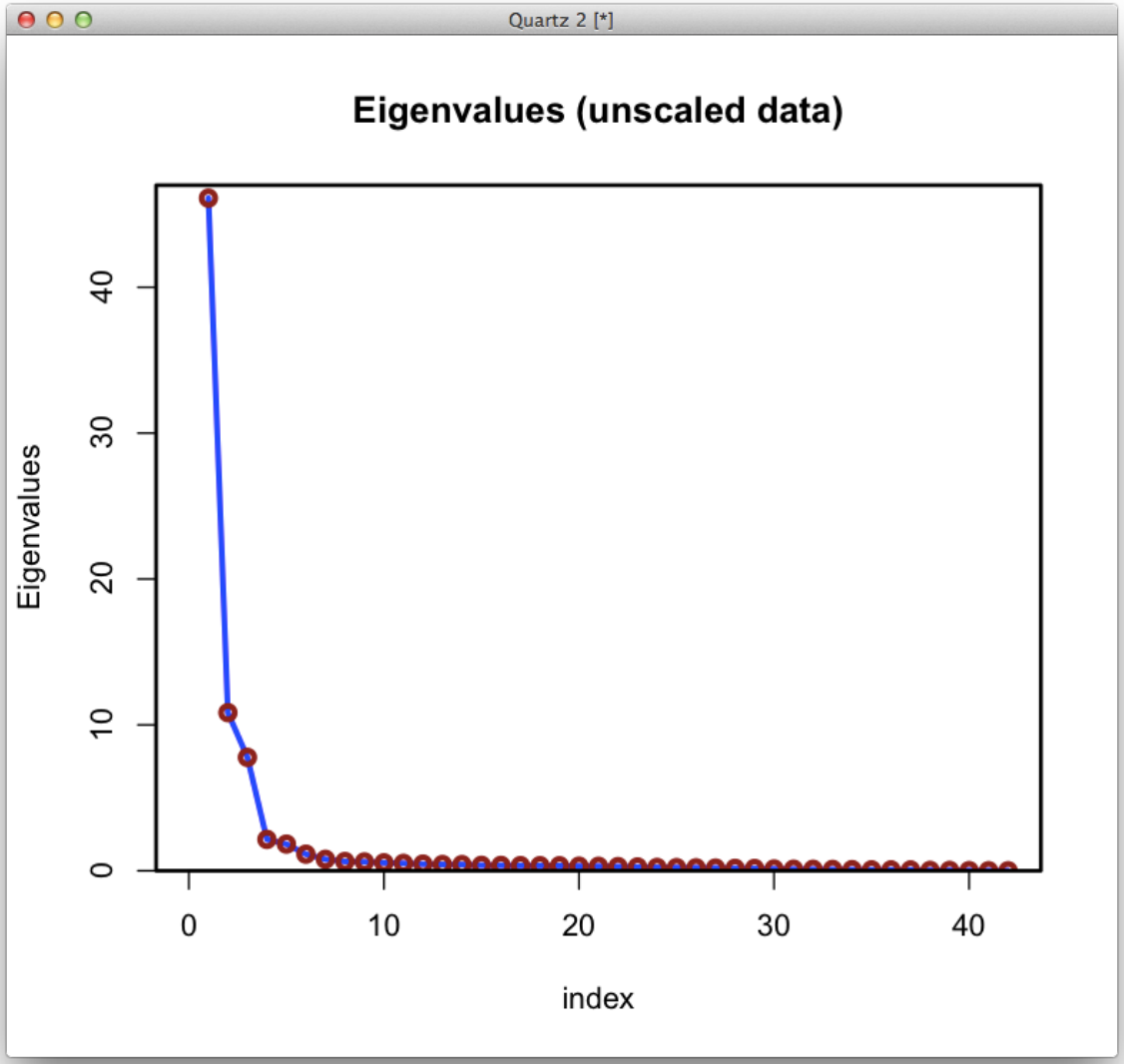
