CSE 291: Unsupervised learning **Spring 2008**

Lecture 7 — Spectral methods

7.1 Linear algebra review

7.1.1 Eigenvalues and eigenvectors

Definition 1. A $d \times d$ matrix $\mathbf{M}$ has *eigenvalue* λ if there is a d-dimensional vector $\mathbf{u} \neq \mathbf{0}$ for which $\mathbf{M}\mathbf{u} = \lambda\mathbf{u}$. This $\mathbf{u}$ is the *eigenvector* corresponding to λ.

In other words, the linear transformation $\mathbf{M}$ maps vector $\mathbf{u}$ into the same direction. It is interesting that *any* linear transformation necessarily has directional fixed points of this kind. The following chain of implications helps in understanding this:

$$\begin{aligned}
& \lambda \text{ is an eigenvalue of } \mathbf{M} \\
\Leftrightarrow\;& \text{there exists } \mathbf{u} \neq \mathbf{0} \text{ with } \mathbf{M}\mathbf{u} = \lambda\mathbf{u} \\
\Leftrightarrow\;& \text{there exists } \mathbf{u} \neq \mathbf{0} \text{ with } (\mathbf{M} - \lambda\mathbf{I})\mathbf{u} = \mathbf{0} \\
\Leftrightarrow\;& (\mathbf{M} - \lambda\mathbf{I}) \text{ is singular (that is, not invertible)} \\
\Leftrightarrow\;& \det(\mathbf{M} - \lambda\mathbf{I}) = 0.
\end{aligned}$$

Now, $\det(\mathbf{M} - \lambda\mathbf{I})$ is a polynomial of degree d in λ. As such it has d roots (although some of them might be complex). This explains the existence of eigenvalues.

A case of great interest is when $\mathbf{M}$ is real-valued and symmetric, because then the eigenvalues are real.

Theorem 2. *Let $\mathbf{M}$ be any real symmetric $d \times d$ matrix. Then:*

1. *$\mathbf{M}$ has d real eigenvalues $\lambda_1, \ldots, \lambda_d$ (not necessarily distinct).*
2. *There is a set of d corresponding eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_d$ that constitute an orthonormal basis of $\mathbb{R}^d$, that is, $\mathbf{u}_i \cdot \mathbf{u}_j = \delta_{ij}$ for all i, j.*

7.1.2 Spectral decomposition

The spectral decomposition recasts a matrix in terms of its eigenvalues and eigenvectors. This representation turns out to be enormously useful.

Theorem 3. *Let $\mathbf{M}$ be a real symmetric $d \times d$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_d$ and corresponding orthonormal eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_d$. Then:*

1. $$\mathbf{M} = \underbrace{\begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_d \\ \downarrow & \downarrow & & \downarrow \end{pmatrix}}_{\text{call this } \mathbf{Q}} \underbrace{\begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_d \end{pmatrix}}_{\mathbf{\Lambda}} \underbrace{\begin{pmatrix} \longleftarrow & \mathbf{u}_1 & \longrightarrow \\ \longleftarrow & \mathbf{u}_2 & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{u}_d & \longrightarrow \end{pmatrix}}_{\mathbf{Q}^T}.$$

2. $\mathbf{M} = \sum_{i=1}^d \lambda_i \mathbf{u}_i \mathbf{u}_i^T$.

Proof. A general proof strategy is to observe that $\mathbf{M}$ represents a linear transformation $\mathbf{x} \mapsto \mathbf{Mx}$ on $\mathbb{R}^d$, and as such, is completely determined by its behavior on *any* set of d linearly independent vectors. For instance, $\{\mathbf{u}_1, \ldots, \mathbf{u}_d\}$ are linearly independent, so any $d \times d$ matrix $\mathbf{N}$ that satisfies $\mathbf{N}\mathbf{u}_i = \mathbf{M}\mathbf{u}_i$ (for all i) is necessarily identical to $\mathbf{M}$.

Let's start by verifying (1). For practice, we'll do this two different ways.

Method One: For any i, we have

$$\mathbf{Q\Lambda Q}^T \mathbf{u}_i \;=\; \mathbf{Q\Lambda e}_i \;=\; \mathbf{Q}\lambda_i \mathbf{e}_i \;=\; \lambda_i \mathbf{Q}\mathbf{e}_i \;=\; \lambda_i \mathbf{u}_i \;=\; \mathbf{M}\mathbf{u}_i.$$

Thus $\mathbf{Q\Lambda Q}^T = \mathbf{M}$.

