Artificial Intelligence and Machine Learning

Unit II

Eigendecomposition, Principal Component Analysis (PCA), 3DMM

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My own latex definitions

$$\gdef\mbf#1{\mathbf{#1}}$$

In [1]:

```
import matplotlib
import matplotlib.pyplot as plt
import numpy as np
%matplotlib inline
#plt.style.use('seaborn-whitegrid')

font = {'family' : 'Times New Roman',
        'weight' : 'bold',
        'size'   : 12}

matplotlib.rc('font', **font)


# Aux functions

def plot_grid(Xs, Ys, axs=None):
    ''' Aux function to plot a grid'''
    t = (np.arange(Xs.size)) # define progression of int for indexing colormap
    if axs:
        axs.plot(0, 0, marker='*', color='r', linestyle='none') #plot origin
        axs.scatter(Xs,Ys, c=t, cmap='jet', marker='.') # scatter x vs y
        axs.axis('scaled') # axis scaled
    else:
        plt.plot(0, 0, marker='*', color='r', linestyle='none') #plot origin
        plt.scatter(Xs,Ys, c=t, cmap='jet', marker='.') # scatter x vs y
        plt.axis('scaled') # axis scaled

def linear_map(A, Xs, Ys):
    '''Map src points with A'''
    # [NxN,NxN] -> NxNx2 # add 3-rd axis, like adding another layer
    src = np.stack((Xs,Ys), axis=Xs.ndim)
    # flatten first two dimension
    # (NN)x2
    src_r = src.reshape(-1,src.shape[-1]) #ask reshape to keep last dimension and adjust the rest
    # 2x2 @ 2x(NN)
    dst = A @ src_r.T # 2xNN
    #(NN)x2 and then reshape as NxNx2
    dst = (dst.T).reshape(src.shape)
    # Access X and Y
    return dst[...,0], dst[...,1]


def plot_points(ax, Xs, Ys, col='red', unit=None, linestyle='solid'):
    '''Plots points'''
    ax.set_aspect('equal')
    ax.grid(True, which='both')
    ax.axhline(y=0, color='gray', linestyle="--")
    ax.axvline(x=0, color='gray',  linestyle="--")
    ax.plot(Xs, Ys, color=col)
    if unit is None:
        plotVectors(ax, [[0,1],[1,0]], ['gray']*2, alpha=1, linestyle=linestyle)
    else:
        plotVectors(ax, unit, [col]*2, alpha=1, linestyle=linestyle)

def plotVectors(ax, vecs, cols, alpha=1, linestyle='solid'):
    '''Plot set of vectors.'''
    for i in range(len(vecs)):
        x = np.concatenate([[0,0], vecs[i]])
        ax.quiver([x[0]],
                  [x[1]],
                  [x[2]],
                  [x[3]],
                  angles='xy', scale_units='xy', scale=1, color=cols[i],
                  alpha=alpha, linestyle=linestyle, linewidth=2)

def angle(v, w):
    return np.arccos(v.dot(w) / (np.linalg.norm(v) * np.linalg.norm(w)))

# let's see it with numpy
nX, nY, res = 10, 10, 21 # boundary of our space + resolution
X = np.linspace(-nX, +nX, res) # give me 21 points linear space from -10, +10
Y = np.linspace(-nX, +nX, res) # give me 21 points linear space from -10, +10
# meshgrid is very useful to evaluate functions on a grid
# z = f(X,Y)
# please see https://numpy.org/doc/stable/reference/generated/numpy.meshgrid.html
Xs, Ys = np.meshgrid(X, Y) #NxN, NxN
```

Slide Correction

First send the PR on Github

Then, only after the PR is approved and accepted fill the form

PR = Pull Request

Recap previous lecture

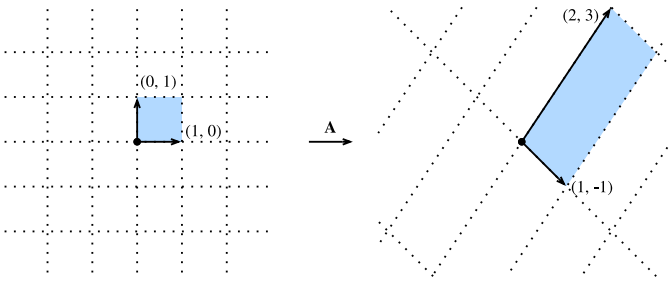
- Vector and Matrix as a formal way to represent data
- Why LA? (data, covariance matrix, calculus)
- Operations (vector to vector, matrix to vector, inner product)
- Geometric Interpretation of the inner product
- Subspaces/Rank/Inverse
- Projection onto a subspace

This lecture material is taken from

- ### Note: you can find PCA on Chapter 12 of [Bishop Book]
- Geometry of the Transformations
- Geometry of Transformations take 2
- This pdf covers this part
- Illustrations and some math part are taken from d2l.ai, eigendecomposition
- Code for Eigendecomposition

Determinant

The geometric view of linear algebra gives an intuitive way to interpret a fundamental quantity known as the *determinant*. Consider the grid image from before, but now with a highlighted region below.



Look at the highlighted square. This is a square with edges given by $(0, 1)$ and $(1, 0)$ and thus it has area one. After $\mathbf{A}$ transforms this square, we see that it becomes a parallelogram. There is no reason this parallelogram should have the same area that we started with, and indeed in the specific case shown here of

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ -1 & 3 \end{bmatrix},$$

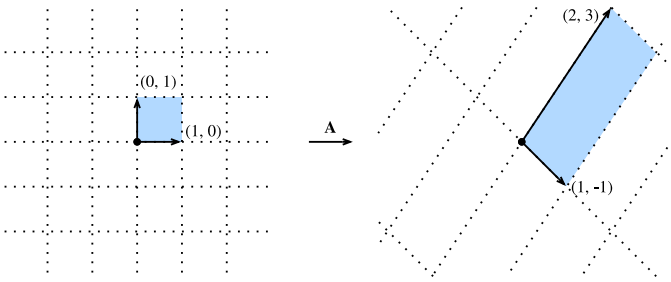
it is an exercise in coordinate geometry to compute the area of this parallelogram and obtain that the area is 5.

In general, if we have a matrix

$$\mathbf{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

we can see with some computation that the area of the resulting parallelogram is $ad - bc$. This area is referred to as the *determinant*.

Determinant $\longrightarrow$ Hyper-volume ratio



Sanity Check: We cannot apply Pythagoras Theorem to compute area because axis are not aligned anymore.

The picture is misleading since axis are **CLOSED to be aligned**.

The angle between $[1, -1]$ and $[2, 3]$ is 101.30993247402021 ```python import numpy as np; X = np.array([[1, -1], [2, 3]]);thetarad = angle(X[0,:],X[1,:]);theta = thetarad*180/np.pi; print(theta)}}

```
The angle between $[1, 0]$ and $[0, 1]$ is 90.

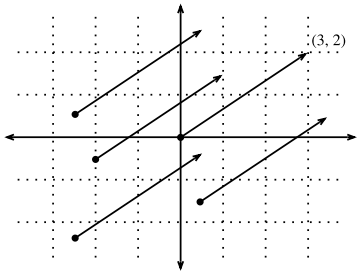
```python
is_basis = False
X = np.array([[1, 0], [0, 1]]) if is_basis else np.array([[1, -1], [2, 3]])
theta_rad = angle(*X)
theta = theta_rad*180/np.pi
print(theta_rad)
```

Transformations of Linear Maps

No transformation! Identity matrix

Translation or Displacement (for now let's leave it a side)

Preserve distances and oriented angles



Isometries (Euclidean): Rotation and Translations

Preserve angles and distances

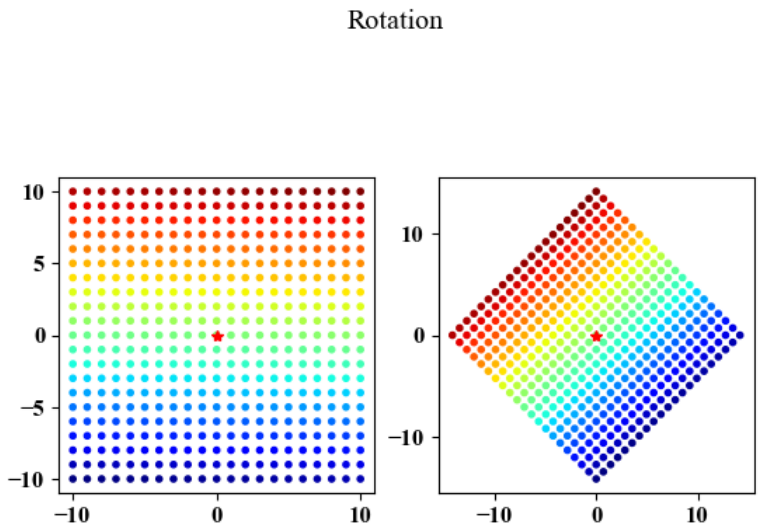
$$A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

This is easily derived by noting that

$$T\left(\begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix}\cos\theta\\ \sin\theta\end{bmatrix}$$
$$T\left(\begin{bmatrix}0\\1\end{bmatrix}\right) = \begin{bmatrix}-\sin\theta\\ \cos\theta\end{bmatrix}.$$
```

In [2]:
```
ang = np.pi/4
A = np.array([[np.cos(ang), -np.sin(ang)],
              [np.sin(ang),np.cos(ang)]])
print(A)
Xd, Yd = linear_map(A, Xs, Ys)
fig, axs = plt.subplots(1,2)
fig.suptitle('Rotation')
plot_grid(Xs,Ys,axs[0])
plot_grid(Xd,Yd,axs[1])
```

```
[[ 0.70710678 -0.70710678]
 [ 0.70710678  0.70710678]]
```



Similarity (Euclidean): scale, reflection (flip), Rotation and Translations

Preserve angles and RATIO between distances

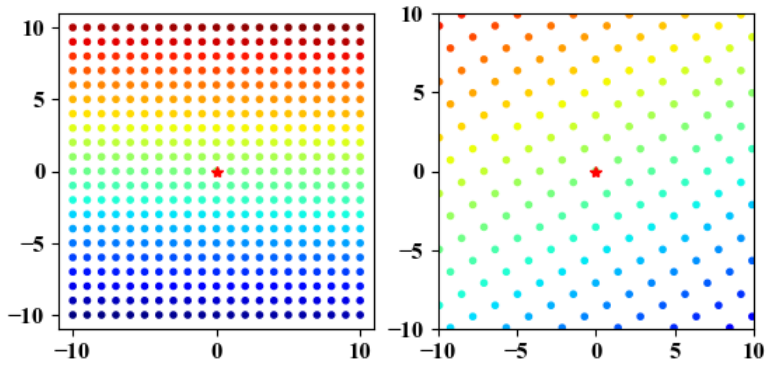
$$A = \begin{bmatrix} s_x \cos\theta & -\sin\theta \\ \sin\theta & s_y \cos\theta \end{bmatrix}$$

This is easily derived by noting that

$$T\left(\begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix} s_x \cos\theta \\ \sin\theta \end{bmatrix}$$
$$T\left(\begin{bmatrix}0\\1\end{bmatrix}\right) = \begin{bmatrix} -\sin\theta \\ s_y \cos\theta \end{bmatrix}.$$

In [3]:
```
ang, scale, clip = np.pi/4, 2, True
A = np.array([[scale*np.cos(ang), -np.sin(ang)],
              [np.sin(ang), scale*np.cos(ang)]])
print(A)
Xd, Yd = linear_map(A, Xs, Ys)
fig, axs = plt.subplots(1, 2)
fig.suptitle('Rotation')
plot_grid(Xs, Ys, axs[0])
plot_grid(Xd, Yd, axs[1])
if clip:
    plt.xlim(-nX, nX)
    plt.ylim(-nY, nY)
```

```
[[ 1.41421356 -0.70710678]
 [ 0.70710678  1.41421356]]
```



Affine: shear, scale, reflection (flip), Rotation and Translations

Preserve parallelism (but NOT angles!)

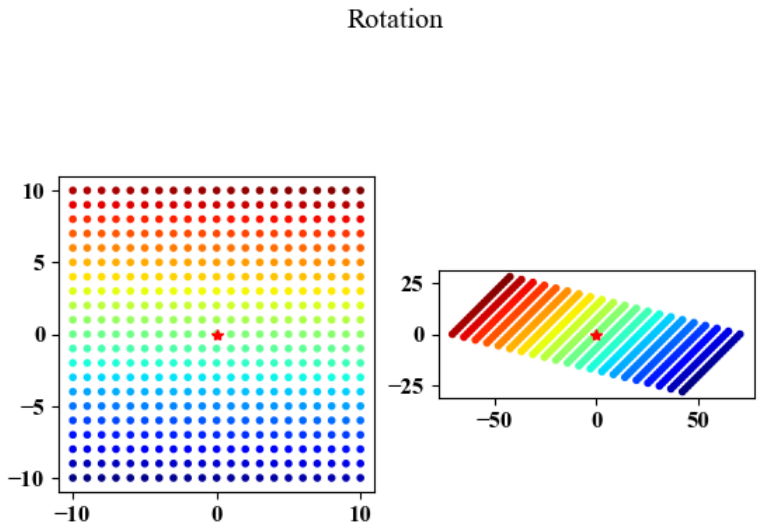
$$A = \begin{bmatrix} s_x \cos\theta & -c_x \sin\theta \\ c_y \sin\theta & s_y \cos\theta \end{bmatrix}$$

This is easily derived by noting that

$$T\left(\begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix} s_x \cos\theta \\ c_y \sin\theta \end{bmatrix}$$
$$T\left(\begin{bmatrix}0\\1\end{bmatrix}\right) = \begin{bmatrix} -c_x \sin\theta \\ s_y \cos\theta \end{bmatrix}.$$

In [4]:
```
ang, scale, cx_shear, cy_shear,clip = np.pi/4, 2, 8, 2, False
A = np.array([[scale*np.cos(ang), -cx_shear*np.sin(ang)],
              [cy_shear*np.sin(ang), scale*np.cos(ang)]])
print(A)
Xd, Yd = linear_map(A, Xs, Ys)
fig, axs = plt.subplots(1, 2)
fig.suptitle('Rotation')
plot_grid(Xs, Ys, axs[0])
plot_grid(Xd, Yd, axs[1])
if clip:
    plt.xlim(-nX, nX)
    plt.ylim(-nY, nY)
```

```
[[ 1.41421356 -5.65685425]
 [ 1.41421356  1.41421356]]
```

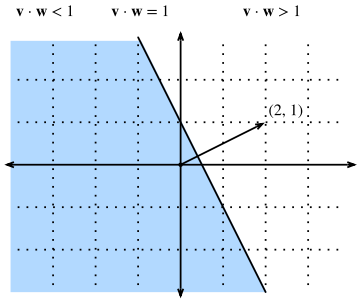


Hyperplanes

Hyperplane: a generalization to higher dimensions of a line ($D = 2$) or of a plane ($D = 3$). In an d-dimensional vector space, a hyperplane has $d - 1$ dimensions and **divides the space into two half-spaces.**

$$\mathbf{wx} + \mathbf{b} = 0$$

where $\mathbf{w}$ is a vector normal to the hyperplane and $\mathbf{b}$ is an offset



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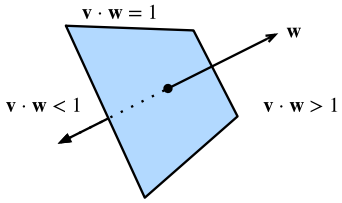
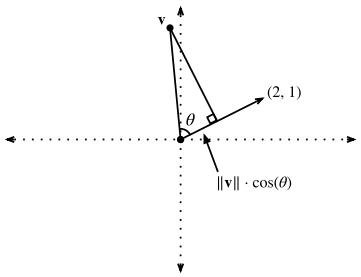


Projection

Suppose that we have two vectors $\mathbf{v}$ and a column vector $\mathbf{w} = [2, 1]^\top$.