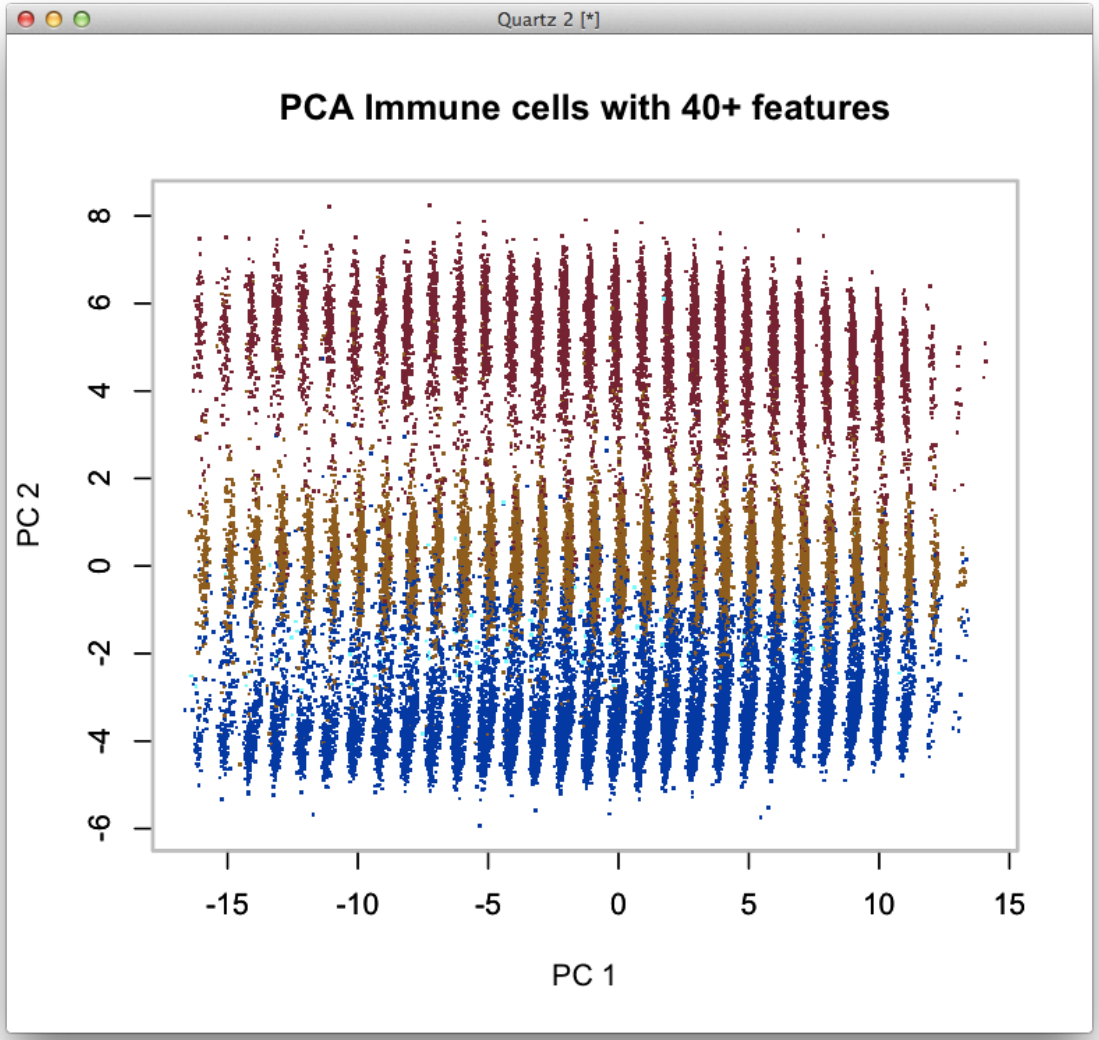


