# Latent Structures and PCA

Daniel Lawson University of Bristol

Lecture 03.1 (v1.0.2)

# Signposting

- In Block 2, we covered:
  - Regression
  - Classical Statistical Testing
  - Resampling - Bootstrap and Cross-Validation
  - Model Selection
- These may be applied directly to data, but what if this is high dimensional?
  - These methods and more can be used in **dimensionality reduced space**.

# Intended Learning Outcomes

- ILO2 Be able to **use and apply basic machine learning** tools
- ILO3 Be able to make and report appropriate inferences from the results of applying basic tools to data

# Latent Structures

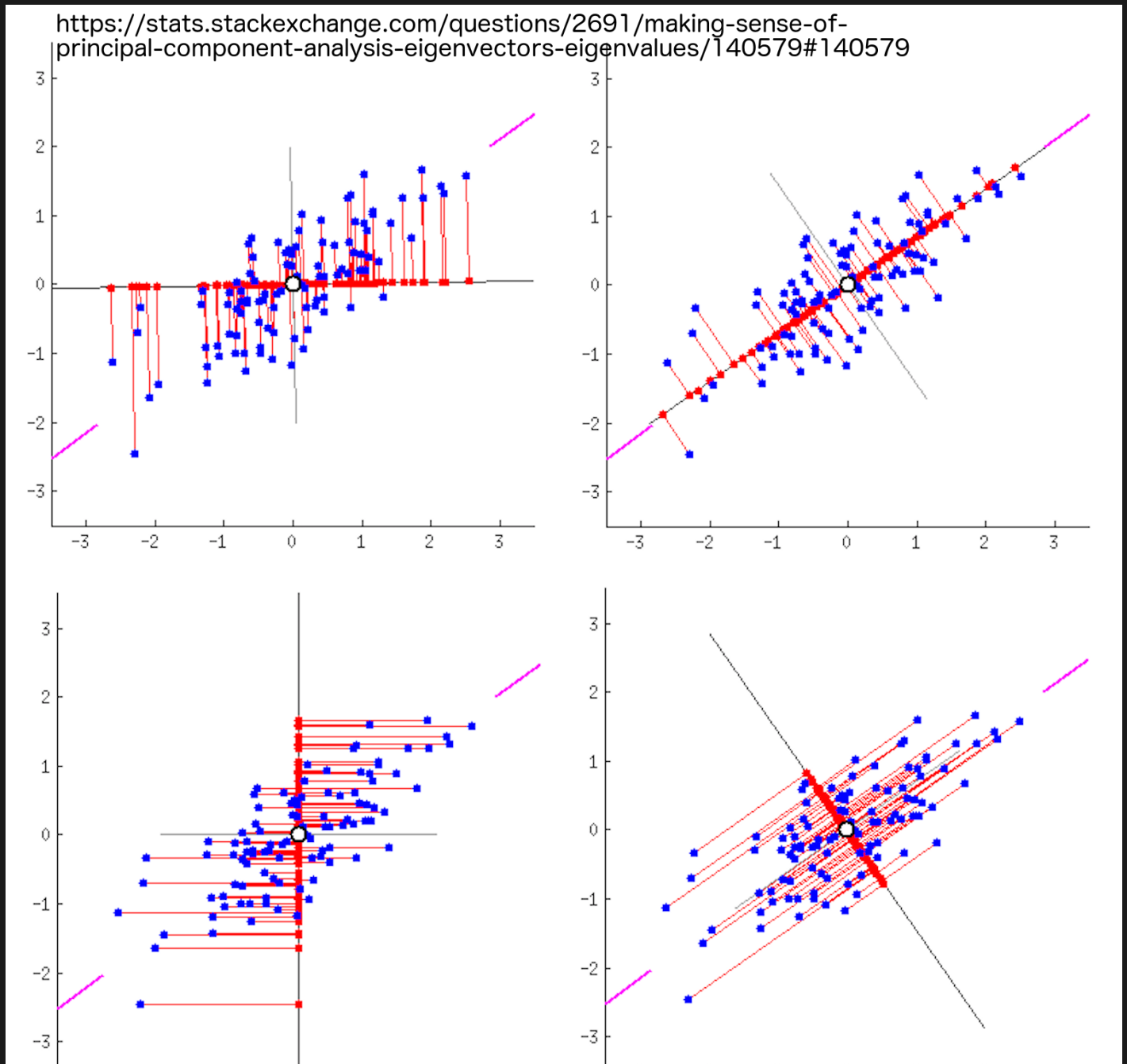
- It is often useful to think of data $X$ being represented in some (usually lower-dimensional) space $\theta$.
- $\theta$ is the **latent space** for $X$.
- Examples:
  - Parameters: $X_i \sim f(\theta_i)$ for some model $f$
  - Kernel representation: $X_i = \sum_{j=1}^{K} K(\theta_i)$
  - Factor analysis
  - Spectral decomposition, Principal Components Analysis, Singular Value Decomposition

# Latent Structure

- What makes this a **latent space** instead of a parameterisation is the modelling done on that space.
- i.e. it is constructed to *mean something*
- If it is done with the intention of making *similar data be close* then we might call this an embedding
- Much care is needed around the words “similar” and “close”!