We want to project $\mathbf{v}$ onto $\mathbf{w}$ or better project v onto the subspace (line in this case) of $\mathbf{w}$.

Recalling trigonometry, we see the formula $\|\mathbf{v}\| \cos(\theta)$ is the length of the projection of the vector $\mathbf{v}$ onto the direction of $\mathbf{w}$



Projection vector onto subspace defined by $\mathbf{w}$

$$\mathbb{P}_{\mathbf{w}}(\mathbf{v}) = \frac{\mathbf{w}\mathbf{w}^T}{\mathbf{w}^T\mathbf{w}}\mathbf{v} = \left(\frac{\mathbf{w}}{||\mathbf{w}||}\right)\left(\frac{\mathbf{w}}{||\mathbf{w}||}\right)^T\mathbf{v}$$

Defining a unit vector $\hat{\mathbf{w}} = \frac{\mathbf{w}}{||\mathbf{w}||}$ we have:

$$\mathbb{P}_{\mathbf{w}}(\mathbf{v}) = \underbrace{\hat{\mathbf{w}}}_{\text{direction}}\left(\underbrace{\hat{\mathbf{w}}^T\mathbf{v}}_{\text{length}}\right)$$

- Projection must be on unit vector $\alpha \cdot \hat{\mathbf{w}}$
- How long in this direction? $\alpha = \hat{\mathbf{w}}^T\mathbf{v}$ that gives the length of **v** onto **w**.
- $\mathbf{w}$ can be also a matrix not a vector (matrix which columns are vectors).

This lecture material is taken from

- Geometry of the Transformations
- Geometry of Transformations take 2
- This pdf covers this part
- Illustrations and some math part are taken from d2l.ai, eigendecomposition
- Code for Eigendecomposition

Today's lecture

Decomposition (Eigen, SVD), PCA (we use projection!)

Applications of PCA

Recap on Calculus

⚠️All the examples are in 2D but generalizes to 3D and N-D

- Machine Learning is about thinking in N-dimensional space
- ...especially for vision problems (images, videos)
- 2D is used for the sake of visualization and clarity in the explanation

Eigendecomposition

Suppose that we have a matrix A with the following entries:

$$\mathbf{A} = \begin{bmatrix} 2 & 0 \\ 0 & -1 \end{bmatrix}.$$

If we apply A to any vector $\mathbf{v} = [x, y]^\top$, we obtain a vector $\mathbf{A}\mathbf{v} = [2x, -y]^\top$. This has an intuitive interpretation: stretch the vector to be twice as wide in the x-direction, and then flip it in the y-direction.

However, there are *some* vectors for which something remains unchanged.

Namely $[1, 0]^\top$ gets sent to $[2, 0]^\top$ and $[0, 1]^\top$ gets sent to $[0, -1]^\top$.

These vectors are still in the same line, and the only modification is that the matrix stretches them by a factor of 2 and -1 respectively. **We call such vectors *eigenvectors* and the factor they are stretched by *eigenvalues*.**

In general, if we can find a number λ and a vector $\mathbf{v}$ such that

$$\underbrace{\mathbf{A}}_{\text{known}}\mathbf{v} = \underbrace{\lambda\mathbf{v}}_{\text{unknown}}$$

We say that $\mathbf{v}$ is an eigenvector for A and λ is an eigenvalue.

Finding Eigenvalues

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0.$$

For the equation to happen, we see that $(\mathbf{A} - \lambda\mathbf{I})$ must compress some direction down to zero, hence it is not invertible, and thus the determinant is zero. Thus, we can find the *eigenvalues* by finding for what λ is $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$. Once we find the eigenvalues, we can solve $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ to find the associated *eigenvector(s)*.

An Example

Let's see this with a more challenging matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 2 & 3 \end{bmatrix}.$$

If we consider $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$, we see this is equivalent to the polynomial equation $0 = (2 - \lambda)(3 - \lambda) - 2 = (4 - \lambda)(1 - \lambda)$. Thus, two eigenvalues are 4 and 1. To find the associated vectors, we then need to solve

$$\begin{bmatrix} 2 & 1 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1x \\ 1y \end{bmatrix} \text{ and } \begin{bmatrix} 2 & 1 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 4x \\ 4y \end{bmatrix}.$$

We can solve this with the vectors $[1, -1]^\top$ and $[1, 2]^\top$ respectively.

In [5]:
```
eigs, eigvects = np.linalg.eig(
                  np.array([[2, 1],
                            [2, 3]]))
print(f'Eigen val:\n {eigs}', end='\n\n')
print(f'EigenVect vect:\n {eigvects}')
# Note that `numpy` normalizes the eigenvectors to be of length one,
# whereas we took ours to be of arbitrary length.
# Additionally, the choice of sign is arbitrary.
# However, the vectors computed are parallel
# to the ones we found by hand with the same eigenvalues.
#help(np.linalg.eig)
```

```
Eigen val:
 [1. 4.]

EigenVect vect:
 [[-0.70710678 -0.4472136 ]
 [ 0.70710678 -0.89442719]]
```

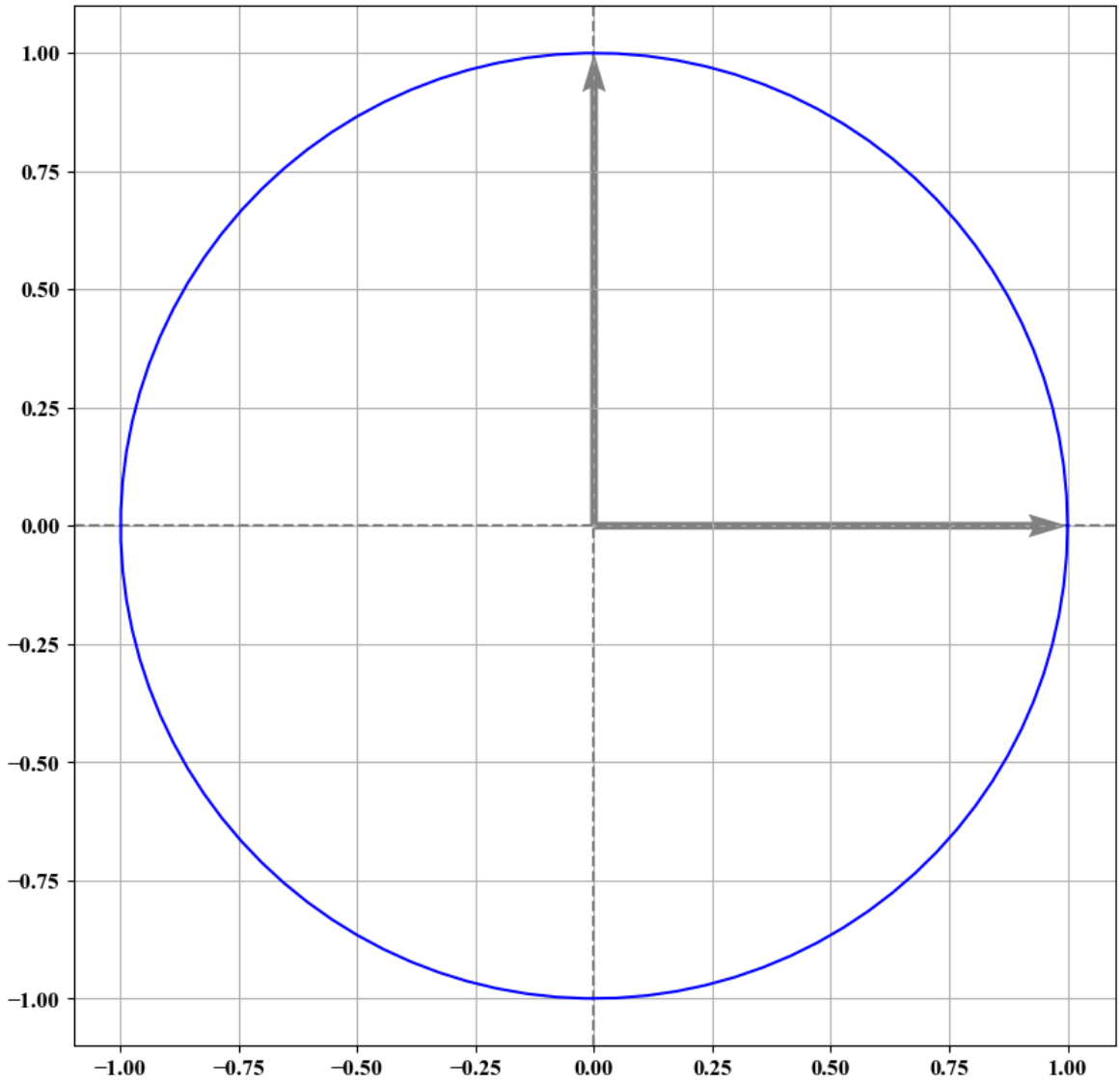
Geometric Interpretation of Eigenvectors

Parametric Unit Sphere

$$\left\{ t \in [0, 2\pi] \mid x = \cos(t), y = \sin(t) \right\} \tag{1}$$

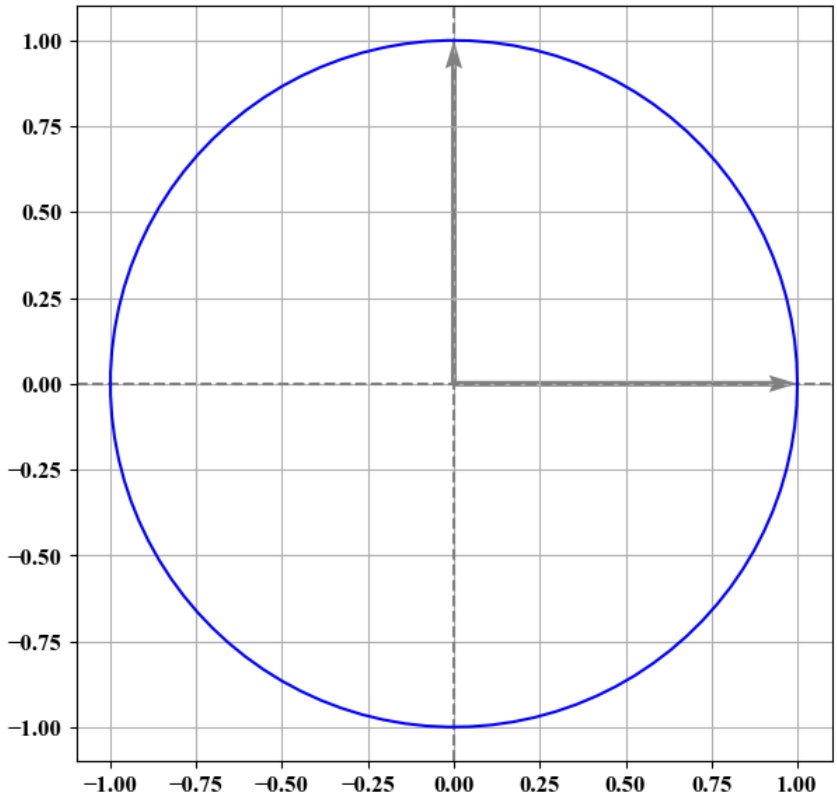
In [6]:
```
fig_dim = 10
### Unit Sphere
# Parametric sphere
t = np.linspace(0, 2*np.pi, 100) # seems a circle but it is not (move resolution to 10)
Xs = np.cos(t)
Ys = np.sin(t)

# Plot
fig, ax = plt.subplots()
fig.set_figheight(fig_dim)
fig.set_figwidth(fig_dim)
plot_points(ax, Xs, Ys, col='blue')
plt.show()
```



In [7]:
```
fig_dim = 7
### Unit Sphere
# Parametric sphere
t = np.linspace(0, 2*np.pi, 100) # seems a circle but it is not (move resolution to 10)
Xs = np.cos(t)
Ys = np.sin(t)

# Plot
fig, ax = plt.subplots()
fig.set_figheight(fig_dim)
fig.set_figwidth(fig_dim)
plot_points(ax, Xs, Ys, col='blue')
plt.show()
```



Linear Transform to Unit Sphere

- For each point $\mathbf{p} = (x, y)$ apply the transform $\mathbf{A}\mathbf{p}^T$
- Plot the result
- We can do it without using for loop (we used it in previous lecture)
  - by stacking all **p** column-wise into a matrix **P**
  - then doing `A@P`
- For now assume:
  - `A` is square

In [8]:
```
# Define a transform
limit = 2.5
# Define a transformation
# A = np.array([[1.5, 1],
#               [1, 1.5]])
A = np.array([[1, -1],
              [-1, 2]])
print(f'Transformation is\n {A}')
```

```
Transformation is
 [[ 1 -1]
 [-1  2]]
```

In [9]:
```
# Map points on the surface
Xd, Yd = linear_map(A, Xs, Ys)
# let's map the basis
Xu_d, Yu_d = linear_map(A, np.array([1,0]), np.array([0,1]))
units_d = np.stack((Xu_d, Yu_d),axis=1)
# Compute the eigenvalues and eigenvectors
eigVals, eigVecs = np.linalg.eig(A)
print('eigVals', eigVals, 'eigVecs', eigVecs, sep='\n'*2)
```