Eigenvalues of the covariance matrix

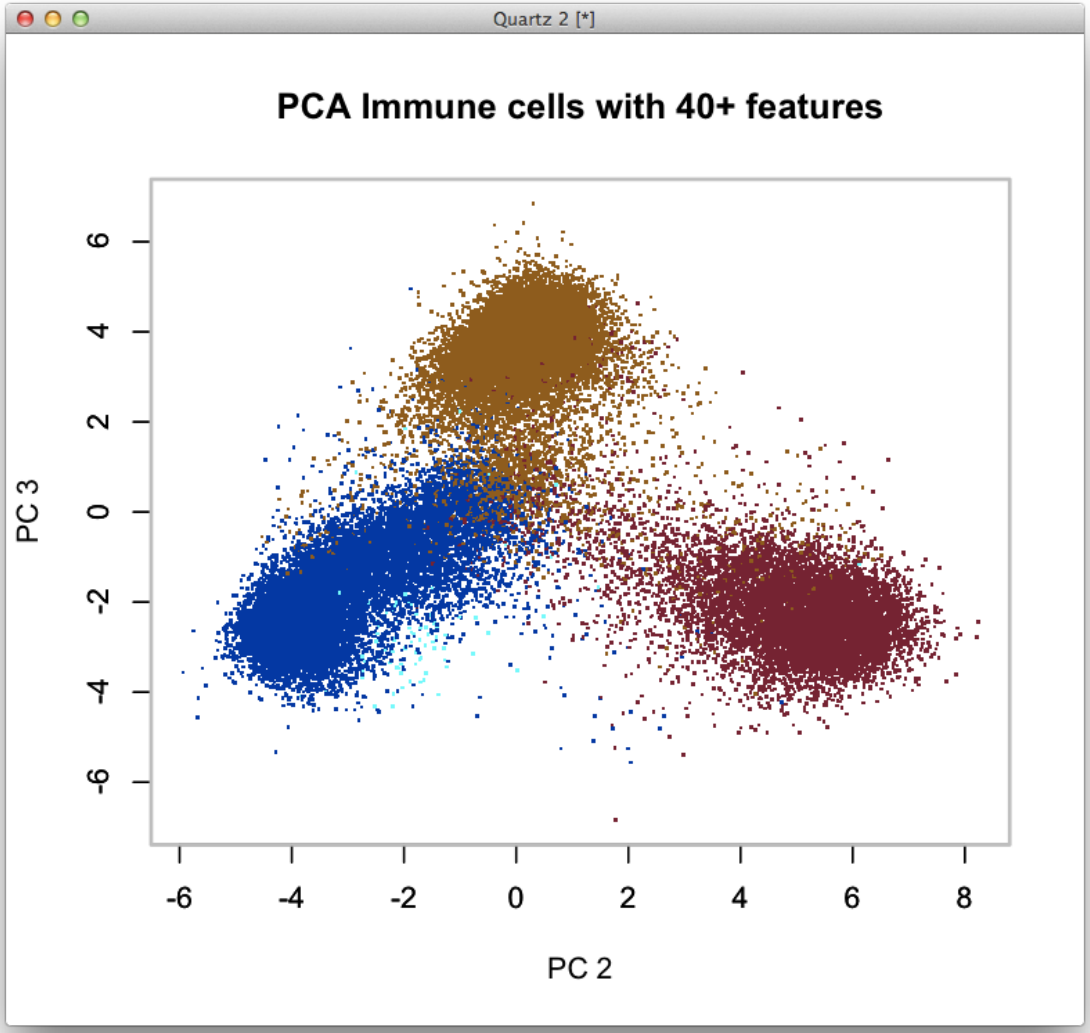


Large variance doesn't mean important pattern

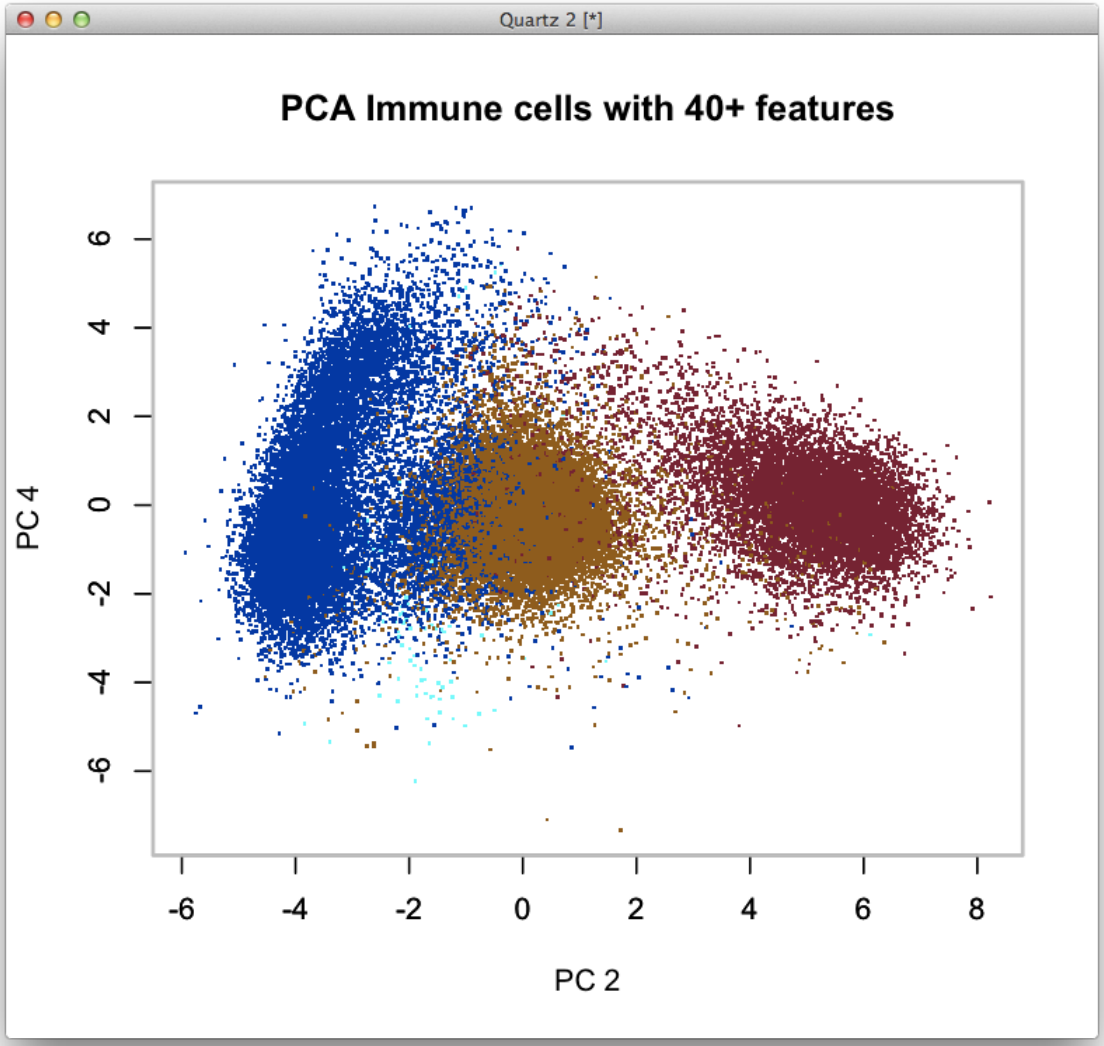
Principal component 1 is just cell length