# PCA Example from Stack Exchange

https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues/140579#140579



# Covariance

- Let $X$ be an $n$ by $m$ matrix.
- Consider that $X$ has been **mean centred**, so that $\mathbb{E}(X_{\cdot,j}) = 0$ for columns $j$. Then:

$$C = \mathrm{Cov}(X) = \frac{1}{n-1} X^T X$$

- this is an unbiased estimator; the factor $1/(n-1)$ arises because we used the data to estimate the mean.
- $C$ is an $m$ by $m$ matrix.
- We might also standardize the variance so that $\mathrm{Var}(X_{\cdot j}) = 1$.

# Principal Components Analysis

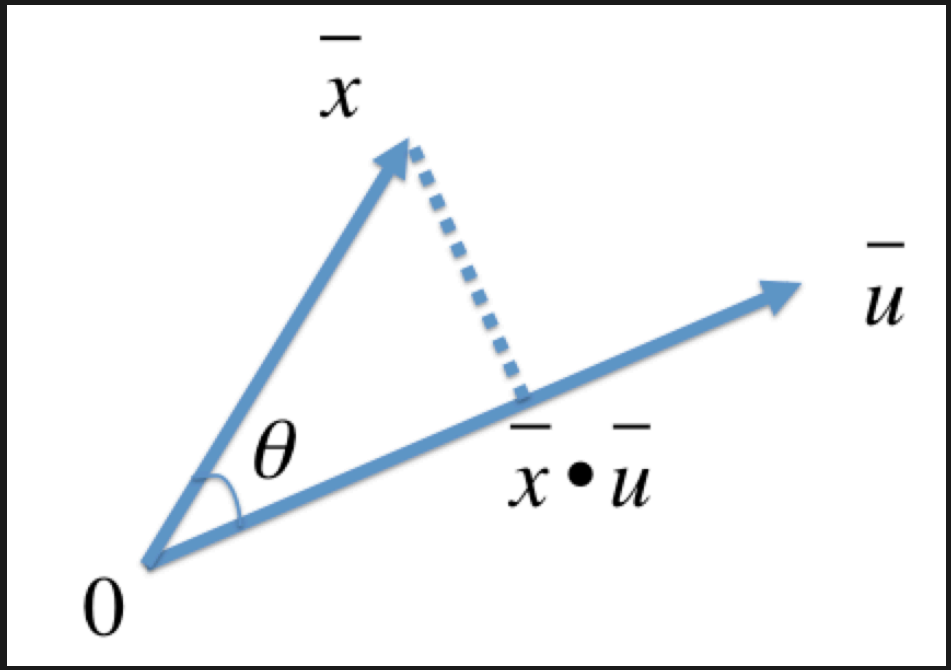
- Consider data $X$ for which we seek the decomposition:

$$C = \mathrm{Cov}(X) = U\Sigma U^T$$

- Where:
  - $D$ is a diagonal matrix of the $m$ **eigenvalues**.
  - $U$ is a matrix of $m$ **eigenvectors** in columns.
- We'll construct this matrix by sequentially:
  - Finding a **projection** of $X$ onto a $k$ dimensional subspace;
  - that **maximises the explained variance**, or equivalently, **minimises the squared error** in the prediction;
  - conditional on this being **orthogonal** to all previous subspaces.

# One dimensional projection

- We will project $X$ onto a subspace $U$.




- In one dimension this is a line defined by $\vec{u}$ of unit length through the origin.
- The projection of $\vec{x}_i$ onto $\vec{u}$ is $(\vec{x}_i \cdot \vec{u})$ in the new coordinate system.
- Recall $\vec{x} \cdot \vec{y} = |\vec{x}||\vec{y}| \cos(\theta)$

# One dimensional projection

- We will compute the projection in the old coordinate system, written $(\vec{x}_i \cdot \vec{u})\vec{u}$.
- Using the properties of $\vec{u}$ the residuals are therefore:

$$||\vec{x}_i - (\vec{x}_i \cdot \vec{u})\vec{u}||^2 = (\vec{x}_i - (\vec{x}_i \cdot \vec{u})\vec{u}) \cdot (\vec{x}_i - (\vec{x}_i \cdot \vec{u})\vec{u}) \quad (1)$$

$$= \vec{x}_i \cdot \vec{x}_i - 2(\vec{u} \cdot \vec{x}_i)^2 + (\vec{u} \cdot \vec{x}_i)^2(\vec{u} \cdot \vec{u}) \quad (2)$$

$$= \vec{x}_i \cdot \vec{x}_i - (\vec{u} \cdot \vec{x}_i)^2 \quad (3)$$

# One dimensional projection

- Averaging over all vectors:

$$MSE(\vec{u}) = \frac{1}{n}\sum_{i=1}^{n} \vec{x}_i \cdot \vec{x}_i - (\vec{u} \cdot \vec{x}_i)^2,$$