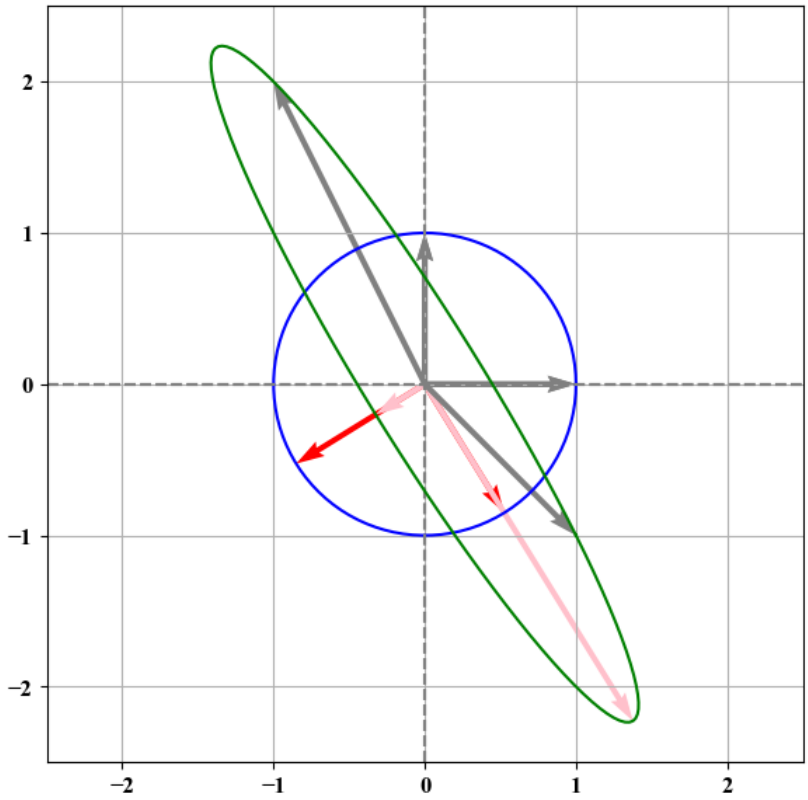
```
eigVals

[0.38196601 2.61803399]

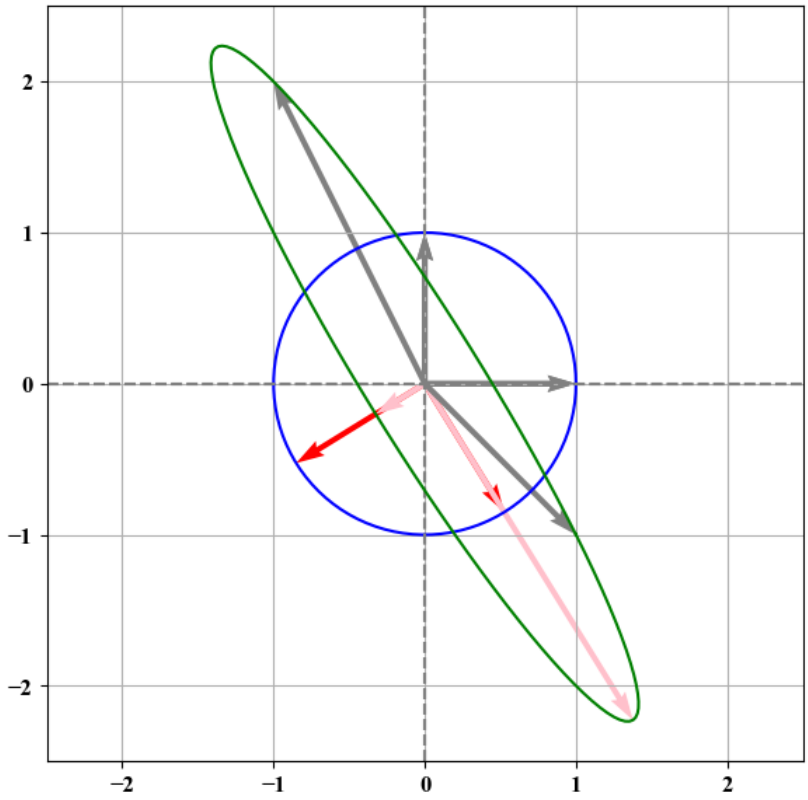
eigVecs

[[-0.85065081  0.52573111]
 [-0.52573111 -0.85065081]]
```

In [10]:
```
# Plot src points and destination points
fig, ax = plt.subplots(1,1)
fig.set_figheight(fig_dim)
fig.set_figwidth(fig_dim)
# Plot src
plot_points(ax, Xs, Ys, col='blue')
# Plot destination
plot_points(ax, Xd, Yd, col='green')
ax.set_aspect('equal')
ax.set_xlim(-limit,limit)
ax.set_ylim(-limit,limit)
# Plot normalized eigenvectors (unit 1)
plotVectors(ax, [eigVecs[:,0], eigVecs[:,1]],
            cols=['red']*2)
# Plot unnormalized eigenvectors (unit 1)
# we have to multiply back to its own eig val
plotVectors(ax, [eigVals[0]*eigVecs[:,0], eigVals[1]*eigVecs[:,1]],
            cols=['pink']*2)
plotVectors(ax, [Xu_d, Yu_d ],
            cols=['gray']*2)
```



In [11]:
```
# Plot src points and destination points
fig, ax = plt.subplots(1,1)
fig.set_figheight(fig_dim)
fig.set_figwidth(fig_dim)
# Plot src
plot_points(ax, Xs, Ys, col='blue')
# Plot destination
plot_points(ax, Xd, Yd, col='green')
ax.set_aspect('equal')
ax.set_xlim(-limit,limit)
ax.set_ylim(-limit,limit)
# Plot normalized eigenvectors (unit 1)
plotVectors(ax, [eigVecs[:,0], eigVecs[:,1]],
            cols=['red']*2)
# Plot unnormalized eigenvectors (unit 1)
# we have to multiply back to its own eig val
plotVectors(ax, [eigVals[0]*eigVecs[:,0], eigVals[1]*eigVecs[:,1]],
            cols=['pink']*2)
plotVectors(ax, [Xu_d, Yu_d ],
            cols=['gray']*2)
```



Interpretations of the determinant with Eigendecomposition

- Symmetric if $A = A^T$ so we can compute eigenvalues
- **The determinant of a matrix is the product of the eigenvalues**
  - So determinant does not capture change in directions (consider only eigenvalues)
  - Just change in the "hyper-volume" (area in 2D).
- **The determinant can be considered as the ratio between**
  - Volume of destination shape/volume of the source shape
  - Ratio of area between ellipse and circle is `np.prod(eigVals)` = {{np.prod(eigVals)}}

Eigendecomposition of Matrices

$$\mathbf{W} = \begin{bmatrix} 1 & 1 \\ -1 & 2 \end{bmatrix},$$

be the matrix where the columns are the eigenvectors of the matrix $\mathbf{A}$. Let

$$\mathbf{\Sigma} = \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix},$$

be the matrix with the associated eigenvalues on the diagonal. Then the definition of eigenvalues and eigenvectors tells us that

$$\mathbf{AW} = \mathbf{W\Sigma}.$$

The matrix W is invertible, so we may multiply both sides by W^{-1} on the right, we see that we may write

$$\mathbf{A} = \mathbf{W\Sigma W}^{-1}.$$

if $\mathbf{W}$ is invertible

Operations on Eigendecompositions

One nice thing about eigendecompositions is that we can write many operations we usually encounter cleanly in terms of the eigendecomposition. As a first example, consider:

$$\mathbf{A}^n = \overbrace{\mathbf{A}\cdots\mathbf{A}}^{n \text{ times}} = \overbrace{(\mathbf{W}\mathbf{\Sigma}\mathbf{W}^{-1})\cdots(\mathbf{W}\mathbf{\Sigma}\mathbf{W}^{-1})}^{n \text{ times}} = \mathbf{W}\overbrace{\mathbf{\Sigma}\cdots\mathbf{\Sigma}}^{n \text{ times}}\mathbf{W}^{-1} = \mathbf{W}\mathbf{\Sigma}^n\mathbf{W}^{-1}.$$

This tells us that for any positive power of a matrix, the eigendecomposition is obtained by just raising the eigenvalues to the same power. The same can be shown for negative powers, so if we want to invert a matrix we need only consider

$$\mathbf{A}^{-1} = \mathbf{W}\mathbf{\Sigma}^{-1}\mathbf{W}^{-1},$$

or in other words, just invert each eigenvalue.

Spectral Theorem

Informal: Given a matrix $\mathbf{A}$ **squared and symmetric**, $\mathbf{A} \in \mathbb{R}^{d\times d}$ and $\mathbf{A} = \mathbf{A}^T$ then:

- All the eigenvalues take **real values**
- The eigenvectors are all **orthogonal**

Practical applications:

- Hessian, Covariance Matrices
- Kernels matrices

Eigendecompositions of Symmetric Matrices

- Hessian
- Covariance Matrices
- PCA
- Kernels etc

Eigendecompositions and Singular Value Decomposition

Method	$\mathbf{A}$	Decomposition
SVD	any	$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$
Eigen	square	$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^{-1}$
Eigen=SVD	square/sym	as above but $\mathbf{U}\mathbf{U}^T = \mathbf{I}$

Decomposition as a Geometric Pipeline

$$\mathbf{A}\mathbf{x} = (\underbrace{\mathbf{U}(\underbrace{\mathbf{\Sigma}\ \underbrace{(\mathbf{U}^{-1}\mathbf{x})}_{\text{1st step/rotate}}}_{\text{2nd step/scale}}\ )}_{\text{3rd step/rotate}})$$

Method	Step 1	Step 2	Step 3
geometry	rotate	scale/reflect axis	rotate/reflect
SVD	$\mathbf{V}^T$	$\mathbf{\Sigma}$	$\mathbf{U}$
geometry	rotate	scale/reflect axis	rotate back/reflect
Eig	$\mathbf{U}^{-1}$	$\mathbf{\Sigma}$	$\mathbf{U}$

Decomposition as a Geometric Pipeline (Code)

In [12]:
```
print('A', A, sep='\n\n')
Sigma, U = np.diag(eigVals), eigVecs
print('Sigma', Sigma, 'U', U, sep='\n\n')
```

```
A

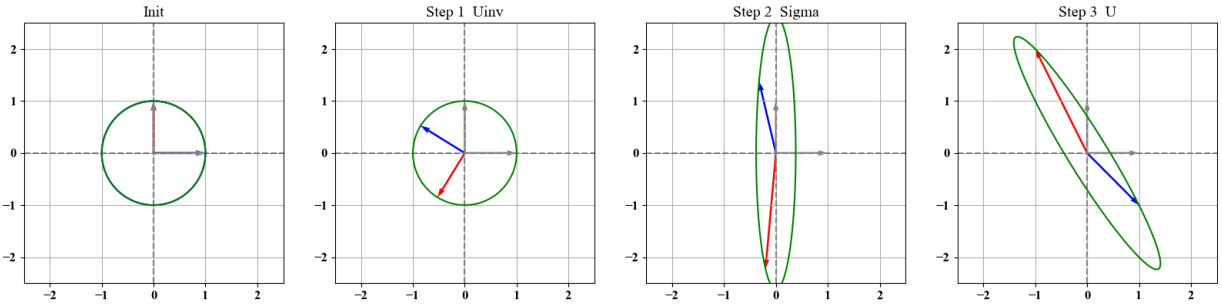
[[ 1 -1]
 [-1  2]]
Sigma

[[0.38196601 0.        ]
 [0.         2.61803399]]

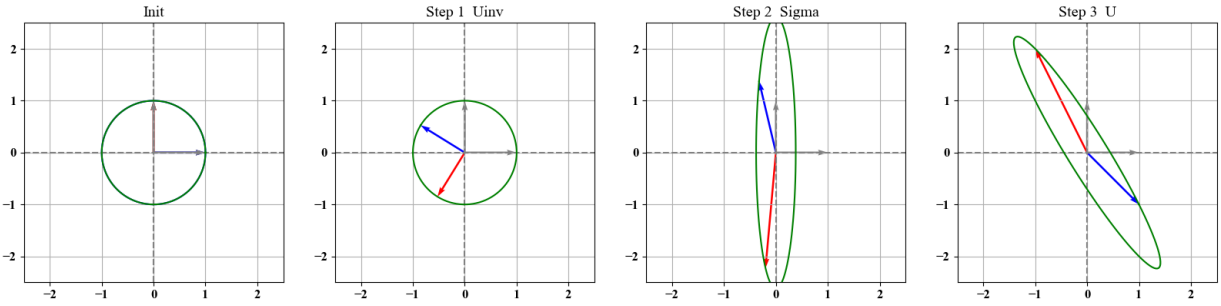
U

[[-0.85065081  0.52573111]
 [-0.52573111 -0.85065081]]
```

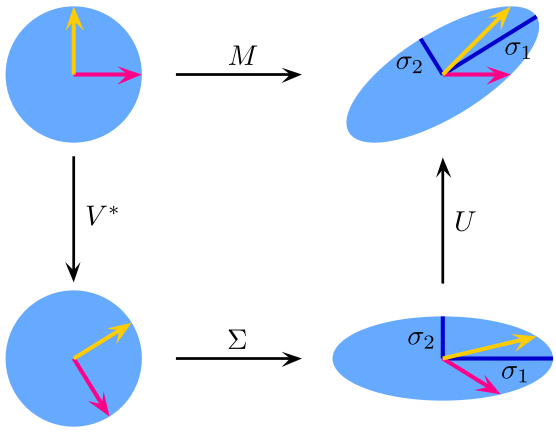
In [13]:
```
# Plot src points and destination points
fig, axes = plt.subplots(1, 4)
fig.set_figheight(20)
fig.set_figwidth(20)
# apply [Id, Uinv, Sigma, U]
Trans = [np.diag((1, 1)), U.T, Sigma, U]
titles = ['Init', 'Step 1  Uinv', 'Step 2  Sigma', 'Step 3  U']
X_orig = np.array([1, 0])
Y_orig = np.array([0, 1])
Xss = np.copy(Xs)
Yss = np.copy(Ys)
for count, (ax, T, title) in enumerate(zip(axes, Trans, titles)):
    ax.set_xlim(-limit, limit)
    ax.set_ylim(-limit, limit)
    ax.set_aspect('equal')
    ax.set_title(title)
    Xss, Yss = linear_map(T, Xss, Yss)
    X_orig, Y_orig = linear_map(T, X_orig, Y_orig)
    if count == 0:
        plot_points(ax, Xs, Ys, col='blue')
    unit_v = np.stack((X_orig, Y_orig), axis=1)
    plotVectors(ax, unit_v, ['blue', 'red'])
    plot_points(ax, Xss, Yss, col='green')
```



In [14]:
```
# Plot src points and destination points
fig, axes = plt.subplots(1, 4)
fig.set_figheight(20)
fig.set_figwidth(20)
# apply [Id, Uinv, Sigma, U]
Trans = [np.diag((1, 1)), U.T, Sigma, U]
titles = ['Init', 'Step 1  Uinv', 'Step 2  Sigma', 'Step 3  U']
X_orig = np.array([1, 0])
Y_orig = np.array([0, 1])
Xss = np.copy(Xs)
Yss = np.copy(Ys)
for count, (ax, T, title) in enumerate(zip(axes, Trans, titles)):
    ax.set_xlim(-limit, limit)
    ax.set_ylim(-limit, limit)
    ax.set_aspect('equal')
    ax.set_title(title)
    Xss, Yss = linear_map(T, Xss, Yss)
    X_orig, Y_orig = linear_map(T, X_orig, Y_orig)
    if count == 0:
        plot_points(ax, Xs, Ys, col='blue')
    unit_v = np.stack((X_orig, Y_orig), axis=1)
    plotVectors(ax, unit_v, ['blue', 'red'])
    plot_points(ax, Xss, Yss, col='green')
```



Geometry of SVD



$$M = U \cdot \Sigma \cdot V^*$$

Source: wikipedia

Principal Component Analysis (PCA)

PCA works in unsupervised learning settings

$$\underbrace{\{\mathbf{x}_i\}_{i=1}^N}_{\text{known}} \sim \underbrace{\mathcal{D}}_{\text{unknown}} \tag{2}$$

Assumptions

- $\mathbf{x}_i \in \mathbb{R}^D$
- $N \geq D$ (number of points higher than number of features; or else, more points than dimensions..for now...)
- $D \geq k$ (where k is the dimension of the subspace on which we will project the points | number of components we will take)

Objective: find a transformation for compressing the data.