Method Two: Since the $\mathbf{u}_i$ are orthonormal, we have $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$. Thus $\mathbf{Q}$ is invertible, with $\mathbf{Q}^{-1} = \mathbf{Q}^T$; whereupon $\mathbf{QQ}^T = \mathbf{I}$. For any i,

$$\mathbf{Q}^T\mathbf{MQe}_i \;=\; \mathbf{Q}^T\mathbf{M}\mathbf{u}_i \;=\; \mathbf{Q}^T\lambda_i\mathbf{u}_i \;=\; \lambda_i\mathbf{Q}^T\mathbf{u}_i \;=\; \lambda_i\mathbf{e}_i \;=\; \mathbf{\Lambda e}_i.$$

Thus $\mathbf{\Lambda} = \mathbf{Q}^T\mathbf{MQ}$, which implies $\mathbf{M} = \mathbf{Q\Lambda Q}^T$.

Now for (2). Again we use the same proof strategy. For any j,

$$\left(\sum_i \lambda_i \mathbf{u}_i \mathbf{u}_i^T\right)\mathbf{u}_j \;=\; \lambda_j \mathbf{u}_j \;=\; \mathbf{M}\mathbf{u}_j.$$

Hence $\mathbf{M} = \sum_i \lambda_i \mathbf{u}_i \mathbf{u}_i^T$. □

7.1.3 Positive semidefinite matrices

We now introduce an important subclass of real symmetric matrices.

Definition 4. A real symmetric $d \times d$ matrix $\mathbf{M}$ is *positive semidefinite* (denoted $\mathbf{M} \succcurlyeq 0$) if $\mathbf{z}^T\mathbf{Mz} \geq 0$ for all $\mathbf{z} \in \mathbb{R}^d$. It is *positive definite* (denoted $\mathbf{M} \succ 0$) if $\mathbf{z}^T\mathbf{Mz} > 0$ for all nonzero $\mathbf{z} \in \mathbb{R}^d$.

Example 5. Consider any random vector $X \in \mathbb{R}^d$, and let $\mu = \mathbb{E}X$ and $\mathbf{S} = \mathbb{E}[(X-\mu)(X-\mu)^T]$ denote its mean and covariance, respectively. Then $\mathbf{S} \succcurlyeq 0$ because for any $\mathbf{z} \in \mathbb{R}^d$,

$$\mathbf{z}^T\mathbf{Sz} \;=\; \mathbf{z}^T\mathbb{E}[(X-\mu)(X-\mu)^T]\mathbf{z} \;=\; \mathbb{E}[(\mathbf{z}^T(X-\mu))((X-\mu)^T\mathbf{z})] \;=\; \mathbb{E}[(\mathbf{z}\cdot(X-\mu))^2] \;\geq\; 0.$$

Positive (semi)definiteness is easily characterized in terms of eigenvalues.

Theorem 6. *Let* $\mathbf{M}$ *be a real symmetric* $d \times d$ *matrix. Then:*

1. $\mathbf{M}$ *is positive semidefinite iff all its eigenvalues* $\lambda_i \geq 0$.
2. $\mathbf{M}$ *is positive definite iff all its eigenvalues* $\lambda_i > 0$.

Proof. Let's prove (1) (the second is similar). Let $\lambda_1, \ldots, \lambda_d$ be the eigenvalues of $\mathbf{M}$, with corresponding eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_d$.

First, suppose $\mathbf{M} \succcurlyeq 0$. Then for all i, $\lambda_i = \mathbf{u}_i^T\mathbf{M}\mathbf{u}_i \geq 0$.

Conversely, suppose that all the $\lambda_i \geq 0$. Then for any $\mathbf{z} \in \mathbb{R}^d$, we have

$$\mathbf{z}^T\mathbf{Mz} \;=\; \mathbf{z}^T\left(\sum_{i=1}^d \lambda_i \mathbf{u}_i \mathbf{u}_i^T\right)\mathbf{z} \;=\; \sum_{i=1}^d \lambda_i (\mathbf{z}\cdot\mathbf{u})^2 \;\geq\; 0.$$

□

7.1.4 The Rayleigh quotient

One of the reasons why eigenvalues are so useful is that they constitute the optimal solution of a very basic quadratic optimization problem.