- But the first term is constant, so we therefore are seeking to **maximise**:

$$\frac{1}{n}\sum_{i=1}^{n} (\vec{u} \cdot \vec{x}_i)^2,$$

- This is the second moment of $\vec{u} \cdot \vec{x}_i$ which can be written as:

$$\mathbb{E}(\vec{u} \cdot \vec{x}_i)^2 + \mathrm{Var}(\vec{u} \cdot \vec{x}_i).$$

- However, the mean of the projection is zero by construction so **minimising the MSE is equivalent to maximising the variance explained**.

# Multiple dimensions

- To work with multiple dimensions:
  - replace the single vector projection $(\vec{u} \cdot \vec{x}_i)\vec{u}$ with a sum over all dimensions $\sum_{k=1}^{K} (\vec{u}_k \cdot \vec{x}_i)\vec{u}_k$.
- In matrix notation, with our conventions, $\vec{U} = XU$
- It is straightforward to show that the cross terms cancel out.
- This is due to the orthogonality constraint.

# Maximising variance

- Using matrix notation,

$$\mathrm{Var}(\vec{U}) = \frac{1}{n-1}(\mathbf{XU})^T(\mathbf{XU}) \tag{4}$$

$$= \mathbf{U}^T \frac{\mathbf{X}^T\mathbf{X}}{n-1}\mathbf{U} \tag{5}$$

$$= \mathbf{U}^T\mathbf{CU} \tag{6}$$

- Where $\mathbf{C}$ is the covariance.
- We need to constrain the search over $\mathbf{U}$ to look for unit vectors.
- We do this with a Lagrange multiplier $\lambda$, which allows unconstrained optimisation of a different problem.
- Lagrange multipliers are important tools for many optimisation problems in Data Science.

# Lagrangian Calculus



## Leveling with Lagrange: An Alternate View of Constrained Optimization

DAN KALMAN
American University
Washington, D.C. 20016
kalman@american.edu

In most calculus books today [**11, 14, 15**], Lagrange multipliers are explained as follows. Say that we wish to find the maximum value of $f$ subject to the condition that $g = 0$. Under certain assumptions about $f$ and $g$, the Lagrange multipliers theorem asserts that at the solution point, the gradient vectors $\nabla f$ and $\nabla g$ are parallel. Therefore, either $\nabla f = \lambda \nabla g$ for some real number $\lambda$, or $\nabla g = 0$. Combined with the equation $g = 0$, this gives necessary conditions for a solution to the constrained optimization problem. We will refer to this as the standard approach to Lagrange multipliers.

An earlier tradition approaches this subject far differently. It defines a new function, $F = f + \lambda g$, that incorporates both the objective function and the constraint, and in which $\lambda$ is considered to be an additional variable. Here, $F$ is referred to as a *Lagrangian function*. The conditions for $F$ to achieve an unconstrained extremum are then determined, and these become necessary conditions for a solution to the original problem. This is the Lagrangian function approach to Lagrange multipliers.

# Optimisation

- For simplicity we'll just add the $k$-th dimension, conditioning on orthogonality to the previous $k-1$
  - This is how many algorithms work in practice
- Constraint: $\mathbf{u}^T\mathbf{u} = 1$. Therefore

$$\mathbb{L}(\mathbf{u}, \lambda) = \mathbf{u}^T\mathbf{c}\mathbf{u} - \lambda(\mathbf{u}^T\mathbf{u} - 1) \tag{7}$$

$$\frac{\partial \mathbb{L}}{\partial \lambda} = \mathbf{u}^T\mathbf{u} - 1 \tag{8}$$

$$\frac{\partial \mathbb{L}}{\partial \mathbf{u}} = 2\mathbf{c}\mathbf{u} - 2\lambda\mathbf{u} \tag{9}$$

- Which can be solved for when the derivatives are zero to get

$$\mathbf{u}^T\mathbf{u} = 1 \tag{10}$$

$$\mathbf{c}\mathbf{u} = \lambda\mathbf{u} \tag{11}$$

# PCA

- We have shown that the **eigenvector** $\mathbf{u}$ and **eigenvalue** $\lambda$ solve:

$$\mathbf{cu} = \lambda \mathbf{u}$$

- The eigenvectors can be arranged into a matrix $U$ with eigenvectors on the columns, and the eigenvalues into a diagonal matrix $\Sigma$. Then:

$$C = U \Sigma U^T$$

- (Care needs to be taken with zero/repeated eigenvalues.)