What does it mean compressing data? Maybe have different meaning

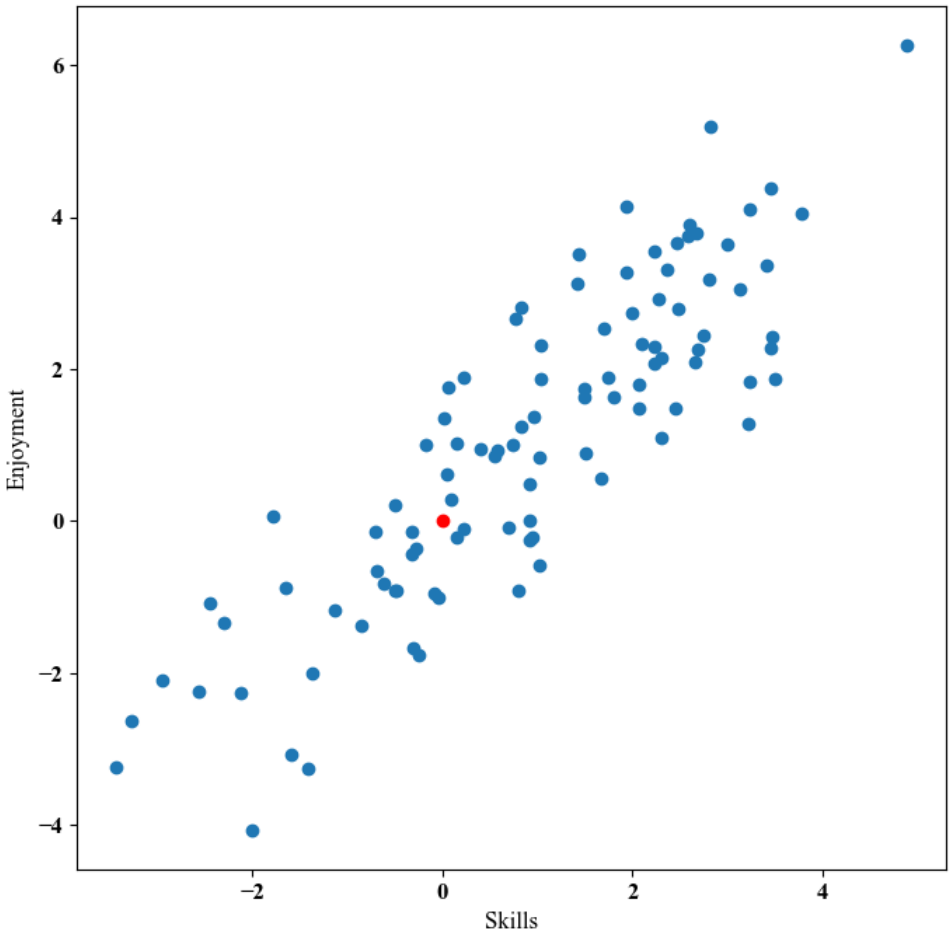
Which kind of transformation?

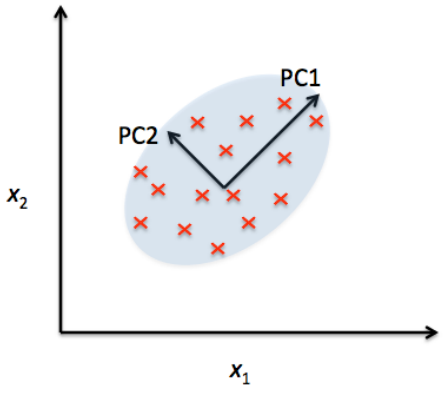
In [15]:
```
########### We know the generative model of the data D ############
np.random.seed(0) # fixing the seed
n_samples=100; cov = [[3, 3], [3, 4]]
# Assumes know the generative model of data
X = np.random.multivariate_normal(mean=[1, 1], cov=cov, size=n_samples)
############################################################
```

In [16]:
```
# import pandas as pd
# pd.DataFrame(X, columns=["x", "y"])
```

In [17]:
```
print(f'num of points {X.shape[0]} in dimension {X.shape[1]}')
fig = plt.figure(figsize=(8,8))
plt.scatter(*X.T)
plt.scatter(0, 0, c='r', marker='o')
plt.ylabel('Enjoyment')
_ = plt.xlabel('Skills')
```

```
num of points 100 in dimension 2
```





Covariance Matrix: the shape of the input matrix matters

- $\mathbf{X} \in \mathbb{R}^{N \times D}$
- N=samples [rows] in D dimensional space [cols]

{{import pandas as pd; pd.DataFrame(X, columns=["x", "y"])}}

then the covariance matrix needs to be $\in \mathbb{R}^{D \times D}$:

$$\mathbf{C} = \frac{1}{N}(\mathbf{X} - \boldsymbol{\mu})^T(\mathbf{X} - \boldsymbol{\mu})$$

Covariance Matrix: the shape of the input matrix matters

- $\mathbf{X} \in \mathbb{R}^{D \times N}$
- N=samples [columns] in D dimensional space [row]

{{import pandas as pd; pd.DataFrame(X.T[:,:10])}}

then the covariance matrix needs to be $\in \mathbb{R}^{D \times D}$:

$$\mathbf{C} = \frac{1}{N}(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^T$$

First Step: Standardize the data

- Assumptions that $\mathbf{X}$ is sampled from multi-variate Gaussian distribution
- **Center all the data in the center (origin). Compute mean and remove it.**
- **[Optional] Rescale all axis so that the standard deviation is one.**

$$\mathbf{X}' \leftarrow \frac{\mathbf{X} - \mu}{\sigma}$$

After: $\mathbf{X}'$ is **standardized**

Objective: find a transformation (subspace) for compressing the data

- Which subspace are we going to find? 🤔
- There could be more than one!

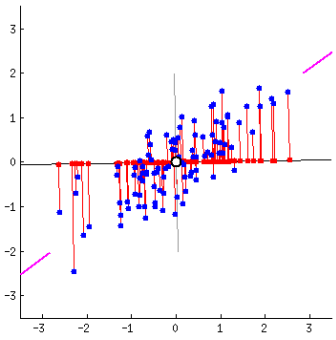
Second Step: Finding the components

- PCA finds a subspace that **maximizes the variance of the data.**
- Given the input D-dimensional space, PCA finds a k-dimensional subspace that maximizes the variance of data.
- Motivation: **compress the dimensions, but keep most of information i.e. preserve tha variance of the data as much as possible**

Play a game

I will show you a point cloud,

you tell me STOP when the variance of the data is maximized on the subspace



Taken from StackExchange

- Find $\mathbf{u} \in \mathbb{R}^D$ s.t. $\|\mathbf{u}\|_2 = 1$ for which you can project the data $\mathbf{x}' = \mathbb{P}_{\mathbf{u}}\mathbf{x}$

$$\mathbb{P}_{\mathbf{u}}\mathbf{x} = \frac{\mathbf{u}\mathbf{u}^T}{\mathbf{u}^T\mathbf{u}}\mathbf{x} = (\mathbf{x}^T\mathbf{u})\mathbf{u}$$

- We have to maximize the variance once projected.
- Which means making the projection of **x** with **u large**:
- We can measure the **size** of the projection with ℓ_2^2 norm.

$$\arg\max_{\mathbf{u}} \frac{1}{N}\sum_i^N \|\mathbb{P}_{\mathbf{u}}\mathbf{x}_i\|_2^2$$

- Find $\mathbf{u} \in \mathbb{R}^k$ s.t. $\|\mathbf{u}\|_2 = 1$ for which you can project the data $\mathbf{x}' = \mathbb{P}_{\mathbf{u}}\mathbf{x}$

$$\mathbb{P}_{\mathbf{u}}\mathbf{x} = \frac{\mathbf{u}\mathbf{u}^T}{\mathbf{u}^T\mathbf{u}}\mathbf{x} = (\mathbf{x}^T\mathbf{u})\mathbf{u}$$

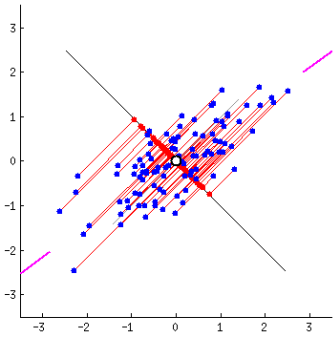
- We have to maximize the variance once projected.
- Which means making the projection of **x** with **u large**:
- We can measure the **size** of the projection with ℓ_2 norm.

$$\arg\max_{\mathbf{u}} \frac{1}{N}\sum_i^N \|\mathbb{P}_{\mathbf{u}}\mathbf{x}\|_2^2 \rightarrow \arg\max_{\mathbf{u}} \frac{1}{N}\sum_i^N \left\|(\mathbf{x}_i^T\mathbf{u})\mathbf{u}\right\|_2^2$$

$$\arg\max_{\mathbf{u}} \frac{1}{N}\sum_i^N \left\|(\mathbf{x}_i^T\mathbf{u})\mathbf{u}\right\|_2^2 = \frac{1}{N}\sum_i^N (\mathbf{x}_i^T\mathbf{u})^2 = \frac{1}{N}\sum_i^N (\mathbf{x}_i^T\mathbf{u})(\mathbf{x}_i^T\mathbf{u}) = \frac{1}{N}\sum_i^N \underbrace{\mathbf{u}^T\mathbf{x}_i}_{\text{reverse dot prod}} \mathbf{x}_i^T\mathbf{u} = \mathbf{u}^T\left(\frac{1}{N}\sum_i^N \mathbf{x}_i\mathbf{x}_i^T\right)\mathbf{u}$$

$$\arg\max_{\mathbf{u}} \mathbf{u}^T\mathbf{C}\mathbf{u} \text{ where } \mathbf{C} = \frac{1}{N}\mathbf{X}\mathbf{X}^T$$

- So the $\mathbf{u}$ that maximizes the data is the **eigenvector** of covariance matrix **C**.
- Remember that $\mathbf{X}$ is "zero mean".
- $\|\mathbf{u}\|_2 = 1$



Taken from StackExchange

Can be used for compressing and reconstructing the data using **U** up to *k* components:

$$\underbrace{\underbrace{\mathbf{x}^T}_{\text{rec}} = \underbrace{\mathbf{U}_{|k}}_{k \mapsto D} \underbrace{\mathbf{U}_{|k}^T}_{D \mapsto k} \underbrace{\mathbf{x}^T}_{\text{orig}}}_{projection}}_{reconstruction}$$

Subspaces in decreasing order of variance

$$(\lambda_1, \mathbf{u}_1), \ldots, (\lambda_d, \mathbf{u}_d) = \text{eig}(\frac{1}{N}\mathbf{X}^T\mathbf{X})$$

Note: *numpy is not guaranteed to return it ordered so you have to sort*

How do we choose the subspace where to cut the dimension?

- From D-dimensional to k-dimension
- Given the spectrum

$$\mathbf{\Sigma} = \text{diag}(\lambda_1, \ldots, \lambda_d)$$

  we can remove the dimension considering the spectrum "energy" and retain e.g. 95% of the variance in data.

