Linear Algebra 2

Lecture #17

Orthogonal projection onto subspaces of \mathbb{R}^n . The method of least squares

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 - A brief review of projections onto subspaces

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A brief review of projections onto subspaces

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Theorem 6.5.1

Let V be a finite-dimensional real or complex vector space, equipped with a scalar product $\langle \cdot, \cdot \rangle$ and the induced norm $|| \cdot ||$. Let U be a subspace of V, and let $\mathbf{x} \in V$. Then there exists a unique vector $\mathbf{x}_U \in U$ that has the property that

$$||\mathbf{x} - \mathbf{x}_U|| = \min_{\mathbf{u} \in U} ||\mathbf{x} - \mathbf{u}||.$$

Moreover, if $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ is an orthogonal basis of U, then this vector \mathbf{x}_U is given by the formula

$$\mathbf{x}_U = \sum_{i=1}^k \operatorname{proj}_{\mathbf{u}_i}(\mathbf{x}) = \sum_{i=1}^k \frac{\langle \mathbf{x}, \mathbf{u}_i \rangle}{\langle \mathbf{u}_i, \mathbf{u}_i \rangle} \mathbf{u}_i.$$

• **Terminology/Notation:** The vector **x**_U from Theorem 6.5.1 is called the *orthogonal projection* of **x** onto U.

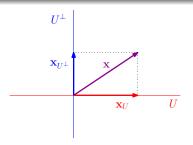
Corollary 6.5.3

Let V be a finite-dimensional real or complex vector space, equipped with a scalar product $\langle \cdot, \cdot \rangle$ and the induced norm $|| \cdot ||$. Let U be a subspace of V, and let $\mathbf{x} \in V$. Then

$$\mathbf{x} = \mathbf{x}_U + \mathbf{x}_{U^{\perp}}.$$

Moreover, this is the unique way of expressing **x** as a sum of a vector in U and a vector in U^{\perp} .^{*a*}

^aThis means that for all $\mathbf{y} \in U$ and $\mathbf{z} \in U^{\perp}$, if $\mathbf{x} = \mathbf{y} + \mathbf{z}$, then $\mathbf{y} = \mathbf{x}_U$ and $\mathbf{z} = \mathbf{x}_{U^{\perp}}$.



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- We can then define the function $\operatorname{proj}_U : V \to V$ by setting $\operatorname{proj}_U(\mathbf{x}) = \mathbf{x}_U$ for all $\mathbf{x} \in V$ (where \mathbf{x}_U is the orthogonal projection of \mathbf{x} onto U, as in Theorem 6.5.1).

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- Clearly, $\operatorname{proj}_U(\mathbf{u}) = \mathbf{u}$ for all $\mathbf{u} \in U$.
- Moreover, we have that $Im(proj_U) = U$ and $proj_U[U] = U$.

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- Clearly, $\operatorname{proj}_U(\mathbf{u}) = \mathbf{u}$ for all $\mathbf{u} \in U$.
- Moreover, we have that $Im(proj_U) = U$ and $proj_U[U] = U$.
- Using the formula from Theorem 6.5.1, we can easily see that the function proj_U is linear.

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• Our goal is to we give formulas for the standard matrices of orthogonal projections onto various subspaces of \mathbb{R}^n .

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 In what follows, it will be convenient to slightly modify the definition of the row space, as follows:

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 In what follows, it will be convenient to slightly modify the definition of the row space, as follows:

$$\operatorname{Row}(A) := \operatorname{Col}(A^T).$$

 So, we (re)defined the row space of a matrix to be the span of the transposes of its rows. • For example, for the matrix

$$A = \begin{bmatrix} 1 & 2 & 1 & 2 \\ 2 & 3 & 2 & 3 \\ 3 & 4 & 3 & 4 \end{bmatrix},$$

we have that

$$A^{T} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 1 & 2 & 3 \\ 2 & 3 & 4 \end{bmatrix},$$

and consequently,

$$\operatorname{Row}(A) = \operatorname{Span}\left(\begin{bmatrix}1\\2\\1\\2\end{bmatrix}, \begin{bmatrix}2\\3\\2\\3\end{bmatrix}, \begin{bmatrix}3\\4\\3\\4\end{bmatrix}\right).$$

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 If this change of definition bothers you, then every time you see Row(□), mentally replace it with Col(□^T).

Let $A \in \mathbb{R}^{n \times m}$. Then $\operatorname{Row}(A)^{\perp} = \operatorname{Nul}(A)$ and $\operatorname{Row}(A) = \operatorname{Nul}(A)^{\perp}$.