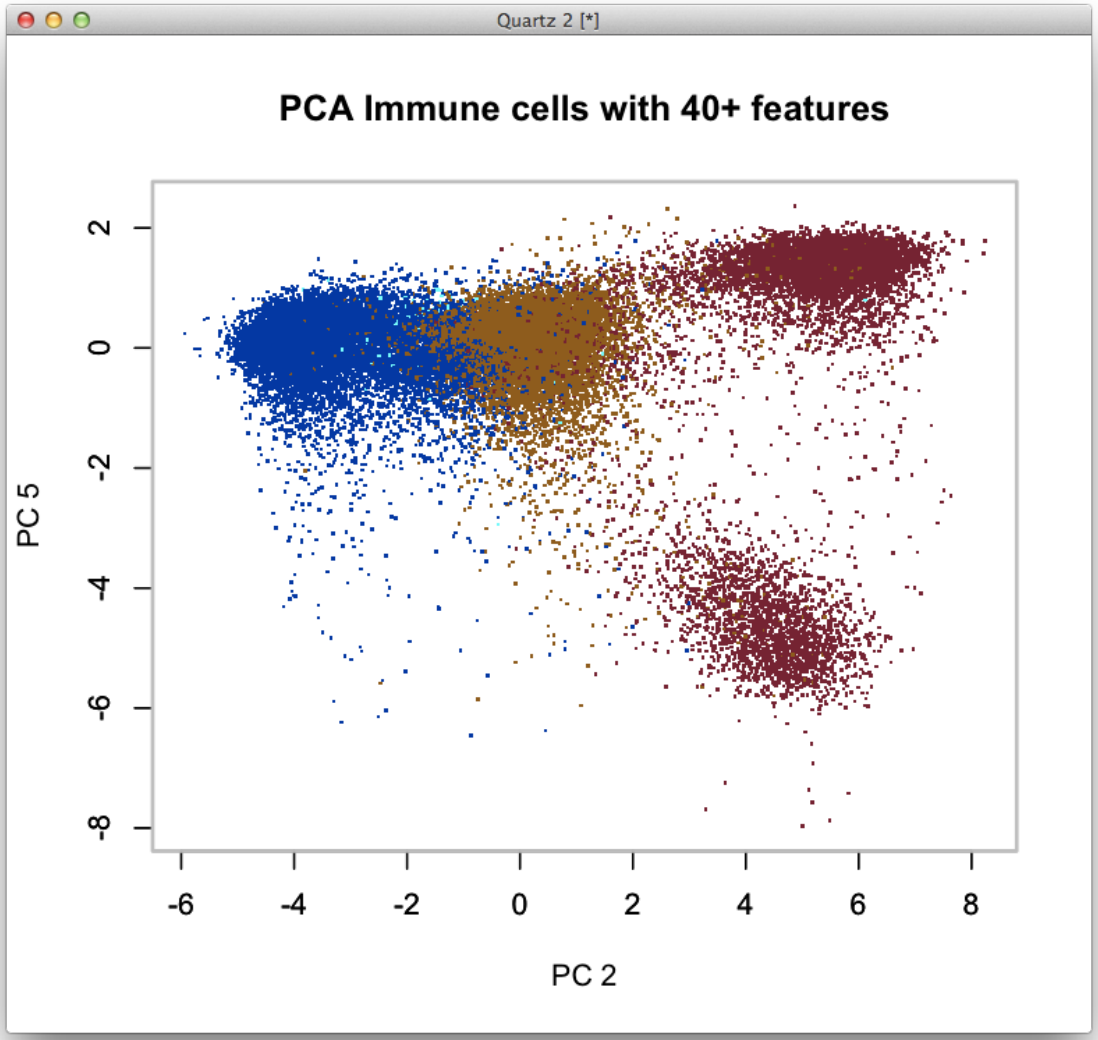
Principal component 2 and 3 show different cell types