That is, keep k components until:

$$\frac{\sum_i^k \lambda_i}{\sum_i^d \lambda_i} \leq 95\%$$

PCA Applications

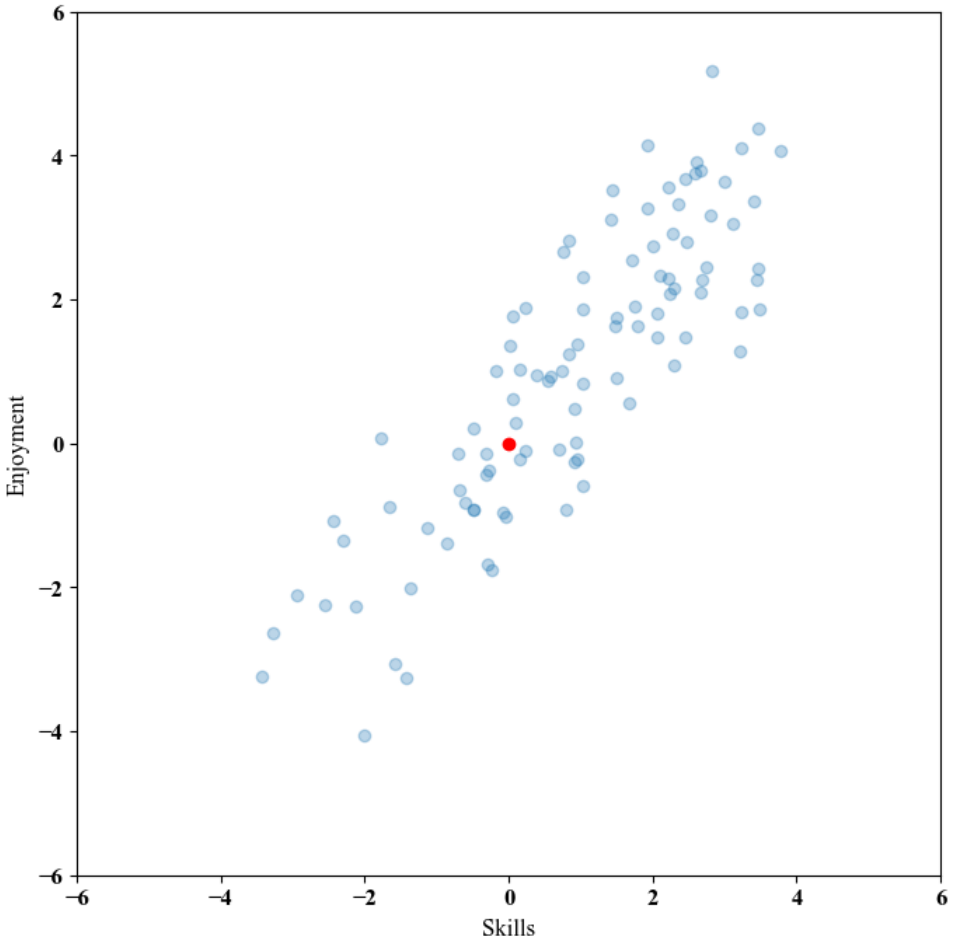
- Visualization
- Dimensionality Reduction
- Reconstructing data and Compression
- Further pre-processing by machine learning algorithms
- Decorrelate the features

Let's go back to our problem

In [18]:
```
print(f'num of points {X.shape[0]} in dimension {X.shape[1]}')
fig = plt.figure(figsize=(8,8))
plt.scatter(*X.T, alpha=0.3)
plt.scatter(0, 0, c='red')
plt.ylabel('Enjoyment')
plt.xlabel('Skills')
plt.axis('scaled')
plt.xlim(-6, 6)
plt.ylim(-6, 6)
```

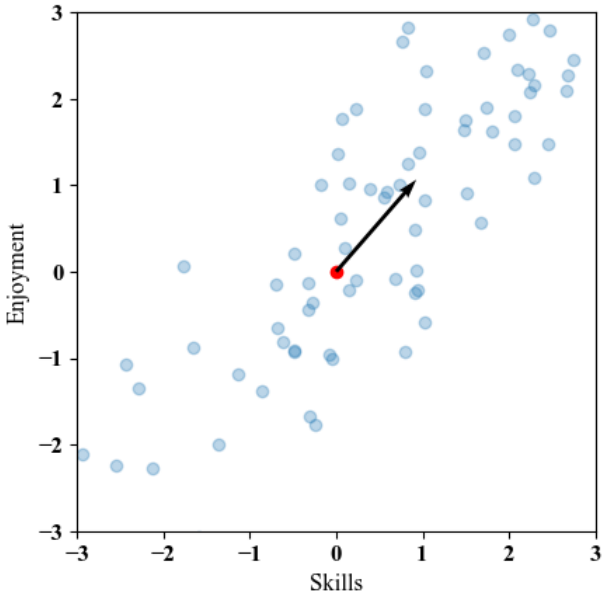
```
num of points 100 in dimension 2
```

Out[18]:
```
(-6.0, 6.0)
```

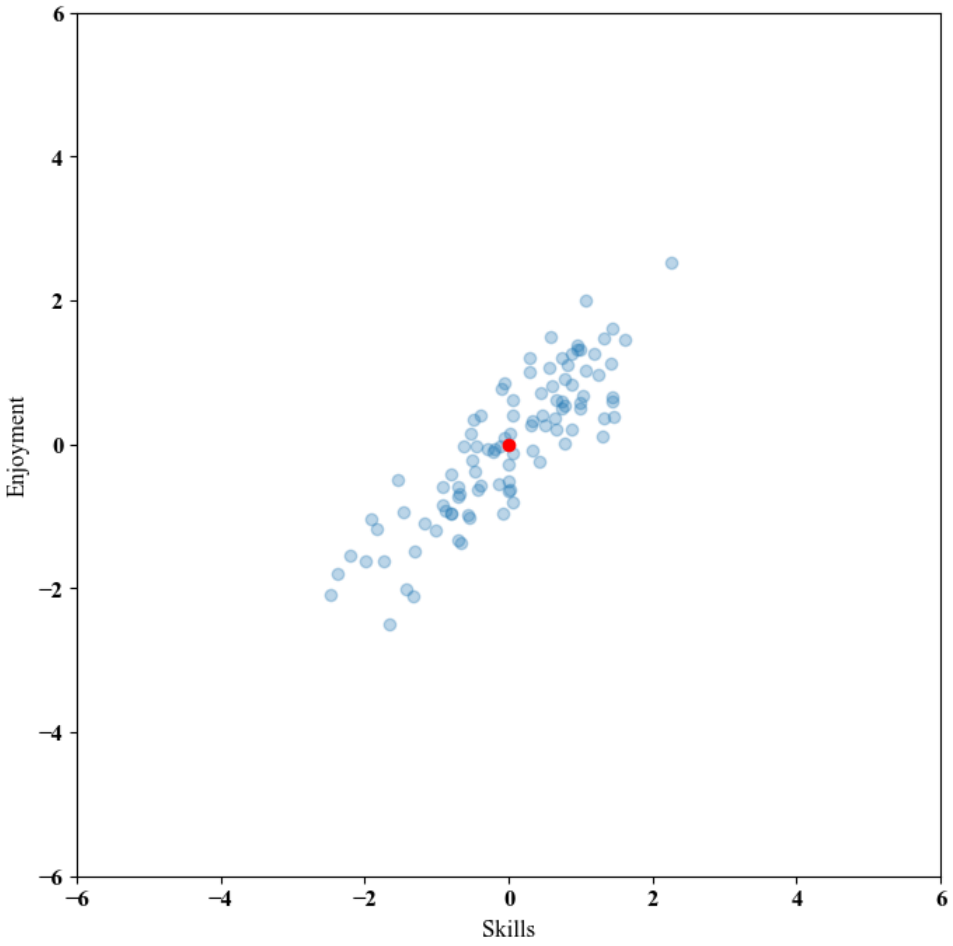


In [19]:
```
# standardize
center = X.mean(axis=0) #X shape is 100x2
std = X.std(axis=0)
Xp = (X-center)/std
```

In [20]:
```
fig = plt.scatter(*X.T, alpha=0.3)
plt.scatter(0, 0, c='red')
plt.quiver(0, 0, *center, angles='xy', scale_units='xy', scale=1)
plt.ylabel('Enjoyment')
plt.xlabel('Skills')
plt.axis('scaled')
plt.xlim(-3, 3)
_=plt.ylim(-3, 3)
#print(center)
```



In [21]:
```
fig = plt.figure(figsize=(8,8))
plt.scatter(*Xp.T, alpha=0.3)
plt.scatter(0, 0, c = 'red')
plt.ylabel('Enjoyment')
plt.xlabel('Skills')
plt.axis('scaled')
plt.xlim(-6, 6)
_=plt.ylim(-6, 6)
```



In [22]:
```
C = np.cov(X, rowvar=False)
Sigma, U = np.linalg.eig(C)
# If rowvar is True (default), then each row represents a variable,
# with observations in the columns. Otherwise, the relationship
# is transposed: each column represents a variable, while the
# rows contain observations.
```

In [23]:
```
C.shape
```

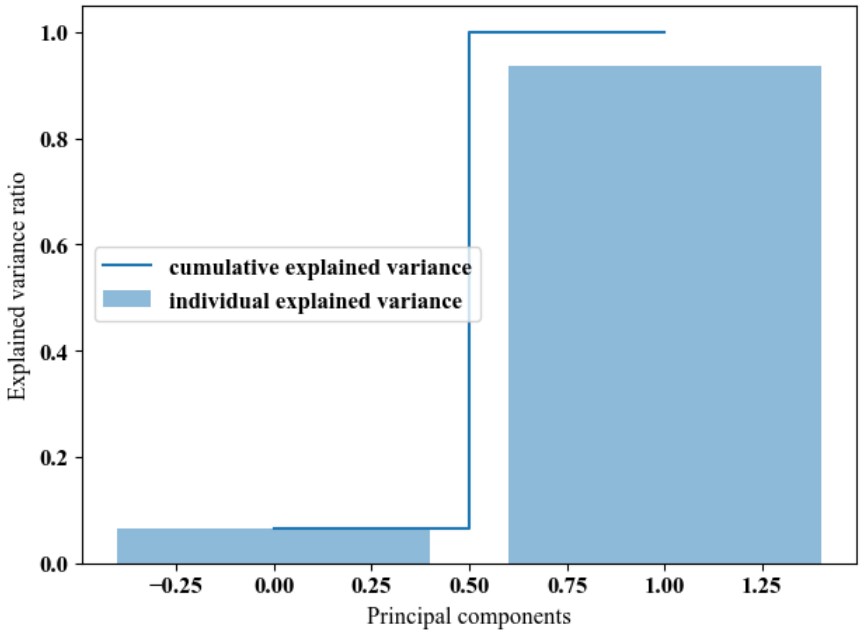
Out[23]:
```
(2, 2)
```

In [24]:
```
Sigma.shape, U.shape, Sigma
```

Out[24]:
```
((2,), (2, 2), array([0.47772418, 6.90110921]))
```

In [25]:
```
total_energy = Sigma.sum()
var_exp = Sigma/total_energy
cum_var_exp = np.cumsum(var_exp)
```

In [26]:
```
plt.bar(range(len(var_exp)), var_exp, alpha=0.5, align='center',
        label='individual explained variance')
plt.step(range(len(var_exp)), cum_var_exp, where='mid',
         label='cumulative explained variance')
plt.ylabel('Explained variance ratio')
plt.xlabel('Principal components')
plt.legend(loc='best')
plt.tight_layout()
plt.show()
Sigma = np.diag(Sigma)
```



PCA for projecting/reconstructing data

$$\text{eig}(\mathbf{C}) \rightarrow \mathbf{\Sigma}, \mathbf{U}$$

$$\mathbf{C} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^T$$

$$\mathbf{U}\mathbf{\Sigma}\mathbf{U}^T = \frac{1}{N}\mathbf{X}\mathbf{X}^T$$

$$\mathbb{P}_{\mathbf{u}}\mathbf{x} = (\mathbf{x}\mathbf{u}^T)\mathbf{u}$$

No compression, no rotation

Can be see as reconstructing the data using **U**:

$$\underbrace{\mathbf{x}^T}_{2\times N} = \underbrace{\mathbf{U}}_{2\times 2}\ \underbrace{\mathbf{U}^T}_{2\times 2}\ \underbrace{\mathbf{x}^T}_{2\times N}$$

In [27]:
```
# Full projection
print(U.shape, U.T.shape, Xp.T.shape)
Xd = U @ U.T @ Xp.T  # Our transformation
print(Xd.shape)
```

```
(2, 2) (2, 2) (2, 100)
(2, 100)
```

In [28]:
```
print('Sigma', Sigma, 'U', U, sep='\n\n')
```

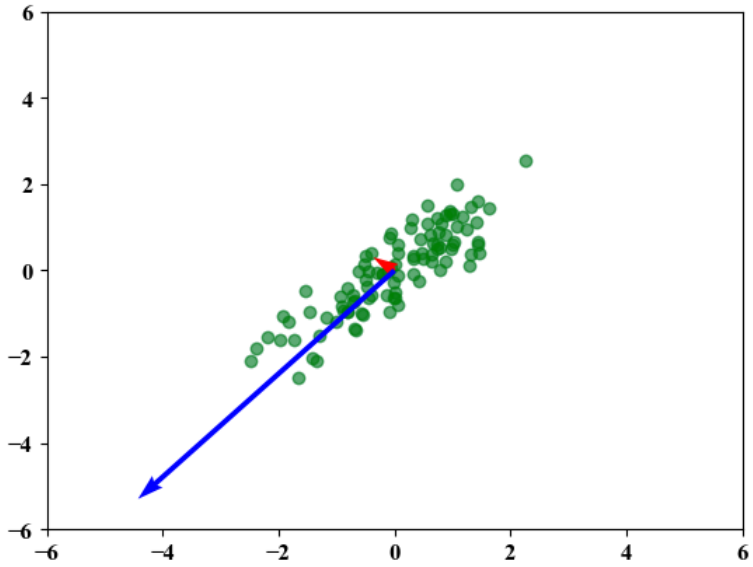
```
Sigma

[[0.47772418 0.        ]
 [0.         6.90110921]]

U

[[-0.76738982 -0.64118083]
 [ 0.64118083 -0.76738982]]
```

In [29]:
```
fig, ax = plt.subplots()
ax.scatter(*Xp.T,alpha=0.3)
ax.scatter(*Xd, color='green', alpha=0.5)
plt.xlim(-6,6)
plt.ylim(-6,6)
plotVectors(ax, [Sigma[0,0]*U[:,0], Sigma[1,1]*U[:,1]], cols=['red','blue'])
```



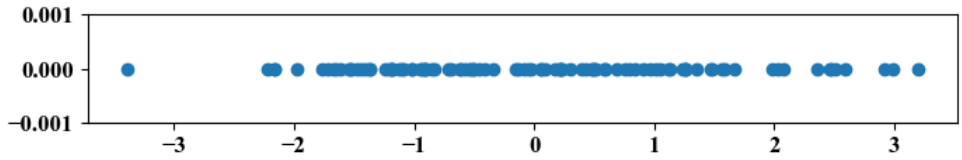
What happens if we use only the first dominant basis (first component)?