Theorem 7. *Let* $\mathbf{M}$ *be a real symmetric* $d \times d$ *matrix with eigenvalues* $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$*, and corresponding eigenvectors* $\mathbf{u}_1, \ldots, \mathbf{u}_d$*. Then:*

$$\max_{\|\mathbf{z}\|=1} \mathbf{z}^T \mathbf{M} \mathbf{z} \;=\; \max_{\mathbf{z} \neq \mathbf{0}} \frac{\mathbf{z}^T \mathbf{M} \mathbf{z}}{\mathbf{z}^T \mathbf{z}} \;=\; \lambda_1$$

$$\min_{\|\mathbf{z}\|=1} \mathbf{z}^T \mathbf{M} \mathbf{z} \;=\; \min_{\mathbf{z} \neq \mathbf{0}} \frac{\mathbf{z}^T \mathbf{M} \mathbf{z}}{\mathbf{z}^T \mathbf{z}} \;=\; \lambda_d$$

and these are realized at $\mathbf{z} = \mathbf{u}_1$ *and* $\mathbf{z} = \mathbf{u}_d$*, respectively.*

Proof. Denote the spectral decomposition by $\mathbf{M} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T$. Then:

$$\begin{aligned}
\max_{\mathbf{z} \neq \mathbf{0}} \frac{\mathbf{z}^T \mathbf{M} \mathbf{z}}{\mathbf{z}^T \mathbf{z}} &= \max_{\mathbf{z} \neq \mathbf{0}} \frac{\mathbf{z}^T \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T \mathbf{z}}{\mathbf{z}^T \mathbf{Q} \mathbf{Q}^T \mathbf{z}} \qquad (\text{since } \mathbf{Q}\mathbf{Q}^T = \mathbf{I}) \\
&= \max_{\mathbf{y} \neq \mathbf{0}} \frac{\mathbf{y}^T \mathbf{\Lambda} \mathbf{y}}{\mathbf{y}^T \mathbf{y}} \qquad (\text{writing } \mathbf{y} = \mathbf{Q}^T \mathbf{z}) \\
&= \max_{\mathbf{y} \neq \mathbf{0}} \frac{\lambda_1 y_1^2 + \cdots + \lambda_d y_d^2}{y_1^2 + \cdots + y_d^2} \;\leq\; \lambda_1,
\end{aligned}$$

where equality is attained in the last step when $\mathbf{y} = \mathbf{e}_1$, that is, $\mathbf{z} = \mathbf{Q}\mathbf{e}_1 = \mathbf{u}_1$. The argument for the minimum is identical. $\square$

Example 8. Suppose random vector $X \in \mathbb{R}^d$ has mean μ and covariance matrix $\mathbf{M}$. Then $\mathbf{z}^T \mathbf{M} \mathbf{z}$ represents the variance of X in direction $\mathbf{z}$:

$$\text{var}(\mathbf{z}^T X) \;=\; \mathbb{E}[(\mathbf{z}^T (X - \mu))^2] \;=\; \mathbb{E}[\mathbf{z}^T (X - \mu)(X - \mu)^T \mathbf{z}] \;=\; \mathbf{z}^T \mathbf{M} \mathbf{z}.$$

Theorem 7 tells us that the direction of maximum variance is $\mathbf{u}_1$, and that of minimum variance is $\mathbf{u}_d$.

Continuing with this example, suppose that we are interested in the k-dimensional subspace (of $\mathbb{R}^d$) that has the most variance. How can this be formalized?

To start with, we will think of a linear projection from $\mathbb{R}^d$ to $\mathbb{R}^k$ as a function $\mathbf{x} \mapsto \mathbf{P}^T \mathbf{x}$, where $\mathbf{P}^T$ is a $k \times d$ matrix with $\mathbf{P}^T \mathbf{P} = \mathbf{I}_k$. The last condition simply says that the rows of the projection matrix are orthonormal.

When a random vector $X \in \mathbb{R}^d$ is subjected to such a projection, the resulting k-dimensional vector has covariance matrix

$$\text{cov}(\mathbf{P}^T X) \;=\; \mathbb{E}[\mathbf{P}^T (X - \mu)(X - \mu)^T \mathbf{P}] \;=\; \mathbf{P}^T \mathbf{M} \mathbf{P}.$$

Often we want to summarize the variance by just a single number rather than an entire matrix; in such cases, we typically use the *trace* of this matrix, and we write $\text{var}(\mathbf{P}^T X) = \text{tr}(\mathbf{P}^T \mathbf{M} \mathbf{P})$. This is also equal to $\mathbb{E}\|\mathbf{P}^T X - \mathbf{P}^T \mu\|^2$. With this terminology established, we can now determine the projection $\mathbf{P}^T$ that maximizes this variance.