# Interpretation

- Our basis $\mathbf{U}$ is **orthonormal**, and
- As $\mathbf{C}$ is a covariance matrix, it is symmetric.
- Therefore the **eigenvectors are orthogonal**.
- The **eigenvalue** (i.e. $\lambda_k$) is the **variance explained** by the $k$-th PC.
- The proportion of **variance explained** by $K$ PCs is $R^2 = \frac{\sum_{k=1}^{K} \lambda_k}{\sum_{m=1}^{M} \lambda_m}$.
- If the data are really in a $K$ dimensional subspace, the eigenvalues beyond that should be 0.

# Singular value decomposition

- PCA and SVD are related:

$$\mathrm{SVD}(X) = UDV^T$$

- and therefore

$$\frac{1}{n-1}X^TX = \frac{1}{n-1}VD^TU^TUDV^T = V\frac{D^TD}{n-1}V^T = V\Sigma V^T$$

- where $\Sigma = D^TD/(n-1)$ are both diagonal matrices.

# Data preparation

```
## Make a 4 column dataset and log-transform
testdata=conndata[,c("orig_bytes","resp_bytes",
                     "orig_ip_bytes","resp_ip_bytes")]
testdata[testdata=="-"]=0
testdata[testdata=="0"]=0
for(i in 1:4) testdata[,i]=log10(as.numeric(testdata[,i])+1)
rownames(testdata)=NULL
```

# Data preparation

```
## Make a 4 column dataset and log-transform
testdata=conndata[,c("orig_bytes","resp_bytes",
                     "orig_ip_bytes","resp_ip_bytes")]