In [30]:
```
Utrunc = U[:,1].reshape(2,-1) # need reshape for matrix mul.
# note [:,1] selects the eigenvector with with more energy (highest eigen value)
# if you have more of them you have to sort, with 2 it is easier it is either this or the other
print()
```

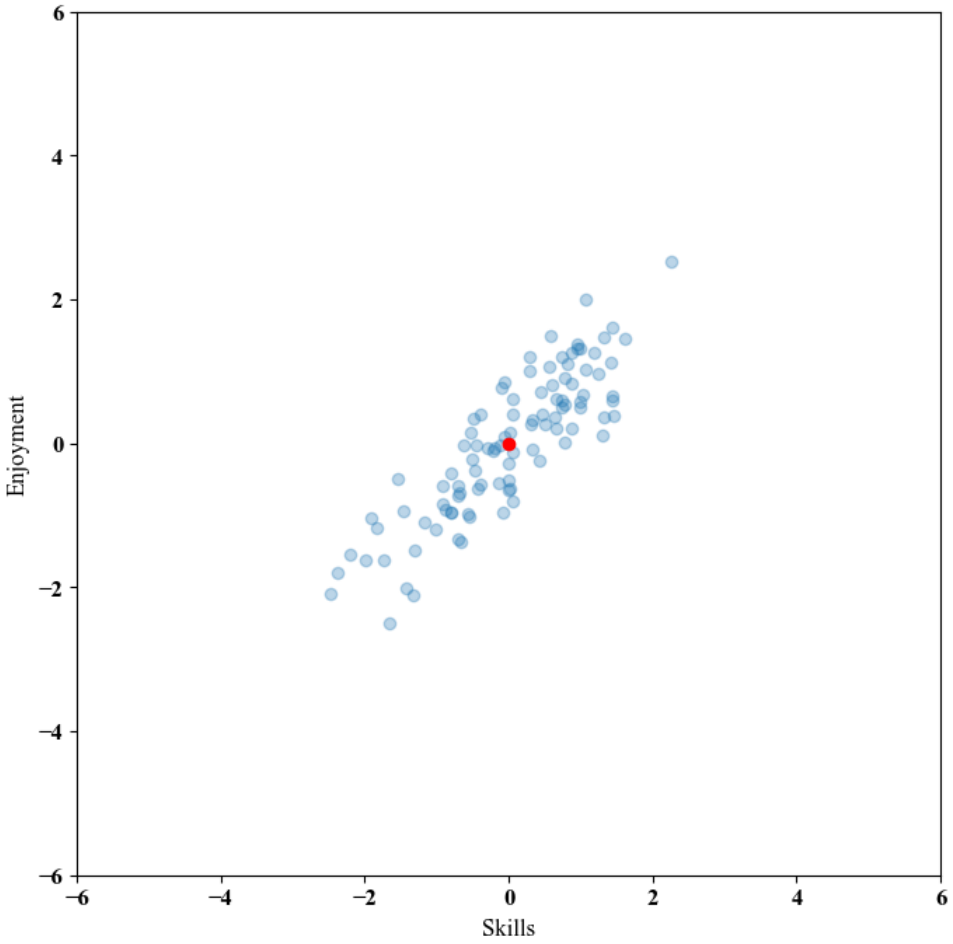
In [31]:
```
# Compressed projection
print('Full projection>', U.shape, U.T.shape, Xp.T.shape)
print('Compressed projection>', Utrunc.shape, Utrunc.T.shape, Xp.T.shape)
Xd = Utrunc.T @ Xp.T  # Our transformation project down = Utrunc.T @ x.T;
print(Xd.shape)
```

```
Full projection> (2, 2) (2, 2) (2, 100)
Compressed projection> (2, 1) (1, 2) (2, 100)
(1, 100)
```

In [32]:
```
fig = plt.figure(figsize=(8,1))
plt.plot(Xd[0, ...].T, [0]*Xd.shape[1], 'o')
_ = plt.ylim(-0.001, 0.001)
```



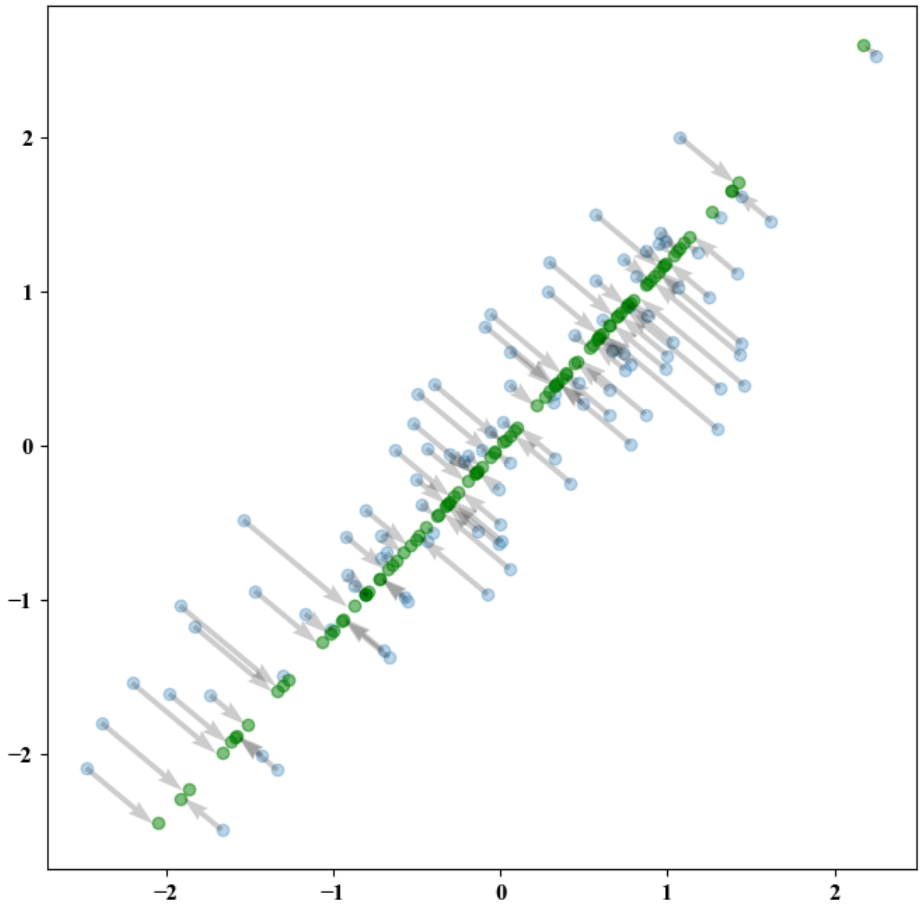
In [33]:
```
fig = plt.figure(figsize=(8,8))
plt.scatter(*Xp.T, alpha=0.3)
plt.scatter(0, 0, c = 'red')
plt.ylabel('Enjoyment')
plt.xlabel('Skills')
plt.axis('scaled')
plt.xlim(-6, 6)
_=plt.ylim(-6, 6)
```



In [34]:
```
# Compressed projection and back-projected
print(U.shape, U.T.shape, Xp.T.shape)
Xd = Utrunc @ Utrunc.T @ Xp.T  # Our transformation A = U @ Ut;
print(Xd.shape)
```

```
(2, 2) (2, 2) (2, 100)
(2, 100)
```

In [35]:
```
fig, ax = plt.subplots()
fig.set_figheight(8)
fig.set_figwidth(8)
ax.scatter(*Xp.T, alpha=0.3)
ax.scatter(*Xd, color='green', alpha=0.5)
_ = ax.quiver(*Xp.T, *(Xd-Xp.T), alpha=0.2, linestyle='dashed',
          linewidth=.4, color='black')  # start, end-start
```



We have reduce the dimensionality of the data since we projected on a line

Can be use for compressing and reconstructing the data using **U** up to *k* components:

$$\underbrace{\mathbf{x}^T}_{\text{rec}} = \underbrace{\underbrace{\mathbf{U}_{|k}}_{k \mapsto D} \underbrace{\mathbf{U}_{|k}^T}_{D \mapsto k} \underbrace{\mathbf{x}^T}_{\text{orig}}}_{projection}}_{reconstruction}$$

PCA Full recipe

$$\mathbf{X}' \leftarrow \frac{\mathbf{X} - \mu}{\boldsymbol{\sigma}}$$

$$\underbrace{\mathbf{x}_p^{T\prime}}_{\text{rec}} = \underbrace{\underbrace{\mathbf{U}_{|k}}_{k \mapsto D} \underbrace{\mathbf{U}_{|k}^T}_{D \mapsto k} \underbrace{\mathbf{x}^{T\prime}}_{\text{orig}}}_{projection}}_{reconstruction}$$

$$\mathbf{x}_p \leftarrow \left(\mathbf{x}_p^{T\prime}\boldsymbol{\sigma}\right) + \mu$$

Artificial Intelligence and Machine Learning

Unit II

PCA in higher dimension, 3DMM, the curse of dimensionality

Iacopo Masi

Recap previous lectures

- Vector and Matrix as a formal way to represent data
- Why LA? (data, covariance matrix, calculus)
- Operations (vector to vector, matrix to vector, inner product)
- Geometric Interpretation of the inner product
- Subspaces/Rank/Inverse
- Projection onto a subspace

This lecture material is taken from

- ### Note: you can find PCA on Chapter 12 of [Bishop Book]
- Geometry of the Transformations
- Geometry of Transformations take 2
- This pdf covers this part
- Illustrations and some math part are taken from d2l.ai, eigendecomposition
- Code for Eigendecomposition

Today's lecture

Recall PCA (we use projection!) and Eigendecomposition

Note: you can find PCA on Chapter 12 of [Bishop Book]

Applications of PCA (3DMM)

PCA Full recipe

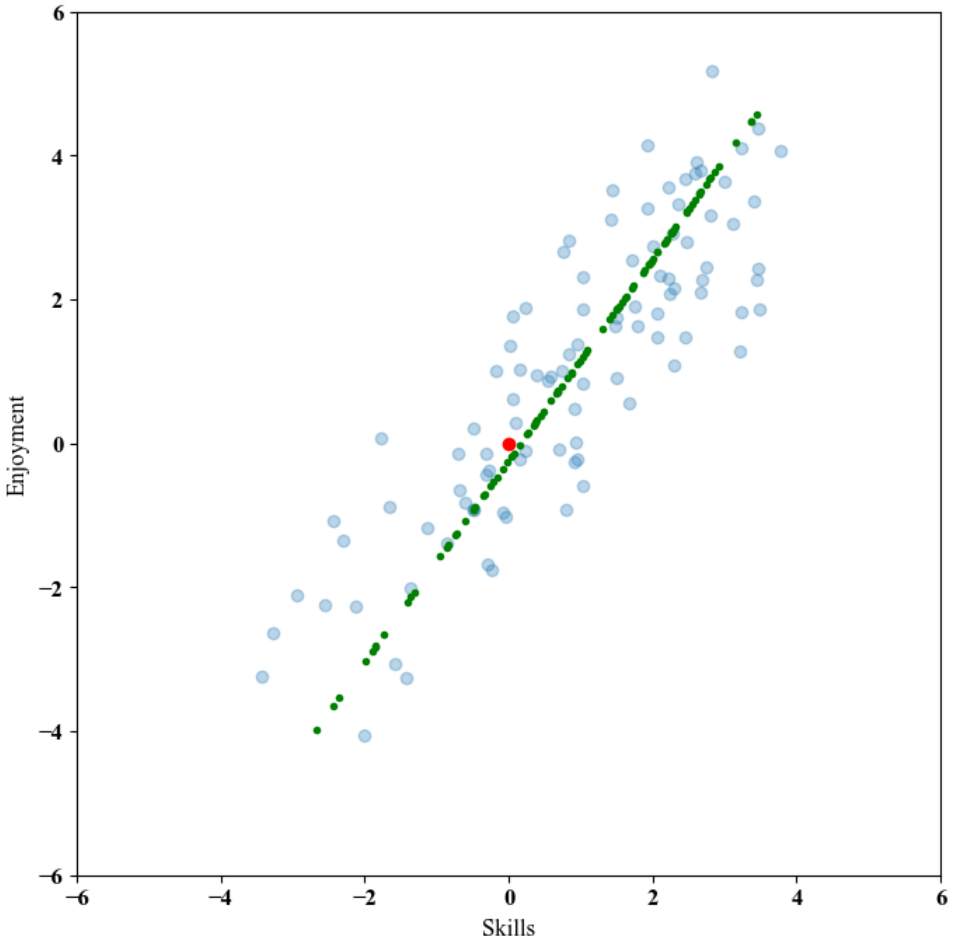
$$\mathbf{X}' \leftarrow \frac{\mathbf{X} - \mu}{\boldsymbol{\sigma}}$$

$$\underbrace{\mathbf{x}_p^{T\prime}}_{\text{rec}} = \underbrace{\underbrace{\underbrace{\mathbf{U}_{|k}}_{k \mapsto D} \underbrace{\mathbf{U}_{|k}^T}_{D \mapsto k}}_{projection} \underbrace{\mathbf{x}^{T\prime}}_{\text{orig}}}_{reconstruction}$$

$$\mathbf{x}_p \leftarrow \left(\mathbf{x}_p^{T\prime}\boldsymbol{\sigma}\right) + \mu$$

In [36]:
```
########################################
plt.figure(figsize=(8,8))
plt.scatter(*X.T, alpha=0.3)
plt.scatter(0, 0, c='red')
plt.ylabel('Enjoyment')
plt.xlabel('Skills')
plt.axis('scaled')
plt.xlim(-6, 6)
plt.ylim(-6, 6)
# Taking reconstruced data and shift it back
##############################
Xd_back = (Xd.T*std)+center
########################
plt.scatter(*Xd_back.T, color='green', marker='.')
```

Out[36]:
```
<matplotlib.collections.PathCollection at 0x7fd5a80e5eb0>
```



Application: PCA to rotate data (make it axis aligned), decorrelate data

in unsupervised way

- For reading images there are multiple library
- One is Pillow `conda install pillow` or `pip install pillow`

In [37]:
```
from PIL import Image
import requests
from io import BytesIO

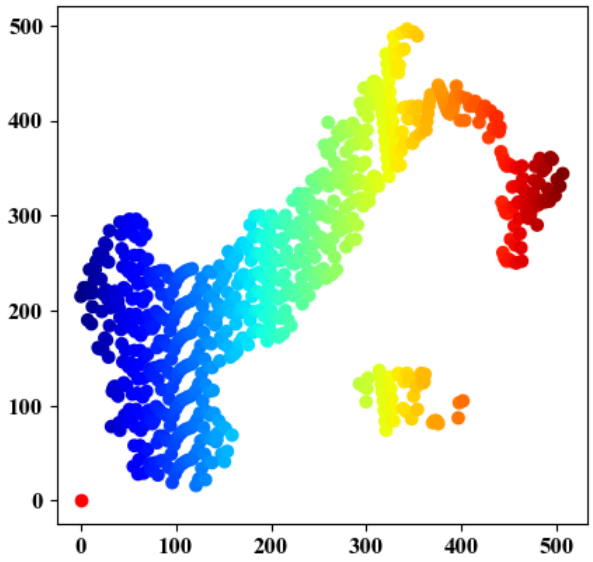
#response = requests.get('https://cdn-icons-png.flaticon.com/512/24/24335.png')
img = Image.open('figs/italy.png')
im = np.array(img)
```

In [38]:
```
img
```

Out[38]:

In [39]:
```
X, Y = np.where(im != 0)
sampling = 100  # to have less points
X, Y = X[::sampling], Y[::sampling]
```

In [40]:
```
fig = plt.scatter(X, Y, c=X, marker='o', cmap='jet')
plt.scatter(0, 0, c='red')
_ = plt.axis('scaled')
```



PCA Application - Rotate the data and decorrelate them - No compression

$$\mathbf{X}' \leftarrow \frac{\mathbf{X} - \mu}{\sigma}$$

$$\underbrace{\mathbf{x}_p^{T\prime}}_{\text{rot}} = \mathbf{U}^T \underbrace{\mathbf{x}^{T\prime}}_{\text{orig}}$$