Theorem 9. *Let* $\mathbf{M}$ *be a real symmetric* $d \times d$ *matrix as in Theorem 7. Pick any* $k \leq d$*.*

$$\max_{\mathbf{P} \in \mathbb{R}^{d \times k}, \mathbf{P}^T \mathbf{P} = \mathbf{I}} \text{tr}(\mathbf{P}^T \mathbf{M} \mathbf{P}) \;=\; \lambda_1 + \cdots + \lambda_k$$

$$\min_{\mathbf{P} \in \mathbb{R}^{d \times k}, \mathbf{P}^T \mathbf{P} = \mathbf{I}} \text{tr}(\mathbf{P}^T \mathbf{M} \mathbf{P}) \;=\; \lambda_{d-k+1} + \cdots + \lambda_d.$$

These are realized when the columns of $\mathbf{P}$ *span the* k*-dimensional subspace spanned by* $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ *and* $\{\mathbf{u}_{d-k+1}, \ldots, \mathbf{u}_d\}$*, respectively.*

Proof. We will prove the result for the maximum; the other case is symmetric. Let $\mathbf{p}_1, \ldots, \mathbf{p}_k$ denote the columns of $\mathbf{P}$. Then

$$\mathrm{tr}\left(\mathbf{P}^T\mathbf{MP}\right) \;=\; \sum_{i=1}^k \mathbf{p}_i^T\mathbf{M}\mathbf{p}_i \;=\; \sum_{i=1}^k \mathbf{p}_i^T\left(\sum_{j=1}^d \lambda_j \mathbf{u}_j\mathbf{u}_j^T\right)\mathbf{p}_i \;=\; \sum_{j=1}^d \lambda_j \sum_{i=1}^k (\mathbf{p}_i \cdot \mathbf{u}_j)^2.$$

We will show that this quantity is at most $\lambda_1 + \cdots + \lambda_k$. To this end, let z_j denote $\sum_{i=1}^k (\mathbf{p}_i \cdot \mathbf{u}_j)^2$; clearly it is nonnegative. We will show that $\sum_j z_j = k$ and that each $z_j \leq 1$; the desired bound is then immediate.

First,

$$\sum_{j=1}^d z_j \;=\; \sum_{i=1}^k\sum_{j=1}^d (\mathbf{p}_i \cdot \mathbf{u}_j)^2 \;=\; \sum_{i=1}^k\sum_{j=1}^d \mathbf{p}_i^T\mathbf{u}_j\mathbf{u}_j^T\mathbf{p}_i \;=\; \sum_{i=1}^k \mathbf{p}_i^T\mathbf{Q}\mathbf{Q}^T\mathbf{p}_i \;=\; \sum_{i=1}^k \|\mathbf{p}_i\|^2 \;=\; k.$$

To upper-bound an individual z_j, start by extending the k orthonormal vectors $\mathbf{p}_1, \ldots, \mathbf{p}_k$ to a full orthonormal basis $\mathbf{p}_1, \ldots, \mathbf{p}_d$ of $\mathbb{R}^d$. Then

$$z_j \;=\; \sum_{i=1}^k (\mathbf{p}_i \cdot \mathbf{u}_j)^2 \;\leq\; \sum_{i=1}^d (\mathbf{p}_i \cdot \mathbf{u}_j)^2 \;=\; \sum_{i=1}^d \mathbf{u}_j^T\mathbf{p}_i\mathbf{p}_i^T\mathbf{u}_j \;=\; \|\mathbf{u}_j^T\|^2 \;=\; 1.$$

It then follows that

$$\mathrm{tr}\left(\mathbf{P}^T\mathbf{MP}\right) \;=\; \sum_{j=1}^d \lambda_j z_j \;\leq\; \lambda_1 + \cdots + \lambda_k,$$

and equality holds when $\mathbf{p}_1, \ldots, \mathbf{p}_k$ span the same space as $\mathbf{u}_1, \ldots, \mathbf{u}_k$. □

7.2 Principal component analysis

Let $X \in \mathbb{R}^d$ be a random vector. We wish to find the single direction that captures as much as possible of the variance of X. Formally: we want $\mathbf{p} \in \mathbb{R}^d$ (the direction) such that $\|\mathbf{p}\| = 1$, so as to maximize $\mathrm{var}(\mathbf{p}^TX)$.

Theorem 10. *The solution to this optimization problem is to make* $\mathbf{p}$ *the principal eigenvector of* $\mathrm{cov}(X)$*.*

Proof. Denote $\mu = \mathbb{E}X$ and $\mathbf{S} = \mathrm{cov}(X) = \mathbb{E}[(X-\mu)(X-\mu)^T]$. For any $\mathbf{p} \in \mathbb{R}^d$, the projection $\mathbf{p}^TX$ has mean $\mathbb{E}[\mathbf{p}^TX] = \mathbf{p}^T\mu$ and variance

$$\mathrm{var}(\mathbf{p}^TX) \;=\; \mathbb{E}[(\mathbf{p}^TX - \mathbf{p}^T\mu)^2] \;=\; \mathbb{E}[\mathbf{p}^T(X-\mu)(X-\mu)^T\mathbf{p}] \;=\; \mathbf{p}^T\mathbf{S}\mathbf{p}.$$

By Theorem 7, this is maximized (over all unit-length $\mathbf{p}$) when $\mathbf{p}$ is the principal eigenvector of $\mathbf{S}$. □

Likewise, the k-dimensional subspace that captures as much as possible of the variance of X is simply the subspace spanned by the top k eigenvectors of $\mathrm{cov}(X)$; call these $\mathbf{u}_1, \ldots, \mathbf{u}_k$.