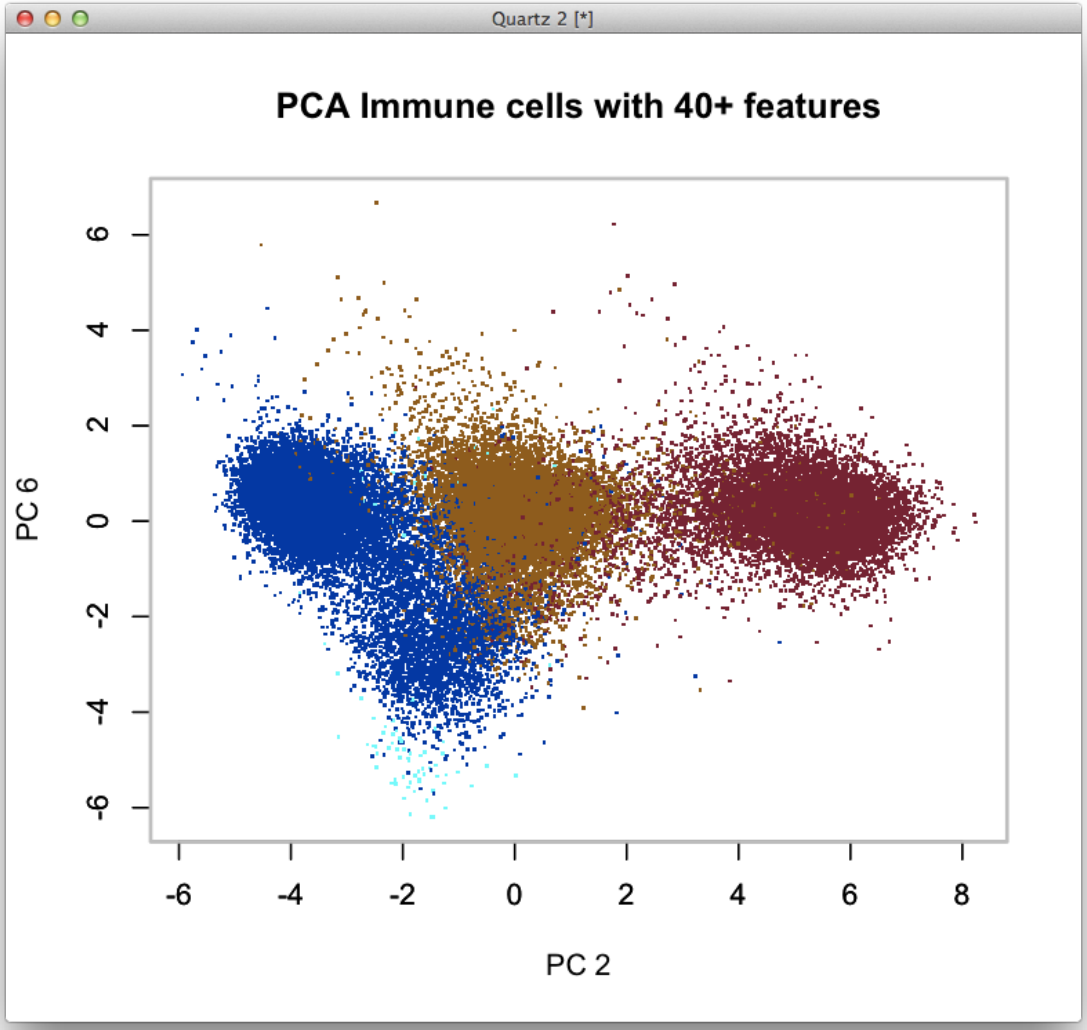
Principal component 4 is not very informative



Principal component 5 is interesting



Principal component 6 is interesting

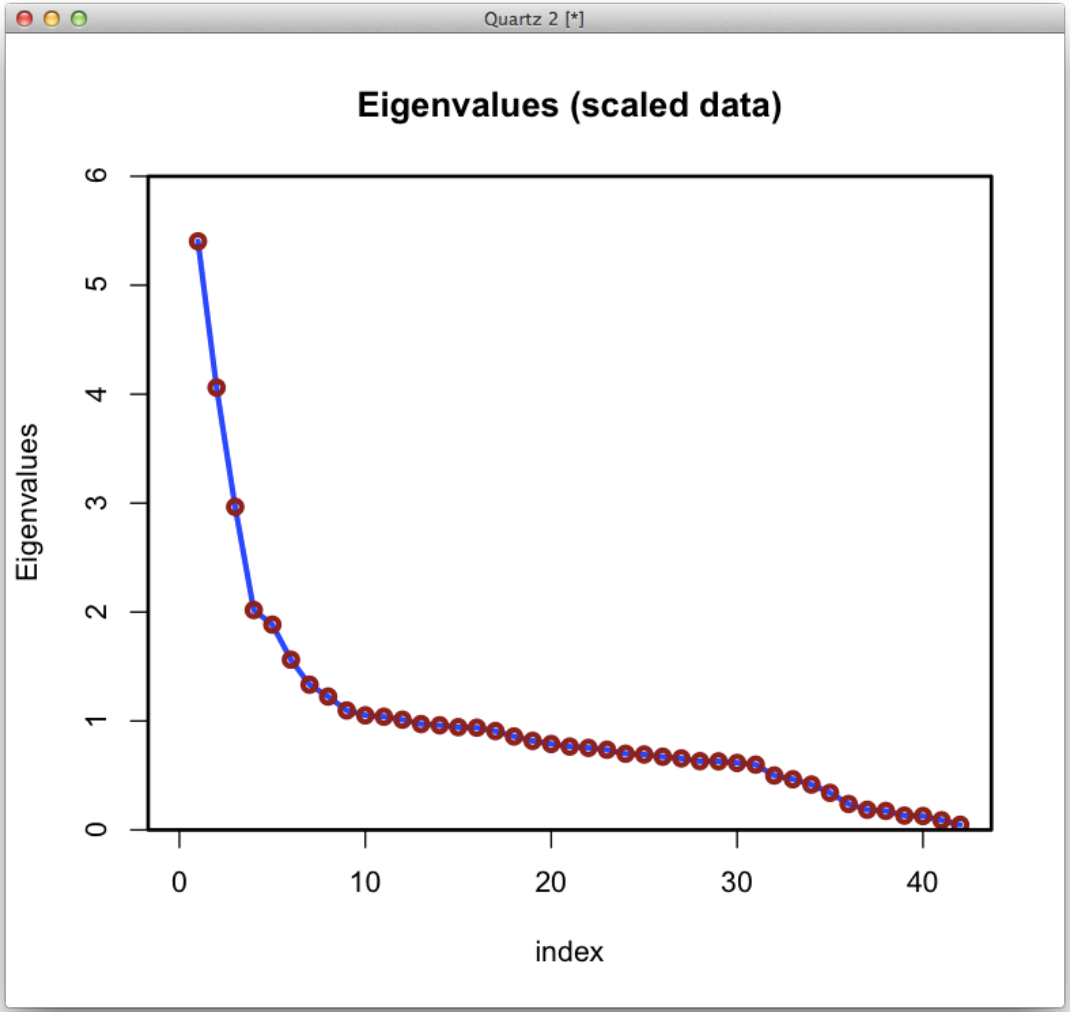


Scaling the data or not in PCA

- Sometimes we need to scale the data for **each** feature have very different value range.
- After scaling the eigenvalues may change significantly.
- Data needs to be investigated case by case