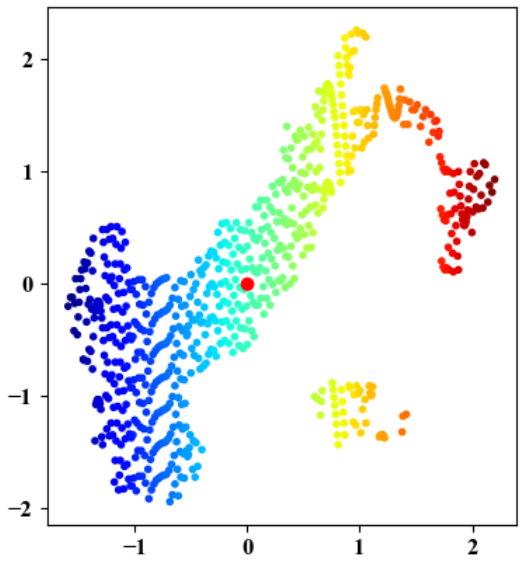
$$\text{Optional:} \quad \mathbf{x}_p \leftarrow \left(\mathbf{x}_p^{T\prime}\sigma\right) + \mu$$

In [41]:
```
pts = np.stack((X, Y), axis=1)
# Nx2
print(f'num of points {pts.shape[0]} in dimension {pts.shape[1]}' )
```

```
num of points 746 in dimension 2
```

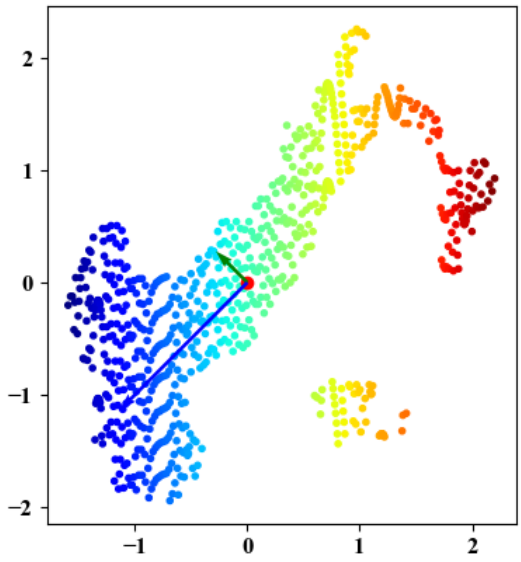
In [42]:
```
# Standardize the data
# (x-mu)/sigma
center = pts.mean(axis=0)
std = pts.std(axis=0)
pts_z = (pts - center)/std
```

In [43]:
```
fig = plt.scatter(*pts_z.T, c=X, marker='.', cmap='jet')
plt.scatter(0,0,c='red')
_ = plt.axis('scaled')
```



In [44]:
```
# np.cov wants features on rows
cov = np.cov(pts_z, rowvar=False)
Sigma, U = np.linalg.eig(cov)
```

In [45]:
```
# plot principal components aka eigenvectors
fig = plt.scatter(*pts_z.T, c=X, marker='.', cmap='jet')
plt.scatter(0,0,c='red')
plotVectors(fig.axes, [Sigma[0]*U[:,0], Sigma[1]*U[:,1]], cols=['green','blue'])
_ = plt.axis('scaled')
```

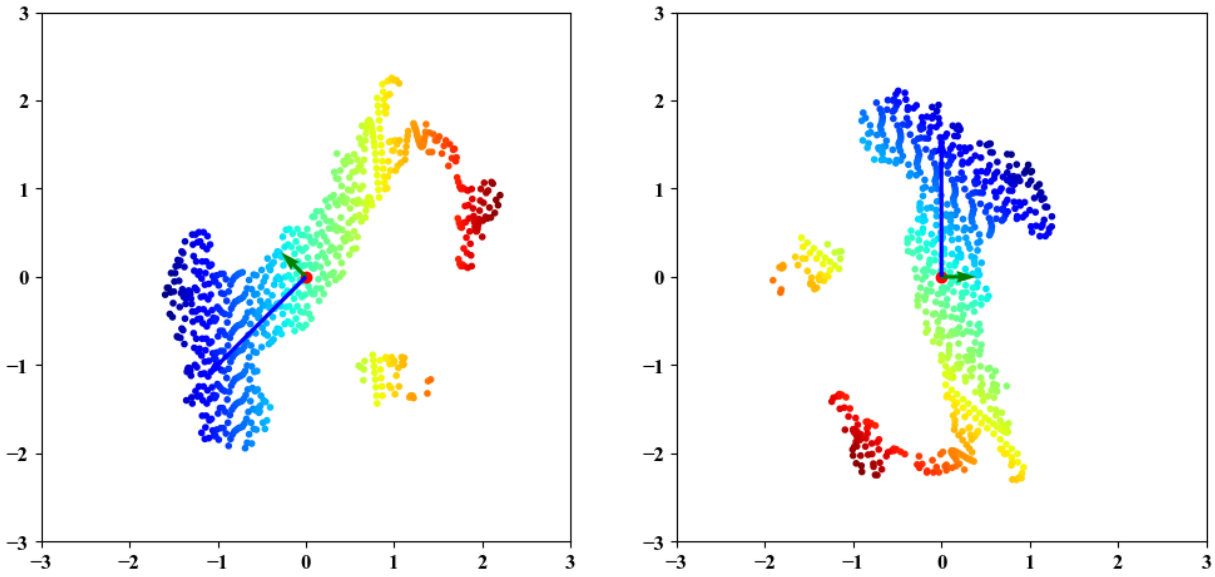


In [46]:
```
# rotate points
rot = U.T@pts_z.T
np.cov(rot,rowvar=True)
```

Out[46]:
```
array([[ 3.95280931e-01, -2.78971477e-16],
       [-2.78971477e-16,  1.60740363e+00]])
```

In [47]:
```
fig, ax = plt.subplots(1,2)
fig.set_figheight(12)
fig.set_figwidth(12)
# First
ax[0].scatter(*pts_z.T, c=X, marker='.', cmap='jet')
ax[0].scatter(0,0,c='red')
plotVectors(ax[0], [Sigma[0]*U[:,0], Sigma[1]*U[:,1]], cols=['green','blue'])
ax[0].set_aspect('equal')
ax[0].set_xlim(-3,3)
ax[0].set_ylim(-3,3)
# second
ax[1].scatter(*rot, c=X, marker='.', cmap='jet')
ax[1].scatter(0,0,c='red')
plotVectors(ax[1], [Sigma[0]*np.array([1,0]), Sigma[1]*np.array([0,1])], cols=['green','blue'])
ax[1].set_aspect('equal')
ax[1].set_xlim(-3,3)
ax[1].set_ylim(-3,3)
```

Out[47]:
```
(-3.0, 3.0)
```



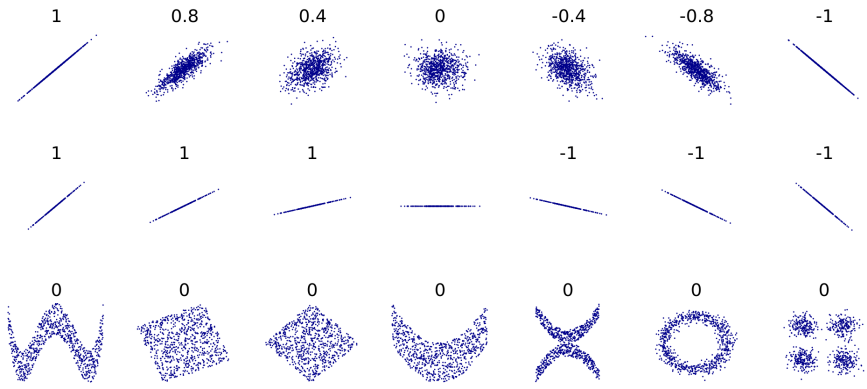
In [48]:
```
np.set_printoptions(suppress=True) #suppress scientific notation, please watch out using this
np.cov(rot, rowvar=True) # rowvar is True becausse matrix is 2xN
# do you know why we get this? and what are the values inside?
```

Out[48]:
```
array([[ 0.39528093, -0.        ],
       [-0.        ,  1.60740363]])
```

Application: Data whitening

What does it mean whitening or sphering?

Do you remember this?



Graphics from Wikipedia

PCA Application - Whitening - No compression

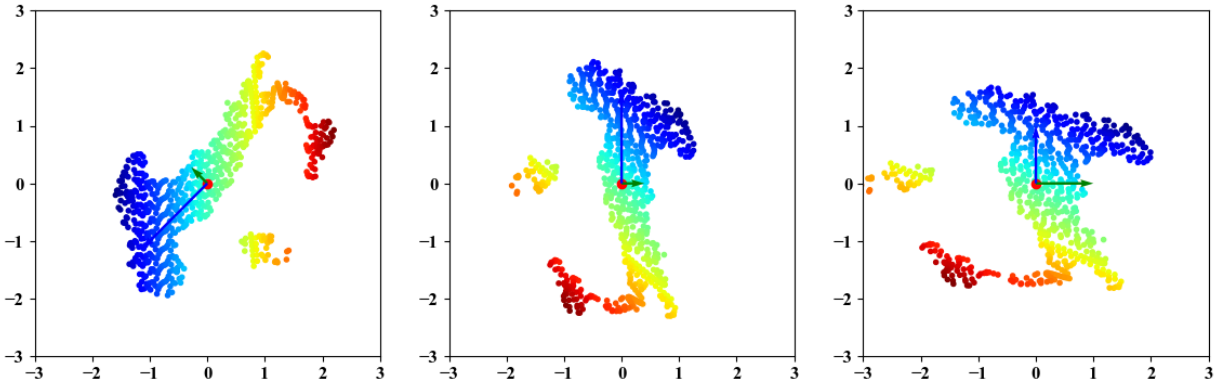
$$\mathbf{X}' \leftarrow \frac{\mathbf{X} - \mu}{\sigma}$$

$$\underbrace{\mathbf{x}_p^{T\prime}}_{\text{dec.}} = \mathbf{\Sigma}^{-1/2}\mathbf{U}^T \quad \underbrace{\mathbf{x}^{T\prime}}_{\text{orig}}$$

In [49]:
```
Sigma_inv_sqrt = np.diag(Sigma**-0.5)
# data is rotated and decorrelated (whitening or sphering)
rot_withening = Sigma_inv_sqrt @ U.T @ pts_z.T
```

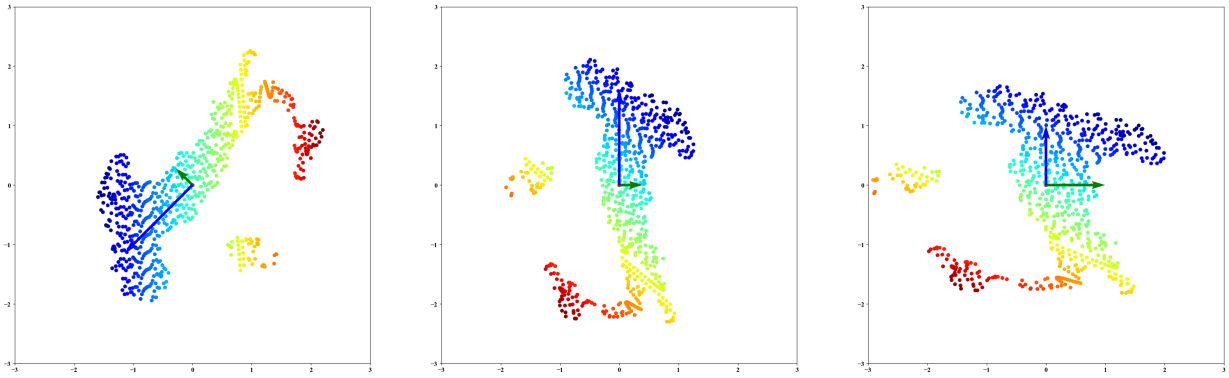
In [50]:
```
fig, ax = plt.subplots(1,3)
fig.set_figheight(14)
fig.set_figwidth(14)
# First
ax[0].scatter(*pts_z.T, c=X, marker='.', cmap='jet')
ax[0].scatter(0,0,c='red')
plotVectors(ax[0], [Sigma[0]*U[:,0], Sigma[1]*U[:,1]], cols=['green','blue'])
ax[0].set_aspect('equal')
ax[0].set_xlim(-3,3)
ax[0].set_ylim(-3,3)
# second
ax[1].scatter(*rot, c=X, marker='.', cmap='jet')
ax[1].scatter(0,0,c='red')
plotVectors(ax[1], [Sigma[0]*np.array([1,0]), Sigma[1]*np.array([0,1])], cols=['green','blue'])
ax[1].set_aspect('equal')
ax[1].set_xlim(-3,3)
ax[1].set_ylim(-3,3)
# third
ax[2].scatter(*rot_withening, c=X, marker='.', cmap='jet')
ax[2].scatter(0,0,c='red')
plotVectors(ax[2], [np.array([1,0]),
                    np.array([0,1])], cols=['green','blue'])
ax[2].set_aspect('equal')
ax[2].set_xlim(-3,3)
ax[2].set_ylim(-3,3)
```

Out[50]:
```
(-3.0, 3.0)
```



In [51]:
```
fig, ax = plt.subplots(1,3); sizeim=40;
fig.set_figheight(sizeim)
fig.set_figwidth(sizeim)
# First
ax[0].scatter(*pts_z.T, c=X, marker='o', cmap='jet')
ax[0].scatter(0,0,c='red')
plotVectors(ax[0], [Sigma[0]*U[:,0], Sigma[1]*U[:,1]], cols=['green','blue'])
ax[0].set_aspect('equal')
ax[0].set_xlim(-3,3)
ax[0].set_ylim(-3,3)
# second
ax[1].scatter(*rot, c=X, marker='o', cmap='jet')
ax[1].scatter(0,0,c='red')
plotVectors(ax[1], [Sigma[0]*np.array([1,0]), Sigma[1]*np.array([0,1])], cols=['green','blue'])
ax[1].set_aspect('equal')
ax[1].set_xlim(-3,3)
ax[1].set_ylim(-3,3)
# third
ax[2].scatter(*rot_withening, c=X, marker='o', cmap='jet')
ax[2].scatter(0,0,c='red')
plotVectors(ax[2], [np.array([1,0]),
                    np.array([0,1])], cols=['green','blue'])
ax[2].set_aspect('equal')
ax[2].set_xlim(-3,3)
ax[2].set_ylim(-3,3)
```

Out[51]: (-3.0, 3.0)



Sanity Check

We take the decorrelated data points and compute the covariance matrix:

$$\mathbf{X}_p\mathbf{X}_p^T$$

if **decorrelated** should get us:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and in more dimensions should give us $\mathbf{I}$ matrix (identity matrix)