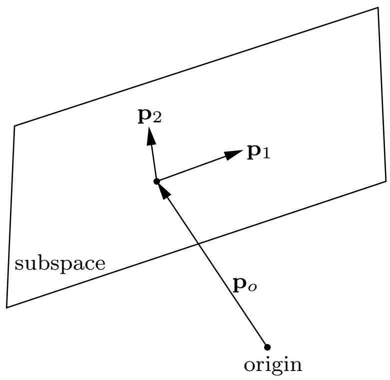
Projection onto these eigenvectors is called *principal component analysis* (PCA). It can be used to reduce the dimension of the data from d to k. Here are the steps:

- Compute the mean μ and covariance matrix $\mathbf{S}$ of the data X.
- Compute the top k eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ of $\mathbf{S}$.
- Project $X \mapsto \mathbf{P}^TX$, where $\mathbf{P}^T$ is the $k \times d$ matrix whose rows are $\mathbf{u}_1, \ldots, \mathbf{u}_k$.

7.2.1 The best approximating affine subspace

We've seen one optimality property of PCA. Here's another: it is the k-dimensional affine subspace that best approximates X, in the sense that the expected squared distance from X to the subspace is minimized.

Let's formalize the problem. A k-dimensional affine subspace is given by a displacement $\mathbf{p}_o \in \mathbb{R}^d$ and a set of (orthonormal) basis vectors $\mathbf{p}_1, \ldots, \mathbf{p}_k \in \mathbb{R}^d$. The subspace itself is then $\{\mathbf{p}_o + \alpha_1 \mathbf{p}_1 + \cdots + \alpha_k \mathbf{p}_k : \alpha_i \in \mathbb{R}\}$.



The projection of $X \in \mathbb{R}^d$ onto this subspace is $\mathbf{P}^T X + \mathbf{p}_o$, where $\mathbf{P}^T$ is the $k \times d$ matrix whose rows are $\mathbf{p}_1, \ldots, \mathbf{p}_k$. Thus, the expected squared distance from X to this subspace is $\mathbb{E}\|X - (\mathbf{P}^T X + \mathbf{p}_o)\|^2$. We wish to find the subspace for which this is minimized.

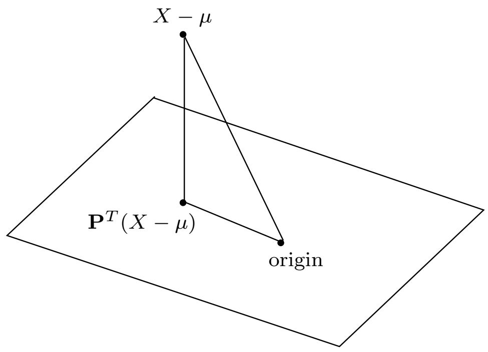
Theorem 11. *Let μ and $\mathbf{S}$ denote the mean and covariance of X, respectively. The solution of this optimization problem is to choose $\mathbf{p}_1, \ldots, \mathbf{p}_k$ to be the top k eigenvectors of $\mathbf{S}$ and to set $\mathbf{p}_o = (\mathbf{I} - \mathbf{P}^T)\mu$.*

Proof. Fix any matrix $\mathbf{P}$; the choice of $\mathbf{p}_o$ that minimizes $\mathbb{E}\|X - (\mathbf{P}^T X + \mathbf{p}_o)\|^2$ is (by calculus) $\mathbf{p}_o = \mathbb{E}[X - \mathbf{P}^T X] = (\mathbf{I} - \mathbf{P}^T)\mu$.

Now let's optimize $\mathbf{P}$. Our cost function is

$$\mathbb{E}\|X - (\mathbf{P}^T X + \mathbf{p}_o)\|^2 \;=\; \mathbb{E}\|(\mathbf{I} - \mathbf{P}^T)(X - \mu)\|^2 \;=\; \mathbb{E}\|X - \mu\|^2 - \mathbb{E}\|\mathbf{P}^T (X - \mu)\|^2,$$

where the second step is simply an invocation of the Pythagorean theorem.