Proof.

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Proof. In view of Theorem 6.4.3(c), it suffices to show that $Row(A)^{\perp} = Nul(A)$.

• Indeed, by Theorem 6.4.3(c), we have that

$$(\operatorname{Row}(A)^{\perp})^{\perp} = \operatorname{Row}(A).$$

• So, if
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, then

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Set

$$A = \begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_n^T \end{bmatrix},$$
so that Row(A) = Span($\mathbf{a}_1, \dots, \mathbf{a}_n$).

Proof (continued). Now, for all vectors $\mathbf{x} \in \mathbb{R}^m$:

 $\mathbf{x} \in$

$$\operatorname{Nul}(A) \iff A\mathbf{x} = \mathbf{0}$$

$$\iff \begin{bmatrix} \mathbf{a}_{1}^{T} \\ \vdots \\ \mathbf{a}_{n}^{T} \end{bmatrix} \mathbf{x} = \mathbf{0}$$

$$\iff \begin{bmatrix} \mathbf{a}_{1} \cdot \mathbf{x} \\ \vdots \\ \mathbf{a}_{n} \cdot \mathbf{x} \end{bmatrix} = \mathbf{0}$$

$$\iff \mathbf{a}_{i} \cdot \mathbf{x} = \mathbf{0} \quad \forall i \in \{1, \dots, n\}$$

$$\iff \mathbf{a}_{i} \perp \mathbf{x} \quad \forall i \in \{1, \dots, n\}$$

$$\iff \mathbf{x} \in \{\mathbf{a}_{1}, \dots, \mathbf{a}_{n}\}^{\perp}$$

$$\stackrel{(*)}{\iff} \mathbf{x} \in \operatorname{Span}(\mathbf{a}_{1}, \dots, \mathbf{a}_{n})^{\perp}$$

$$\iff \mathbf{x} \in \operatorname{Row}(A)^{\perp},$$

where (*) follows from the fact that $\{\mathbf{a}_1, \ldots, \mathbf{a}_m\}^{\perp} = \operatorname{Span}(\mathbf{a}_1, \ldots, \mathbf{a}_m)^{\perp}$ (by Proposition 6.4.2). This proves that $\operatorname{Nul}(A) = \operatorname{Row}(A)^{\perp}$, and we are done. \Box

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Let $A \in \mathbb{R}^{n \times m}$. Then all the following hold:

$$I Nul(A^T A) = Nul(A);$$

$$rank(A^T A) = rank(A)$$

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Suppose first that $\mathbf{x} \in Nul(A)$. Then $A\mathbf{x} = \mathbf{0}$, and consequently, $A^T A \mathbf{x} = \mathbf{0}$. So, $\mathbf{x} \in Nul(A^T A)$.

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Let $A \in \mathbb{R}^{n \times m}$. Then all the following hold:

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Proof (continued). Suppose, conversely, that $\mathbf{x} \in \text{Nul}(A^T A)$.

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$$\mathbf{x}^T A^T A \mathbf{x} = (A \mathbf{x})^T (A \mathbf{x}) = (A \mathbf{x}) \cdot (A \mathbf{x}) = ||A \mathbf{x}||^2;$$

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consequently, $||A\mathbf{x}||^2 = 0$.

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consequently, $||A\mathbf{x}||^2 = 0$. It follows that $||A\mathbf{x}|| = 0$, and therefore, $A\mathbf{x} = \mathbf{0}$, i.e. $\mathbf{x} \in \text{Nul}(A)$. This proves (a).

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Let $A \in \mathbb{R}^{n \times m}$. Then all the following hold:

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Proof (continued). For (b), we observe that

$$Row(A^{T}A) = Nul(A^{T}A)^{\perp}$$
by Theorem 6.6.1
$$= Nul(A)^{\perp}$$
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Let $A \in \mathbb{R}^{n \times m}$. Then all the following hold:

$$rank(A^T A) = rank(A).$$

Proof (continued). Finally, for (c), we have the following:

$$\operatorname{rank}(A^{T}A) = \operatorname{dim}(\operatorname{Row}(A^{T}A))$$
 by Theorem 3.3.9

$$= \dim(\operatorname{Row}(A))$$
 by (b)

$$=$$
 rank(A) by Theorem 3.3.9.

This completes the argument. \Box

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

$$\mathbf{x}_C = A(A^T A)^{-1} A^T \mathbf{x}.$$

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First, note that $A^T A \in \mathbb{R}^{m \times m}$, and that by Corollary 6.6.2(a), we have that rank $(A^T A) = \operatorname{rank}(A) = m$.