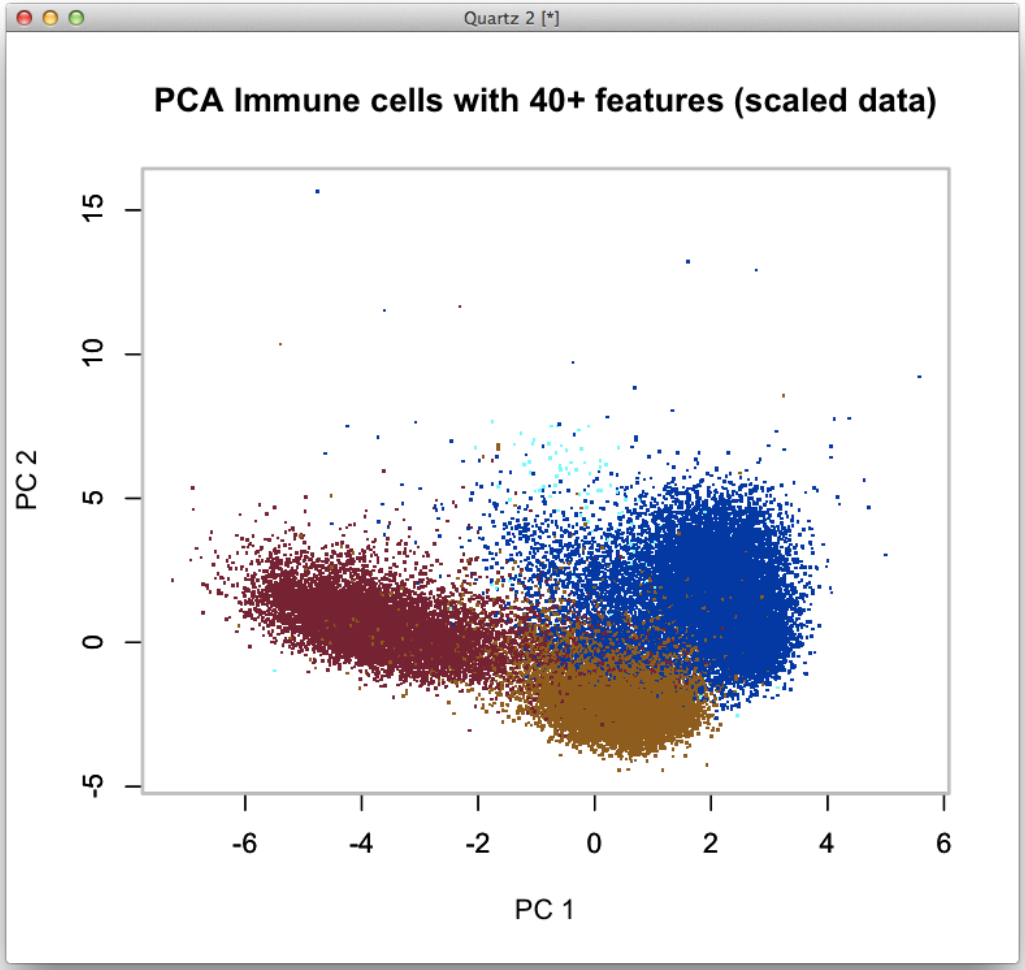
Eigenvalues of the covariance matrix (scaled data)

Eigenvalues do not drop off very quickly



Principal component 1 & 2 (scaled data)

Even the first 2 PCs don't separate the different types of cell very well



Q. Which of these are true?

A. Feature selection should be conducted with domain knowledge

B. Important feature may not show big variance

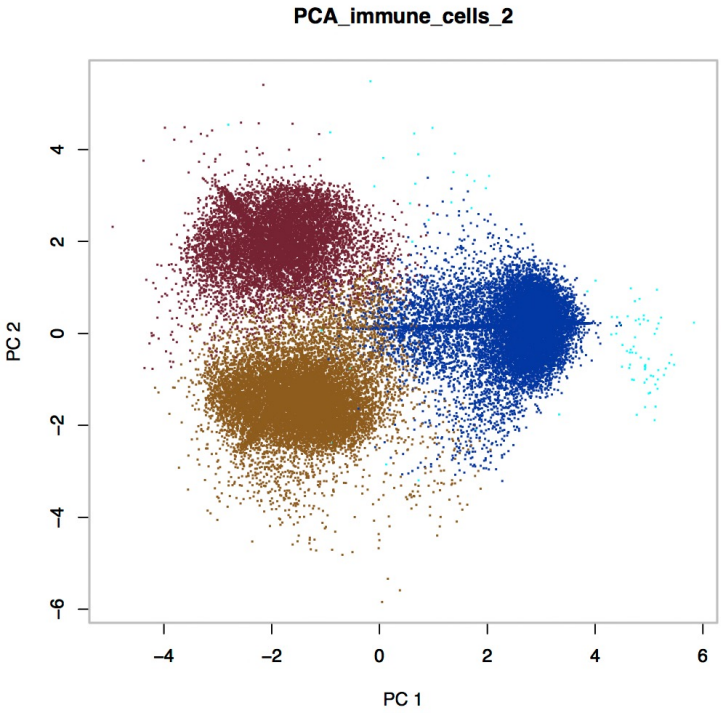
C. Scaling doesn’t change eigenvalues of covariance matrix