testdata[testdata=="-"]=0
testdata[testdata=="0"]=0
for(i in 1:4) testdata[,i]=log10(as.numeric(testdata[,i])+1)
rownames(testdata)=NULL

## Make a test dataset for example purposes
set.seed(1)
myindex=sample(1:dim(testdata)[1],2000)
testdata_sample=testdata[myindex,]
## And categories, for plotting purposes
testdatacat=as.factor(paste(conndata[,"proto"],
    conndata[,"service"],sep="_"))[myindex]
```

# Do the decompositions

```
## The direct (naive) way to standardize
testdata_scaled <- apply(testdata_sample, 2, scale)

## But we need to standardize *samples*
testdata_t=t(testdata_scaled)
testdata_t_scaled <- apply(testdata_t, 2, scale)
```

# Do the decompositions

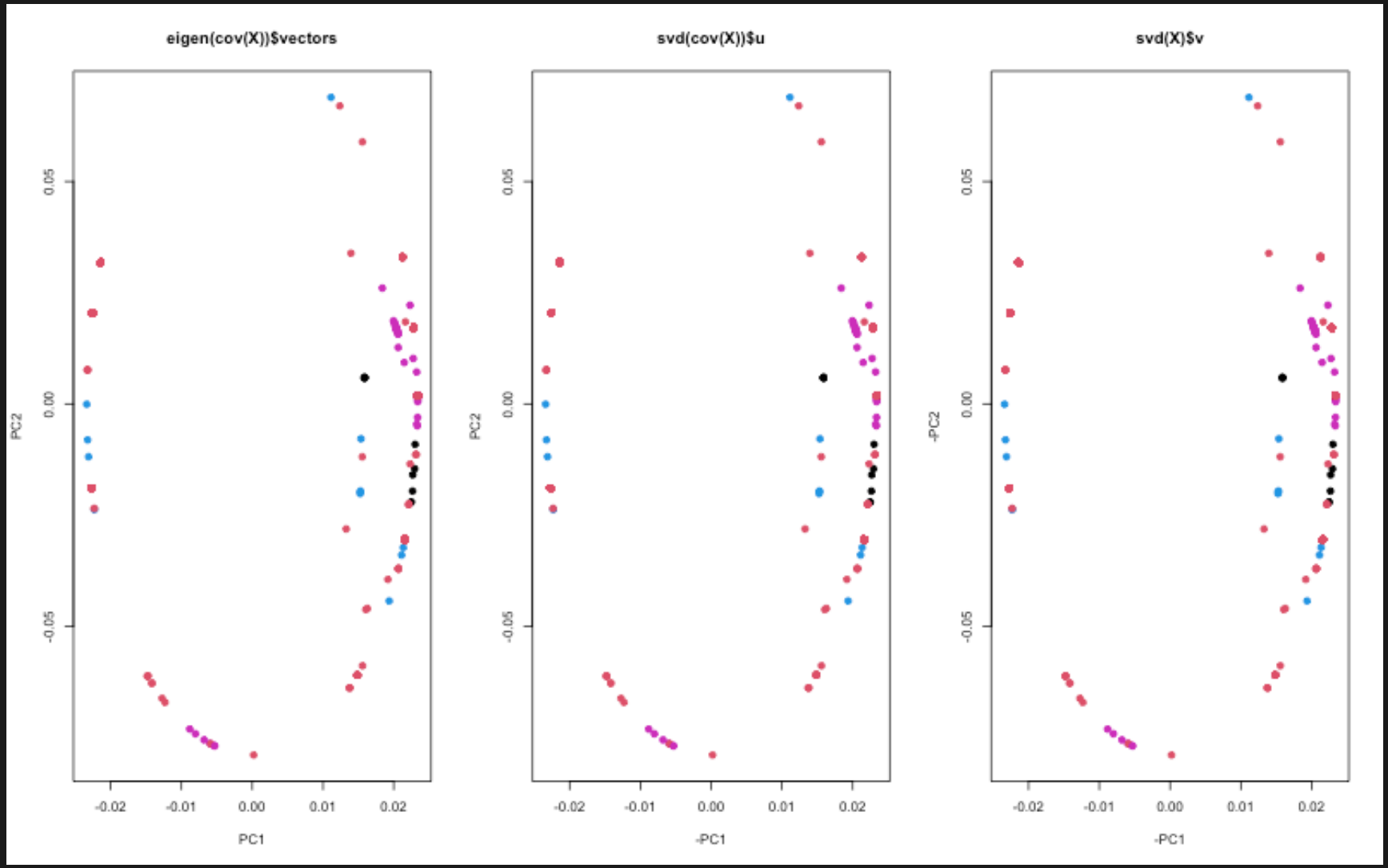
```r
## The direct (naive) way to standardize
testdata_scaled <- apply(testdata_sample, 2, scale)

## But we need to standardize *samples*
testdata_t=t(testdata_scaled)
testdata_t_scaled <- apply(testdata_t, 2, scale)

## Different ways to compute Spectral decompositions
testdata.cov <- cov(testdata_t_scaled)
testdata.eigen <- eigen(testdata.cov)
testdata.cov.svd <- svd(testdata.cov)

# Faster: SVD on the original data matrix
testdata.svd <- svd(testdata_t_scaled)
testdata.prcomp <- prcomp(testdata_t_scaled)
```