Therefore, we need to maximize $\mathbb{E}\|\mathbf{P}^T (X - \mu)\|^2 = \mathrm{var}(\mathbf{P}^T X)$, and we've already seen how to do this in Theorem 10 and the ensuing discussion. $\square$

7.2.2 The projection that best preserves interpoint distances

Suppose we want to find the k-dimensional projection that minimizes the expected distortion in interpoint distances. More precisely, we want to find the $k \times d$ projection matrix $\mathbf{P}^T$ (with $\mathbf{P}^T\mathbf{P} = \mathbf{I}_k$) such that, for i.i.d. random vectors X and Y, expected squared distortion $\mathbb{E}[\|X - Y\|^2 - \|\mathbf{P}^T X - \mathbf{P}^T Y\|^2]$ is minimized (of course, the term in brackets is always positive).

Theorem 12. *The solution is to make the rows of* $\mathbf{P}^T$ *the top* k *eigenvectors of* $\mathrm{cov}(X)$.

Proof. This time we want to maximize

$$\mathbb{E}\|\mathbf{P}^T X - \mathbf{P}^T Y\|^2 \;=\; 2\,\mathbb{E}\|\mathbf{P}^T X - \mathbf{P}^T \mu\|^2 \;=\; 2\,\mathrm{var}(\mathbf{P}^T X),$$

and once again we're back to our original problem. □

This is emphatically not the same as finding the *linear transformation* (that is, not necessarily a projection) $\mathbf{P}^T$ for which $\mathbb{E}\left|\|X - Y\|^2 - \|\mathbf{P}^T X - \mathbf{P}^T Y\|^2\right|$ is minimized. The random projection method that we saw earlier falls in this latter camp, because it consists of a projection *followed by a scaling by* $\sqrt{d/k}$.

7.2.3 A prelude to k-means clustering

Suppose that for random vector $X \in \mathbb{R}^d$, the optimal k-means centers are $\mu_1^*, \ldots, \mu_k^*$, with cost

$$\textsc{opt} \;=\; \mathbb{E}\|X - (\text{nearest } \mu_i^*)\|^2.$$

If instead, we project X into the k-dimensional PCA subspace, and find the best k centers $\mu_1, \ldots, \mu_k$ *in that subspace*, how bad can these centers be?

Theorem 13. $\mathrm{cost}(\mu_1, \ldots, \mu_k) \le 2 \cdot \textsc{opt}$.

Proof. Without loss of generality $\mathbb{E}X = \mathbf{0}$ and the PCA mapping is $X \mapsto \mathbf{P}^T X$. Since $\mu_1, \ldots, \mu_k$ are the best centers for $\mathbf{P}^T X$, it follows that

$$\mathbb{E}\|\mathbf{P}^T X - (\text{nearest } \mu_i)\|^2 \;\le\; \mathbb{E}\|\mathbf{P}^T(X - (\text{nearest } \mu_i^*))\|^2 \;\le\; \mathbb{E}\|X - (\text{nearest } \mu_i^*)\|^2 \;=\; \textsc{opt}.$$

Let $X \mapsto \mathbf{A}^T X$ denote projection onto the subspace spanned by $\mu_1^*, \ldots, \mu_k^*$. From our earlier result on approximating affine subspaces, we know that $\mathbb{E}\|X - \mathbf{P}^T X\|^2 \le \mathbb{E}\|X - \mathbf{A}^T X\|^2$. Thus

$$\begin{aligned}
\mathrm{cost}(\mu_1, \ldots, \mu_k) &= \mathbb{E}\|X - (\text{nearest } \mu_i)\|^2 \\
&= \mathbb{E}\|\mathbf{P}^T X - (\text{nearest } \mu_i)\|^2 + \mathbb{E}\|X - \mathbf{P}^T X\|^2 \qquad \text{(Pythagorean theorem)} \\
&\le \textsc{opt} + \mathbb{E}\|X - \mathbf{A}^T X\|^2 \\
&\le \textsc{opt} + \mathbb{E}\|X - (\text{nearest } \mu_i^*)\|^2 \;=\; 2 \cdot \textsc{opt}.
\end{aligned}$$

□

7.3 Singular value decomposition

For any real symmetric $d \times d$ matrix $\mathbf{M}$, we can find its eigenvalues $\lambda_1 \ge \cdots \ge \lambda_d$ and corresponding orthonormal eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_d$, and write

$$\mathbf{M} \;=\; \sum_{i=1}^{d} \lambda_i \mathbf{u}_i \mathbf{u}_i^T.$$

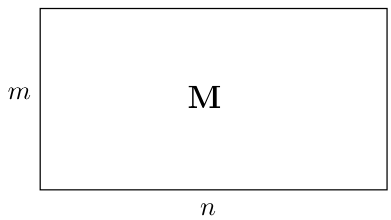
The best rank-k approximation to $\mathbf{M}$ is

$$\mathbf{M}_k \;=\; \sum_{i=1}^{k} \lambda_i \mathbf{u}_i \mathbf{u}_i^T,$$

in the sense that this minimizes $\|\mathbf{M} - \mathbf{M}_k\|_F^2$ over all rank-k matrices. (Here $\|\cdot\|_F$ denotes Frobenius norm; it is the same as L_2 norm if you imagine the matrix rearranged into a very long vector.)