D. A & B

Learning to classify

- Given a set of feature vectors x_i, where each has a class label y_i, we want to train a classifier that maps unlabeled data with the same features to its label.

CD45	CD19	CD11b	CD3e	Type
6.59564671	1.297765164	7.073280884	1.155202366	1
6.742586812	4.692018952	3.145976639	1.572686963	4
6.300680301	1.20613983	6.393630905	1.424572629	2
5.455310882	0.958837541	6.149306002	1.493503124	1
5.725565772	1.719787885	5.998232014	1.310208305	1
5.552847151	0.881373587	6.02155471	0.881373587	3



Binary classifiers

- A binary classifier maps each feature vector to one of two classes.
- For example, you can train the classifier to:
  - Predict a gain or loss of an investment
  - Predict if a gene is beneficial to survival or not
  - …

Multiclass classifiers

- A multiclass classifier maps each feature vector to one of three or more classes.
- For example, you can train the classifier to:
  - Predict the cell type given cells' measurement
  - Predict if an image is showing tree, or flower or car, etc
  - ...

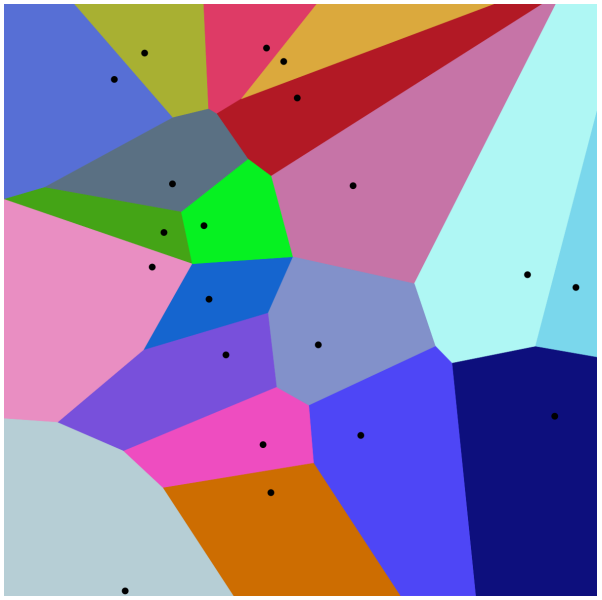
Given our knowledge of probability and statistics, can you think of any classifiers?

Given our knowledge of probability and statistics, can you think of any classifiers?

- We will cover classifiers such as nearest neighbor, decision tree, random forest, Naïve Bayesian and support vector machine.

Nearest neighbors classifier

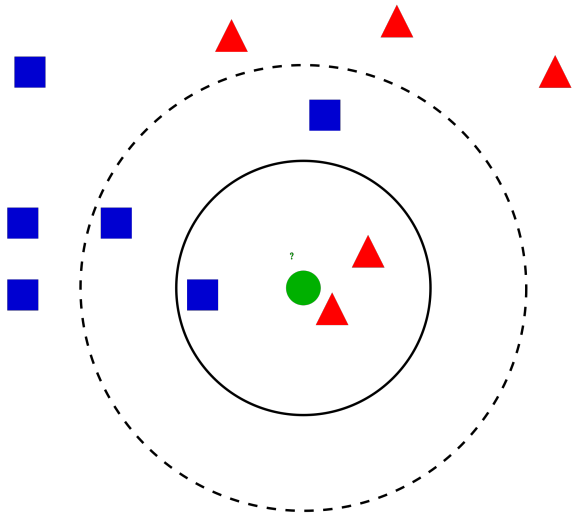
- Given an unlabeled feature vector
  - Calculate the distance from **x**
  - Find the closest labeled $\mathbf{x}_i$
  - Assign the same label to **x**
- Practical issues
  - We need a distance metric
  - We should first standardize the data
  - Classification may be less effective for very high dimensions



Source: wikipedia

Variants of nearest neighbors classifier

- In k-nearest neighbors, the classifier:
  - Looks at the k nearest labeled feature vectors $\mathbf{x}_i$
  - Assigns a label to **x** based on a majority vote



- In (k, ℓ)-nearest neighbors, the classifier:
  - Looks at the k nearest labeled feature vectors
  - Assigns a label to **x** if at least ℓ of them agree on the classification

How do we know if our classifier is good?