# PCA/SVD/Covariance plots



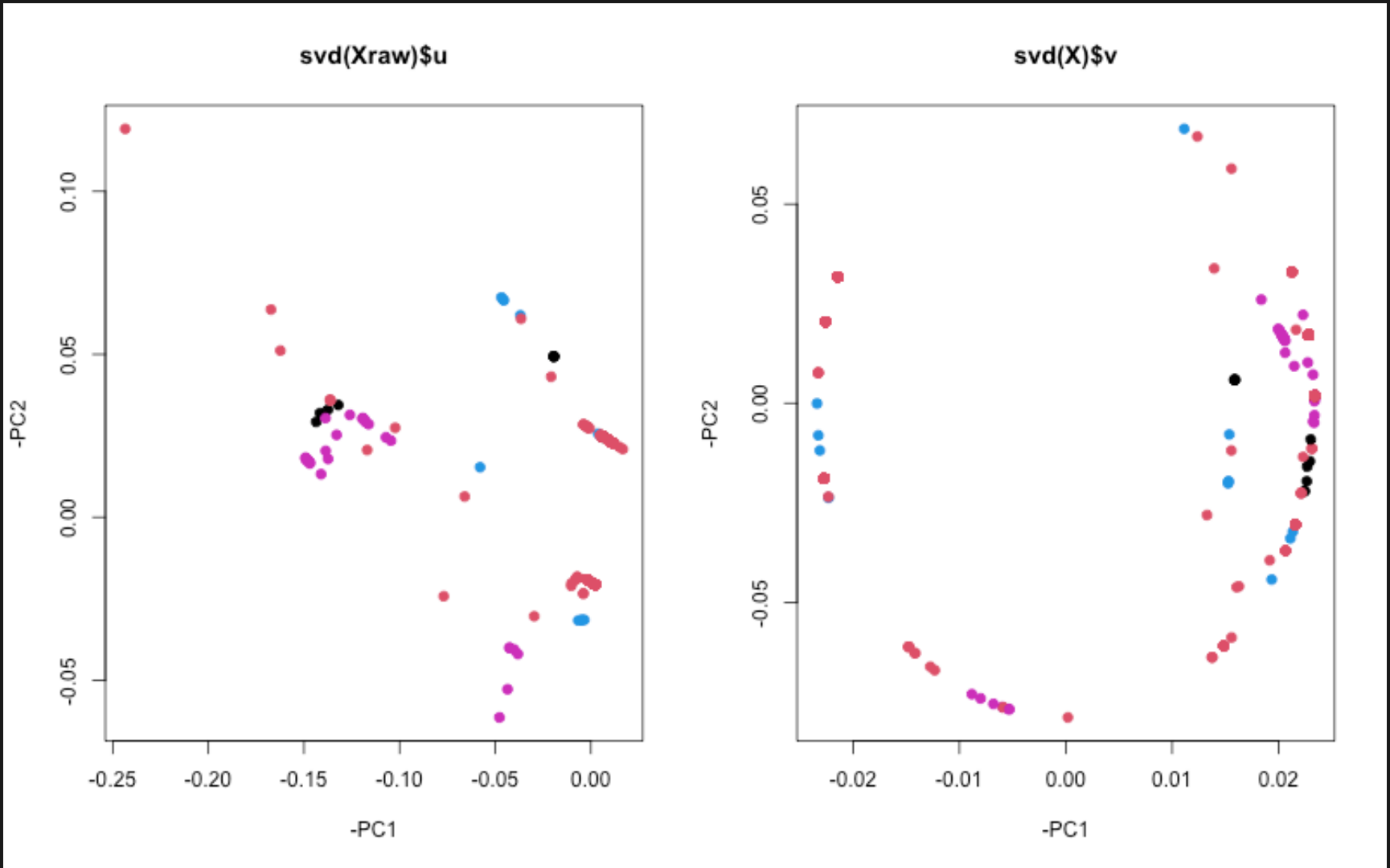
# Plotting code

```
png("../media/03.1.1-EigenExample.png",height=500,width=800)
par(mfrow=c(1,3))
plot(testdata.eigen$vectors[,1],
testdata.eigen$vectors[,2],xlab="PC1",ylab="PC2",
    main="eigen(cov(X))$vectors",
    col=as.numeric(testdatacat),pch=19,cex=0.5)
plot(-testdata.cov.svd$u[,1],
    -testdata.cov.svd$u[,2],xlab="-PC1",
    ylab="PC2",main="svd(cov(X))$u",
    col=as.numeric(testdatacat),pch=19,cex=0.5)
plot(-testdata.svd$v[,1],
    -testdata.svd$v[,2],xlab="-PC1",ylab="-PC2",
    main="svd(X)$v",
    col=as.numeric(testdatacat),pch=19,cex=0.5)
dev.off()
```

