

$$\begin{aligned}
\max_{u: \|u\|_2=1} u^T \Sigma u &= \max_{u: \|u\|_2=1} u^T V \Lambda V^T u \\
&= \max_{u: \|u\|_2=1} (V^T u)^T \Lambda V^T u
\end{aligned}$$

Here is an aside: note through this one line proof that left-multiplying a vector by an orthogonal (or rotation) matrix preserves the length of the vector:

$$\|V^T u\|_2 = \sqrt{(V^T u)^T (V^T u)} = \sqrt{u^T V V^T u} = \sqrt{u^T u} = \|u\|_2$$

I define a new variable $z = V^T u$, and maximize over this variable. Note that because V is invertible, there is a one to one mapping between u and z . Also note that the constraint is the same because the length of the vector u does not change when multiplied by an orthogonal matrix.

$$\max_{z: \|z\|_2=1} z^T \Lambda z = \max_z \sum_{i=1}^d \lambda_i z_i^2 \quad : \quad \sum_{i=1}^d z_i^2 = 1$$

From this new formulation, it is obvious to see that we can maximize this by throwing all of our eggs into one basket and setting $z_i^* = 1$ if i is the index of the largest eigenvalue, and $z_i^* = 0$ otherwise. Thus,

$$z^* = V^T u^* \implies u^* = V z^* = v_1$$

where v_1 is the "principle" eigenvector, and corresponds to λ_1 . Plugging this into the objective function, we see that the optimal value is λ_1 .