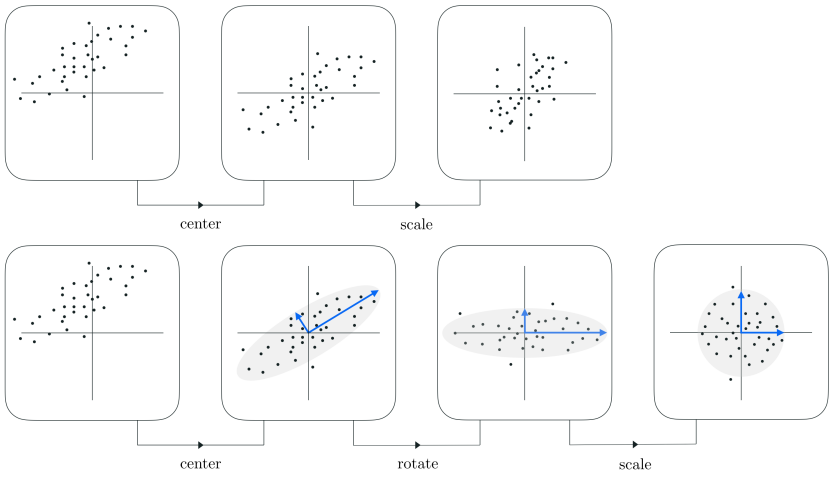
In [52]:
```
np.cov(rot_withening, rowvar=True) # rowvar is True becausse matrix is 2xN
```

Out[52]:
```
array([[ 1., -0.],
       [-0.,  1.]])
```

We can also "prove" it that induced decorrelated and "sphered" points:

$$\underbrace{\mathbf{x}_p^{T\prime}}_{\text{dec.}} = \mathbf{\Sigma}^{-1/2}\mathbf{U}^T \quad \underbrace{\mathbf{x}^{T\prime}}_{\text{orig}}$$

Sphering vs Standardization



PCA in Computer Graphics: 3D Morphable Models (3DMM)

- A set of 3D faces point cloud matrix $\mathbf{X} = \{\mathbf{S}_i\}_{i=1}^{M}$ with $\mathbf{S}_i \in \mathbf{R}^{3N}$ and M are the samples we have.
- $\mathbf{S}_i = [x_1, y_1, z_1, \ldots, x_N, y_N, z_N,]$ point cloud stack in a vector.
- **Assumption**: The point cloud is **vertex-aligned** (usually this implies dense registration, not easy to achieve)
- **Assumption**: $\mathbf{S} \sim \mathcal{N}(\mu, \mathbf{\Sigma})$ faces are modeled as a multi-variate Gaussian distribution.

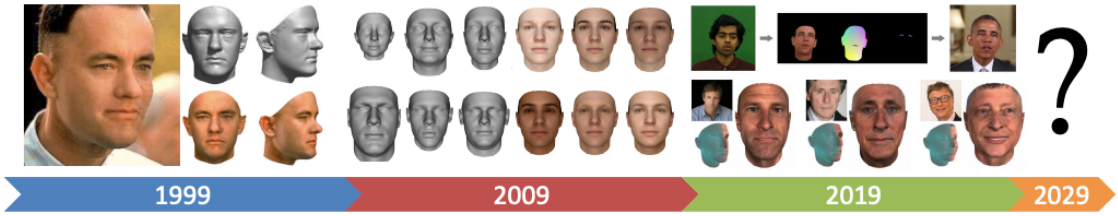


Figure Credit 3DMM, Past Present and Future

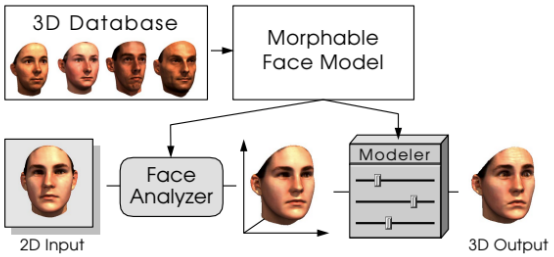


Fig. 2. The visual abstract of the seminal work by Blanz and Vetter [1999]. It proposes a statistical model for faces to perform 3D reconstruction from 2D images and a parametric face space which enables controlled manipulation.

Credits Blanz and Vetter, 1999

3D Face modeling with PCA

$\mathbf{S'} = \hat{\mathbf{S}} + \sum_i^{M-1} \alpha_i \mathbf{U}_i$ where:

- $\hat{\mathbf{S}}$ is the mean shape
- and $\mathbf{U}_i$ are the $M-1$ principal components that you can compute by learning PCA on $\mathbf{X} = \{\mathbf{S}_i\}_{i=1}^{M}$

A (new) 3D face is defined once you know $\boldsymbol{\alpha}$

- $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_k]$ scales each principal component
- Similar to say:
  - OK, this is the average face (fixed for everyone)
  - but I want to edit the average to add `0.25 * male (1st component)` + `-0.12 * caucasian (2nd component)` + `...`

3D Face modeling with PCA

$\mathbf{S'} = \hat{\mathbf{S}} + \sum_i^{M-1} \alpha_i \mathbf{U}_i$ where:

PCA assumes the data generation process is a **multivariate Gaussian distribution (i.e. a Gaussian/Normal distribution but in 3N-D).**

$$\underbrace{\{\mathbf{S}_i\}_{i=1}^{M}}_{\text{known}} \sim \underbrace{\mathcal{N}(\hat{\mathbf{S}}, \mathbf{Cov}_S)}_{\text{multivariate Gaussian assumption}} \approx \underbrace{\mathcal{D}}_{\text{unknown}}$$

- Given a face $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_k]$ you can compute how much it is likely of "being a face" under $\mathcal{N}(\hat{\mathbf{S}}, \mathbf{Cov}_S)$
- $\boldsymbol{\alpha} = [0.2, \ldots, 0.24]$ is **more probable** of being a face (you get something **regular**)
- $\boldsymbol{\alpha} = [0.1, \ldots, -1.24]$ is **less probable** of being a face (you get something **irregular**)

A common technique for data compression known as Principal Component Analysis (PCA) [15, 31] performs a basis transformation to an orthogonal coordinate system formed by the eigenvectors s_i and t_i of the covariance matrices (in descending order according to their eigenvalues)[2]:

$$S_{model} = \overline{S} + \sum_{i=1}^{m-1} \alpha_i s_i \,, \quad T_{model} = \overline{T} + \sum_{i=1}^{m-1} \beta_i t_i \,, \qquad (1)$$

$\vec{\alpha}, \vec{\beta} \in \Re^{m-1}$. The probability for coefficients $\vec{\alpha}$ is given by

$$p(\vec{\alpha}) \sim exp[-\frac{1}{2} \sum_{i=1}^{m-1} (\alpha_i / \sigma_i)^2], \qquad (2)$$

0:00 / 2:03

Principal Components refers to Variations in Faces

- 1st component: gender or age (most variation)
- 2nd component: face size (moderate variation)
- .....
- last component: nose size etc (least variation)

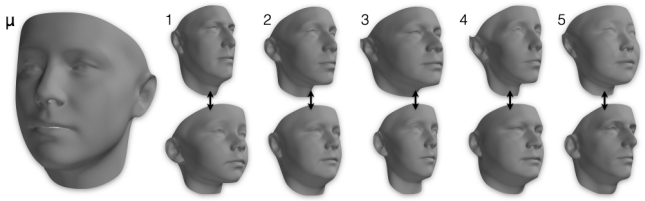


Figure 4: Visualisations of the first five principal components of shape for LSFM, each visualised as additions and subtractions away from the mean (also shown, *left*).

Figure credit Booth et al. 3DMM in the Wild

Click here for interactive demo - FLAME - Max Planck

Expressiveness

$\mathbf{S'} = \hat{\mathbf{S}} + \sum_i^{M-1} \alpha_i \mathbf{U}_i$ where:

- $\hat{\mathbf{S}}$ is the mean shape
- and $\mathbf{U}_i$ are the $M-1$ principal components that you can compute by learning PCA on $\mathbf{X} = \{\mathbf{S}_i\}_{i=1}^{M}$.

Part-based 3DMM

- The expressiveness of the model can be increased by dividing faces into **independent sub-regions** that are morphed independently, for example into eyes, nose, mouth and a surrounding region.
- Since **all faces are assumed to be in correspondence**, it is sufficient to define these regions on a reference face. This segmentation is equivalent to sub-dividing the vector space of faces into **independent subspaces**.
- A complete 3D face is generated by computing linear combinations for each segment separately and **blending** them at the borders according to an algorithm proposed for images by a blending algorithm

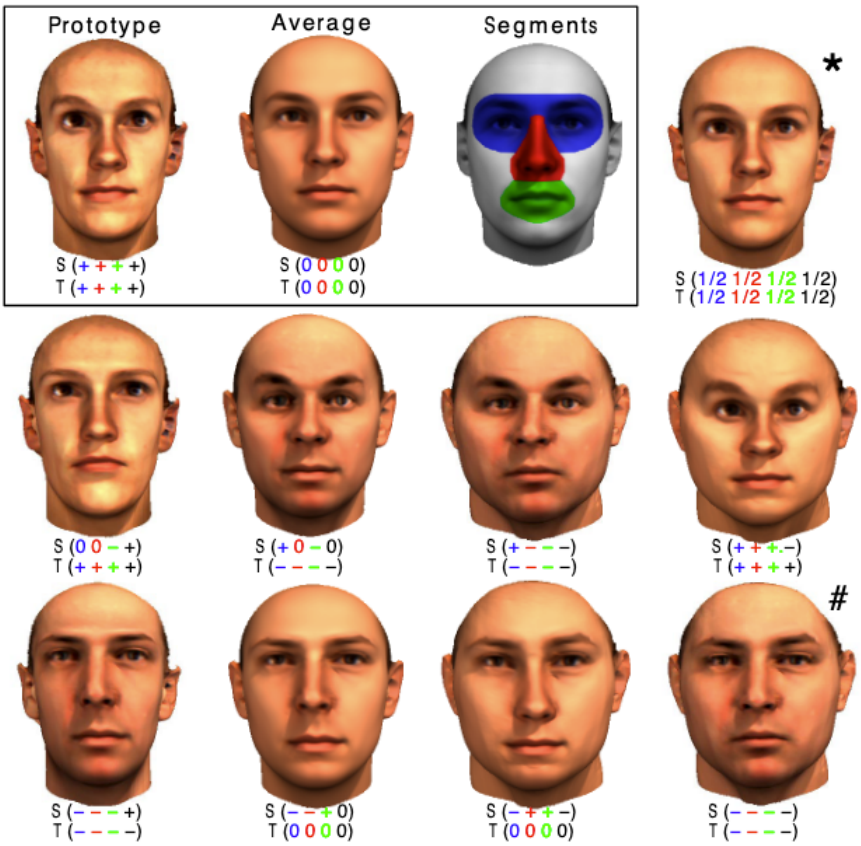


Figure 2: A single prototype adds a large variety of new faces to the morphable model. The deviation of a prototype from the average is added (+) or subtracted (-) from the average. A standard morph (*) is located halfway between average and the prototype. Subtracting the differences from the average yields an 'anti'-face (#). Adding and subtracting deviations independently for shape (S) and texture (T) on each of four segments produces a number of distinct faces.

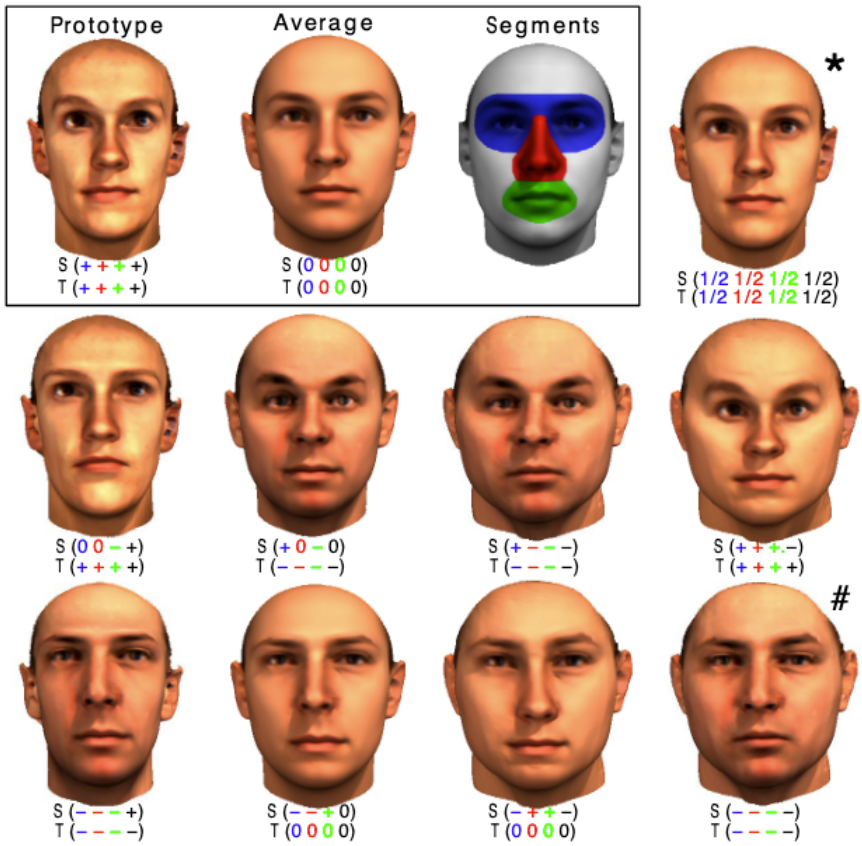


Figure 2: A single prototype adds a large variety of new faces to the morphable model. The deviation of a prototype from the average is added (+) or subtracted (-) from the average. A standard morph (*) is located halfway between average and the prototype. Subtracting the differences from the average yields an 'anti'-face (#). Adding and subtracting deviations independently for shape (S) and texture (T) on each of four segments produces a number of distinct faces.

Two more real world examples

Morphable Models are everywhere - Snapfeet App

Body Morphable Models @ Max Planck Institute for Intelligent Systems

Up next: PCA in High Dimensional Space

- Demonstration with images
- You can think of an image $\mathbf{I} \in \mathbb{R}^{W \times H}$ as a point/vector in high dimension.
- For an image 128×128 now our D dimension is very high. $D = 128^2 = (2^7)^2 = 2^{14} \approx 16K$

- Let's double the image $128 \mapsto 256$

- For an image 256×256 now our D dimension is very high. $D = 256^2 = (2^8)^2 = 2^{16} \approx 65K$
- Doubling a side, increases the dimension four times, for two-dimensional nature of images.

PCA is in sklearn but implementing it manually is for understanding

```
from sklearn.decomposition import PCA
pca = PCA(n_components=2)
pca.fit(X)
```

In case you have to use it in industry/thesis, you will rely on `sklearn`

i.e. "not reinventing the wheel" but academically it is good to do it manually