In many applications, $\mathbf{M}_k$ is an adequate approximation of $\mathbf{M}$ even for fairly small values of k. And it is conveniently compact, of size $O(kd)$.

But what if we are dealing with a matrix $\mathbf{M}$ that is not square; say it is $m \times n$ with $m \leq n$:



To find a compact approximation in such cases, we look at $\mathbf{M}^T\mathbf{M}$ or $\mathbf{M}\mathbf{M}^T$, which are square. Eigendecompositions of these matrices lead to a good representation of $\mathbf{M}$.

7.3.1 The relationship between $\mathbf{M}\mathbf{M}^T$ and $\mathbf{M}^T\mathbf{M}$

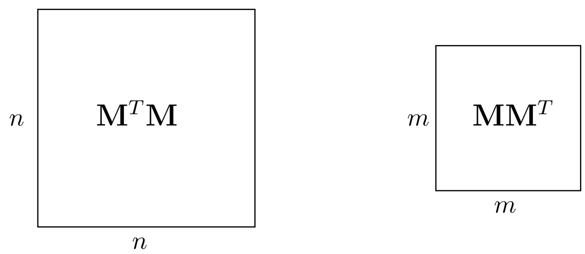
Lemma 14. $\mathbf{M}^T\mathbf{M}$ *and* $\mathbf{M}\mathbf{M}^T$ *are symmetric positive semidefinite matrices.*

Proof. We'll do $\mathbf{M}^T\mathbf{M}$; the other is similar. First off, it is symmetric:

$$(\mathbf{M}^T\mathbf{M})_{ij} \;=\; \sum_k (\mathbf{M}^T)_{ik}\mathbf{M}_{kj} \;=\; \sum_k \mathbf{M}_{ki}\mathbf{M}_{kj} \;=\; \sum_k (\mathbf{M}^T)_{jk}\mathbf{M}_{ki} \;=\; (\mathbf{M}^T\mathbf{M})_{ji}.$$

Next, $\mathbf{M}^T\mathbf{M} \succcurlyeq 0$ since for any $\mathbf{z} \in \mathbb{R}^n$, we have $\mathbf{z}^T\mathbf{M}^T\mathbf{M}\mathbf{z} = \|\mathbf{M}\mathbf{z}\|^2 \geq 0$. □

Which one should we use, $\mathbf{M}^T\mathbf{M}$ or $\mathbf{M}\mathbf{M}^T$? Well, they are of different sizes, $n \times n$ and $m \times m$ respectively.



Ideally, we'd prefer to deal with the smaller of two, $\mathbf{M}\mathbf{M}^T$, especially since eigenvalue computations are expensive. Fortunately, it turns out the two matrices have the same (non-zero) eigenvalues!

Lemma 15. *If* λ *is an eigenvalue of* $\mathbf{M}^T\mathbf{M}$ *with eigenvector* $\mathbf{u}$*, then*

- **either:** (i) λ *is an eigenvalue of* $\mathbf{M}\mathbf{M}^T$ *with eigenvector* $\mathbf{M}\mathbf{u}$*,*
- **or** (ii) $\lambda = 0$ *and* $\mathbf{M}\mathbf{u} = \mathbf{0}$.

Proof. Say $\lambda \neq 0$; we'll prove that condition (i) holds. First of all, $\mathbf{M}^T\mathbf{M}\mathbf{u} = \lambda\mathbf{u} \neq \mathbf{0}$, so certainly $\mathbf{M}\mathbf{u} \neq \mathbf{0}$. It is an eigenvector of $\mathbf{M}\mathbf{M}^T$ with eigenvalue λ, since

$$\mathbf{M}\mathbf{M}^T(\mathbf{M}\mathbf{u}) \;=\; \mathbf{M}(\mathbf{M}^T\mathbf{M}\mathbf{u}) \;=\; \mathbf{M}(\lambda\mathbf{u}) \;=\; \lambda(\mathbf{M}\mathbf{u}).$$