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First, note that $A^T A \in \mathbb{R}^{m \times m}$, and that by Corollary 6.6.2(a), we have that rank $(A^T A) = \operatorname{rank}(A) = m$. So, by the Invertible Matrix Theorem, $A^T A$ is invertible, and we see that $(A^T A)^{-1}$ is defined and belongs to $\mathbb{R}^{m \times m}$.

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First, note that $A^T A \in \mathbb{R}^{m \times m}$, and that by Corollary 6.6.2(a), we have that rank $(A^T A) = \operatorname{rank}(A) = m$. So, by the Invertible Matrix Theorem, $A^T A$ is invertible, and we see that $(A^T A)^{-1}$ is defined and belongs to $\mathbb{R}^{m \times m}$. Since $A \in \mathbb{R}^{n \times m}$, $(A^T A)^{-1} \in \mathbb{R}^{m \times m}$, and $A^T \in \mathbb{R}^{m \times n}$, we see that $A(A^T A)^{-1}A^T \in \mathbb{R}^{n \times n}$;

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

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Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

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Proof. Fix $\mathbf{x} \in \mathbb{R}^n$. We must first check that the expression $A(A^T A)^{-1}A^T \mathbf{x}$ is defined and belongs to C = Col(A).

First, note that $A^T A \in \mathbb{R}^{m \times m}$, and that by Corollary 6.6.2(a), we have that rank $(A^T A) = \operatorname{rank}(A) = m$. So, by the Invertible Matrix Theorem, $A^T A$ is invertible, and we see that $(A^T A)^{-1}$ is defined and belongs to $\mathbb{R}^{m \times m}$. Since $A \in \mathbb{R}^{n \times m}$, $(A^T A)^{-1} \in \mathbb{R}^{m \times m}$, and $A^T \in \mathbb{R}^{m \times n}$, we see that $A(A^T A)^{-1}A^T \in \mathbb{R}^{n \times n}$; since $\mathbf{x} \in \mathbb{R}^n$, we see that $A(A^T A)^{-1}A^T \mathbf{x}$ is defined and belongs to \mathbb{R}^n . Meanwhile, $(A^T A)^{-1}A^T \mathbf{x}$ is a vector in \mathbb{R}^m , and so (next slide):

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

$$\mathbf{x}_C = A(A^T A)^{-1} A^T \mathbf{x}.$$

Proof (continued).

$$A(A^{T}A)^{-1}A^{T}\mathbf{x} = \underbrace{A}_{\in\mathbb{R}^{n\times m}}\left(\underbrace{(A^{T}A)^{-1}A^{T}\mathbf{x}}_{\in\mathbb{R}^{m}}\right)$$

is a linear combination of the columns of A. By definition, this means that $A(A^T A)^{-1}A^T \mathbf{x} \in \text{Col}(A) = C$.

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

 $\mathbf{x}_C = A(A^T A)^{-1} A^T \mathbf{x}.$

Proof (continued). In view of Corollary 6.5.3, it is now enough to prove that $(\mathbf{x} - A(A^T A)^{-1}A^T \mathbf{x}) \in C^{\perp}$, for it will then follow that $\mathbf{x}_C = A(A^T A)^{-1}A^T \mathbf{x}$, which is what we need to show.

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

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• Indeed, if we can show that $(\mathbf{x} - A(A^T A)^{-1}A^T \mathbf{x}) \in C^{\perp}$, then we get that

$$\mathbf{x} = \underbrace{A(A^T A)^{-1} A^T \mathbf{x}}_{\in C} + (\underbrace{\mathbf{x} - A(A^T A)^{-1} A^T \mathbf{x}}_{\in C^{\perp}}),$$

which (by Corollary 6.5.3) implies that $\mathbf{x}_C = A(A^T A)^{-1} A^T \mathbf{x}$ and $\mathbf{x}_{C^{\perp}} = \mathbf{x} - A(A^T A)^{-1} A^T \mathbf{x}$.

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

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Proof (continued). But note that

$$C^{\perp} = \operatorname{Col}(A)^{\perp} = \operatorname{Row}(A^{T})^{\perp} \stackrel{(*)}{=} \operatorname{Nul}(A^{T}),$$

where (*) follows from Theorem 6.6.1.