# Scaling matters

```
testdata.direct.svd <- svd(testdata_scaled)
png("../media/03.1.2-SVDscaling.png",height=500,width=800)
par(mfrow=c(1,2))
plot(-testdata.direct.svd$u[,1],
     -testdata.direct.svd$u[,2],
     xlab="-PC1",ylab="-PC2",main="svd(Xraw)$u",
     col=as.numeric(testdatacat),pch=19,cex=0.5)
plot(-testdata.svd$v[,1],
     -testdata.svd$v[,2],xlab="-PC1",
     ylab="-PC2",main="svd(X)$v",
     col=as.numeric(testdatacat),pch=19,cex=0.5)
dev.off()
```

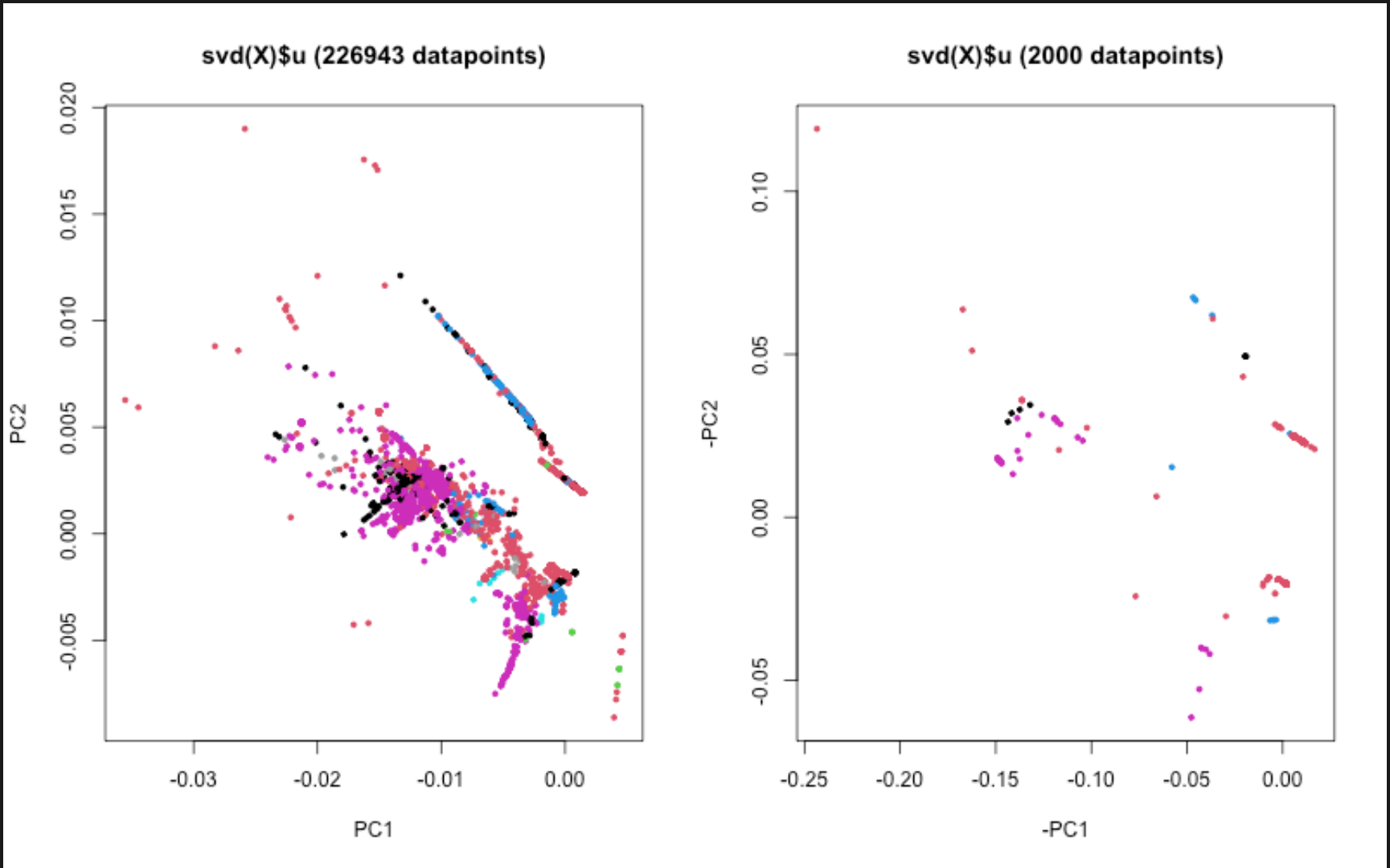
# Scaling matters



# Some notes

- The mean usually shows up in PC1 if you leave it in
- Here, mean centring $X$ to $\tilde{X}$ is weird; its re-weighting features differently for each observation!
- $SVD(X)$ and $SVD(\mathrm{Cov}(\tilde{X}))$ usually contain the same structure, elucidated differently
- When there are many fewer features than observations, working with $X$ directly is **much faster**
- This is because we work with an $M^2$ covariance matrix.
- If the number of features is higher than the number of datapoints, working with Covariance makes sense.

# Full data


svd(X)$u (226943 datapoints)
PC2
0.020
0.015
0.010
0.005
0.000
-0.005
-0.03
-0.02
-0.01
0.00
PC1
svd(X)$u (2000 datapoints)
-PC2
0.10
0.05
0.00
-0.05
-0.25
-0.20
-0.15
-0.10
-0.05
0.00
-PC1

# Full data

```
testdata_all_scaled <- apply(testdata, 2, scale)
dim(testdata_all_scaled)
## [1] 226943      4
testdata_all.svd=svd(testdata_all_scaled)

testdatacat_all <-
    as.factor(paste(conndata[,"proto"],
    conndata[,"service"],sep="_"))
```

# How many PCs?

- This last insight is often used to select only those PCs whose eigenvalues are "large enough" to justify inclusion. There are many procedures, including:
  - **scree plot**, looking for an elbow in the distribution
  - **EVs > 1**, justified by random graph theory
  - **Tracey-Widom theory**, with a similar prediction
  - **Horn's criterion**, based on simulating random matrices for the remaining matrix structure after $K$ are chosen
  - **Velicer's MAP criterion**, similar
- In practice they are all similar, and any can be "wrong", so common sense should be applied.
- What is always true is that Eigenvectors associated with Eigenvalues that are "too small" will contain some noise, even if they still contain a signal.