Next, suppose $\lambda = 0$; we'll establish condition (ii). Notice that

$$\|\mathbf{M}\mathbf{u}\|^2 \;=\; \mathbf{u}^T\mathbf{M}^T\mathbf{M}\mathbf{u} \;=\; \mathbf{u}^T(\mathbf{M}^T\mathbf{M}\mathbf{u}) \;=\; \mathbf{u}^T(\lambda\mathbf{u}) \;=\; 0.$$

Thus it must be the case that $\mathbf{M}\mathbf{u} = \mathbf{0}$. □

7.3.2 A spectral decomposition for rectangular matrices

Let's summarize the consequences of Lemma 15. We have two square matrices, a large one ($\mathbf{M}^T\mathbf{M}$) of size $n \times n$ and a smaller one ($\mathbf{M}\mathbf{M}^T$) of size $m \times m$. Let the eigenvalues of the large matrix be $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, with corresponding orthonormal eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$. From the lemma, we know that at most m of the eigenvalues are nonzero.

The smaller matrix $\mathbf{M}\mathbf{M}^T$ has eigenvalues $\lambda_1, \ldots, \lambda_m$, and corresponding orthonormal eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_m$. The lemma suggests that $\mathbf{v}_i = \mathbf{M}\mathbf{u}_i$; this is certainly a valid set of eigenvectors, but they are not necessarily normalized to unit length. So instead we set

$$\mathbf{v}_i \;=\; \frac{\mathbf{M}\mathbf{u}_i}{\|\mathbf{M}\mathbf{u}_i\|} \;=\; \frac{\mathbf{M}\mathbf{u}_i}{\sqrt{\mathbf{u}_i^T\mathbf{M}^T\mathbf{M}\mathbf{u}_i}} \;=\; \frac{\mathbf{M}\mathbf{u}_i}{\sqrt{\lambda_i}}.$$

This finally gives us the *singular value decomposition*, a spectral decomposition for general matrices.

Theorem 16. *Let* $\mathbf{M}$ *be a rectangular* $m \times n$ *matrix with* $m \leq n$. *Define* $\lambda_i, \mathbf{u}_i, \mathbf{v}_i$ *as above. Then*

$$\mathbf{M} \;=\; \underbrace{\begin{pmatrix} \uparrow & \uparrow & & \uparrow \\ \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_m \\ \downarrow & \downarrow & & \downarrow \end{pmatrix}}_{\mathbf{Q}_1,\ \text{size } m \times m} \underbrace{\left(\begin{array}{cccc|c} \sqrt{\lambda_1} & & & 0 & \\ & \sqrt{\lambda_2} & & & 0 \\ & & \ddots & & \\ 0 & & & \sqrt{\lambda_m} & \end{array}\right)}_{\mathbf{\Sigma},\ \text{size } m \times n} \underbrace{\begin{pmatrix} \longleftarrow & \mathbf{u}_1 & \longrightarrow \\ \longleftarrow & \mathbf{u}_2 & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{u}_n & \longrightarrow \end{pmatrix}}_{\mathbf{Q}_2^T,\ \text{size } n \times n}.$$

Proof. We will check that $\mathbf{\Sigma} = \mathbf{Q}_1^T\mathbf{M}\mathbf{Q}_2$. By our proof strategy from Theorem 3, it is enough to verify that both sides have the same effect on $\mathbf{e}_i$ for all $1 \leq i \leq n$. For any such i,

$$\mathbf{Q}_1^T\mathbf{M}\mathbf{Q}_2\mathbf{e}_i \;=\; \mathbf{Q}_1^T\mathbf{M}\mathbf{u}_i \;=\; \left\{\begin{array}{ll} \mathbf{Q}_1^T\sqrt{\lambda_i}\mathbf{v}_i & \text{if } i \leq m \\ \mathbf{0} & \text{if } i > m \end{array}\right\} \;=\; \left\{\begin{array}{ll} \sqrt{\lambda_i}\mathbf{e}_i & \text{if } i \leq m \\ \mathbf{0} & \text{if } i > m \end{array}\right\} \;=\; \mathbf{\Sigma}\mathbf{e}_i.$$

□

The alternative form of the singular value decomposition is

$$\mathbf{M} \;=\; \sum_{i=1}^{m} \sqrt{\lambda_i}\mathbf{v}_i\mathbf{u}_i^T,$$

which immediately yields a rank-k approximation

$$\mathbf{M}_k \;=\; \sum_{i=1}^{k} \sqrt{\lambda_i}\mathbf{v}_i\mathbf{u}_i^T.$$

As in the square case, $\mathbf{M}_k$ is the rank-k matrix that minimizes $\|\mathbf{M} - \mathbf{M}_k\|_F^2$.