- We want the classifier to avoid some mistakes on unlabeled data that we will see in run time.
- **Problem 1**: some mistakes may be more costly than others

  We can tabulate the types of error and define a loss function
- **Problem 2**: It's hard to know the true labels of the run-time data

  We must separate the labeled data into a training set and test/validation set

Performance of a binary classifier

- A binary classifier can make two types of errors
  - False positive (**FP**)
  - False negative (**FN**)
- Sometimes one type of error is more costly
  - Drug effect test
  - Crime detection
- We can tabulate the performance in a class confusion matrix

Actual	Predicted		
		Negative	Positive
	Negative	True Negative	False Positive
	Positive	False Negative	True Positive

TN	FP
15	3
7	25
FN	TP

Performance of a binary classifier

- A loss function assigns costs to mistakes
- The 0-1 loss function treats FPs and FNs the same
  - Assigns loss 1 to every mistake
  - Assigns loss 0 to every correct decision

Actual	Predicted		
		Negative	Positive
	Negative	True Negative	False Positive
	Positive	False Negative	True Positive

- Under the 0-1 loss function
  - accuracy= $\frac{TP+TN}{TP+TN+FP+FN}$
- The baseline is 50% which we get by random decision.

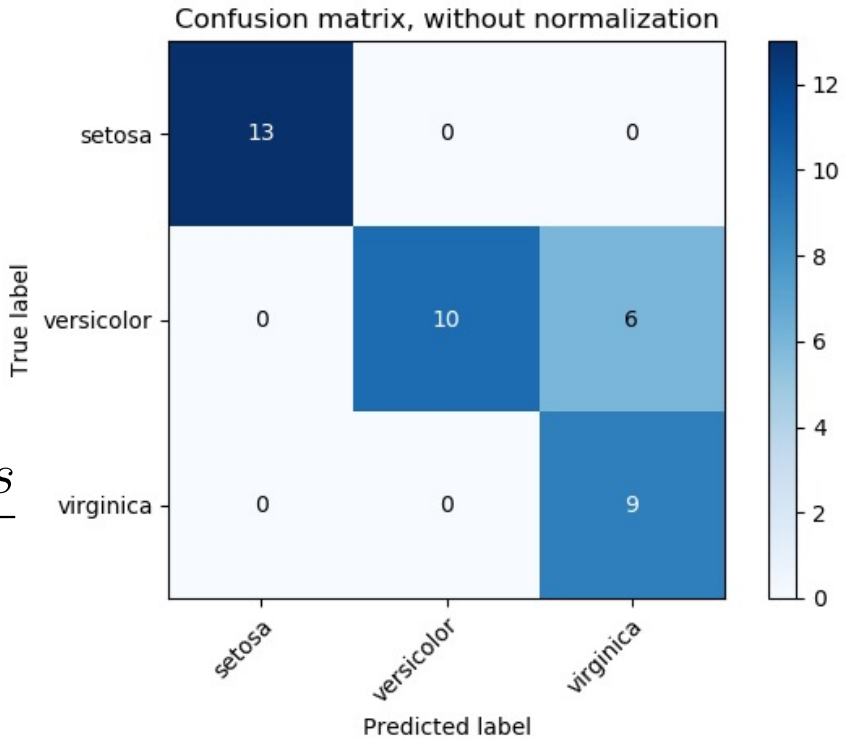
Performance of a multiclass classifier

- Assuming there are **c** classes:
- The class confusion matrix is c × c
- Under the 0-1 loss function

accuracy= $\frac{sum\ of\ diagonal\ terms}{sum\ of\ all\ terms}$

ie. in the right example, accuracy = 32/38=84%

- The baseline accuracy is 1/c.



Source: scikit-learn

Training set vs. validation/test set

- We expect a classifier to perform worse on run-time data
  - Sometimes it will perform much worse: an **overfitting** in training
  - An extreme case is: the classifier correctly labeled 100% when the input is in the training set, but otherwise makes a random guess
- To protect against overfitting, we separate training set from validation/test set
  - **Training set** for training the classifier
  - **Validation/test set** is for evaluating the performance
- It's common to reserve at least 10% of the data for testing

Cross-validation

- If we don't want to "waste" labeled data on validation, we can use **cross-validation** to see if our training method is sound.
- Split the labeled data into training and validation sets in multiple ways
- For each split (called a **fold**)
  - Train a classifier on the training set
  - Evaluate its accuracy on the validation set
- Average the accuracy to evaluate the training methodology

How many trained models I can have for the leave one out cross-validation?

If I have a data set that has 50 labeled data entries, how many leave-one-out validations I can have?

A. 50

B. 49

C. 50*49

How many trained models can I have with this cross-validation?

If I have a data set that has 51 labeled data entries, I divide them into three folds (17,17,17). How many trained models can I have?

***The common practice of using fold is to divide the samples into equal sized k groups and reserve one of the group as the test data set.**

Assignments

- Read Chapter 11 of the textbook
- Next time: Decision tree, Random forest classifier
- Prepare for midterm2 exam (11/12)
  - Lec 11-Lec 17, Chapter 6-10

Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. “Probability and Statistical Inference”
- Morris H. Degroot and Mark J. Schervish "Probability and Statistics”

See you next time

See You!