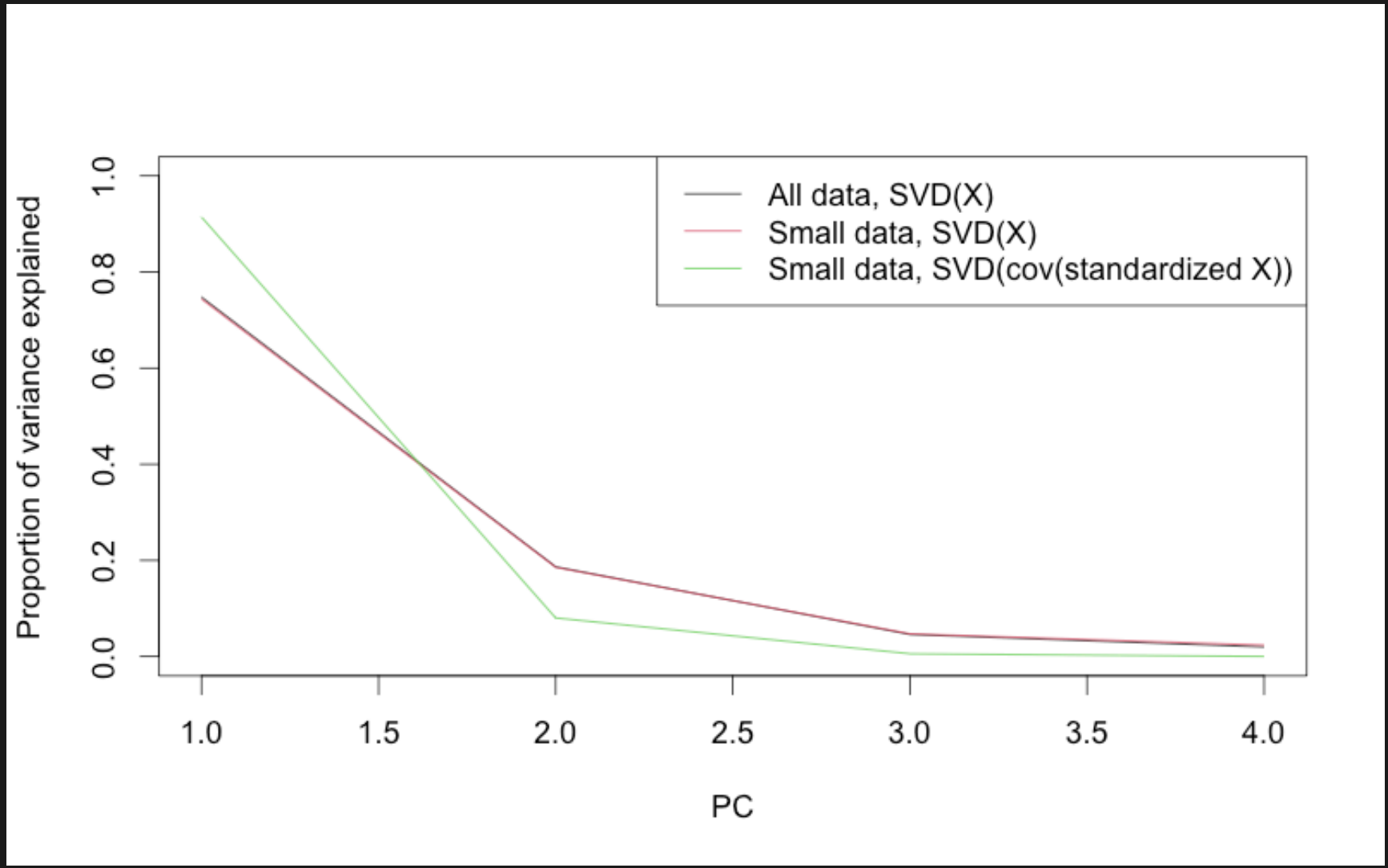
# How many PCs?

- Here we have only 4 features. And we mean centred, which removes a degree of freedom. So the data should lie on a 3D subspace:

```
> round(testdata.eigen$values[1:4],8)
[1] 1859.25164  124.70157   16.04679    0.00000
> round(((testdata.svd$d)^2)/3,8)
[1] 1859.25164  124.70157   16.04679    0.00000
```

- Scaling by the number of features is not important for the SVD when computing the *proportion* of variance explained. Just square the singular values.

# Variance Explained



# Important properties:

- If $X$ is **positive definite**, its eigenvalues are $> 0$.
- If $X$ is **positive semi-definite**, its eigenvalues are $\geq 0$.
- positive definite: If $\forall v \neq 0$ then $v \cdot xv > 0$
- positive semi-definite: If $\forall v \neq 0$ then $v \cdot xv \geq 0$
- The matrix $A$ is **orthogonal** if $A^T = A^{-1}$. This is true iff all column vectors of $A$ are orthonormal, and (equivalently) the row vectors are too. All eigenvalues of an orthogonal matrix are 1.
- If $X$ is square and non-degenerate (distinct eigenvalues), its eigenvectors $U$ form an **orthonormal basis**.

# Projections are idempotent

- Once you project a vector into a subspace, projecting it again does nothing. Such projections $P$ are called **idempotent**:

$$P^K = P$$

- Spectral projections have this property.

# R commands for matrix operations

```r
A %*% B # matrix multiplication
t(A) # matrix transpose
diag(A) # diagonal vector of A
diag(x) # a diagonal matrix formed of the vector x
det(A) # determinant
sum(diag(A)) # trace
solve(A) # matrix inverse
eigen(A) # Eigenvalue decomposition
svd(A) # Singular Value Decomposition
```

# Reflection

- You should:
  - Be able to intuitively explain PCA, and perform simple calculations using it
  - Be able to relate PCA to SVD both mathematically and intuitively
  - Be able to deploy either appropriately on real data
- What is Spectral Decomposition doing? Why is it a good idea?
- How is it different to a model?
- What might it mean that two datapoints are "close" in a PCA plot?
- What might go wrong when making a 2-D PCA plot?

# Signposting

- We will look at **clustering** - both on the raw data but also on PCs, which can often be used to avoid discrete features posing a problem as well as being efficient.
- We'll explore PCA in the Workshop.
- Further reading could include:
  - Cosma Shalizi's Advanced Data Analysis, Lecture 18
  - Boyd and Vandenberghe: Convex Optimization is an excellent and thorough resource.
  - I showed Kalman: Leveling with Lagrange: An Alternate View of Constrained Optimization