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$$A^{T}\left(\mathbf{x}-A(A^{T}A)^{-1}A^{T}\mathbf{x}\right) = A^{T}\mathbf{x}-\underbrace{A^{T}A(A^{T}A)^{-1}}_{=I_{m}}A^{T}\mathbf{x} = \mathbf{0}.$$

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Proof (continued). But note that

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This proves that $\mathbf{x} - A(A^T A)^{-1}A^T \mathbf{x} \in \text{Nul}(A^T)$, and we are done. \Box

 Theorem 6.6.3: If A ∈ ℝ^{n×m} has full column rank, then A(A^TA)⁻¹A^T is the standard matrix of orthogonal projection onto Col(A).

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 - But what if rank(A) < m?
 - In that case, we let *B* be the matrix obtained from *A* by deleting all the non-pivot columns of *A*.
 - By Theorem 3.3.4, the columns of B form a basis of Col(A), and we see that Col(A) = Col(B).

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 - If rank(A) = m (i.e. A has full column rank), then the matrix that we need is $A(A^TA)^{-1}A^T$, as per Theorem 6.6.3.
 - But what if rank(A) < m?
 - In that case, we let *B* be the matrix obtained from *A* by deleting all the non-pivot columns of *A*.
 - By Theorem 3.3.4, the columns of B form a basis of Col(A), and we see that Col(A) = Col(B).
 - Moreover, all the columns of *B* are pivot columns, and so *B* has full column rank.

- Theorem 6.6.3: If A ∈ ℝ^{n×m} has full column rank, then A(A^TA)⁻¹A^T is the standard matrix of orthogonal projection onto Col(A).
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 - If rank(A) = m (i.e. A has full column rank), then the matrix that we need is $A(A^TA)^{-1}A^T$, as per Theorem 6.6.3.
 - But what if rank(A) < m?
 - In that case, we let *B* be the matrix obtained from *A* by deleting all the non-pivot columns of *A*.
 - By Theorem 3.3.4, the columns of B form a basis of Col(A), and we see that Col(A) = Col(B).
 - Moreover, all the columns of *B* are pivot columns, and so *B* has full column rank.
 - But now the matrix *B* satisfies the hypotheses of Theorem 6.6.3. So, the standard matrix of orthogonal projection onto Col(A) = Col(B) is $B(B^TB)^{-1}B^T$.

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank m (i.e. A is a matrix of full column rank). Then the matrix $A(A^T A)^{-1}A^T$ is the standard matrix of orthogonal projection onto Col(A), that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto C := Col(A) is given by

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 $\mathbf{x}_C = A(A^T A)^{-1} A^T \mathbf{x}.$

Corollary 6.6.4

Let **a** be a non-zero vector in \mathbb{R}^n . Then the standard matrix of projection onto the line $L := \text{Span}(\mathbf{a})$ is the matrix

$$\mathbf{a}(\mathbf{a}^{\mathsf{T}}\mathbf{a})^{-1}\mathbf{a}^{\mathsf{T}} = \mathbf{a}(\mathbf{a}\cdot\mathbf{a})^{-1}\mathbf{a}^{\mathsf{T}} = \frac{1}{\mathbf{a}\cdot\mathbf{a}}\mathbf{a}\mathbf{a}^{\mathsf{T}}$$

Consequently, for every vector $\mathbf{x} \in \mathbb{R}^n$, we have that

$$\mathbf{x}_L = \operatorname{proj}_L(\mathbf{x}) = \frac{1}{\mathbf{a} \cdot \mathbf{a}} \mathbf{a} \mathbf{a}^T \mathbf{x}.$$

Proof. This is a special case of Theorem 6.6.3 for $A = |\mathbf{a}|$.

Let U be a subspace of \mathbb{R}^n , and let $P \in \mathbb{R}^{n \times n}$ be the standard matrix of proj_{U^{\perp}}. Then $I_n - P$ is the standard matrix of proj_{U^{\perp}}, that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto U^{\perp} is given by $\mathbf{x}_{U^{\perp}} = (I_n - P)\mathbf{x}$.

Proof.

Let U be a subspace of \mathbb{R}^n , and let $P \in \mathbb{R}^{n \times n}$ be the standard matrix of proj_U. Then $I_n - P$ is the standard matrix of proj_{U^{\perp}}, that is, for all $\mathbf{x} \in \mathbb{R}^n$, the orthogonal projection of \mathbf{x} onto U^{\perp} is given by $\mathbf{x}_{U^{\perp}} = (I_n - P)\mathbf{x}$.

Proof. We observe that for all $\mathbf{x} \in \mathbb{R}^n$, we have that

$$(I_n - P)\mathbf{x} = I_n\mathbf{x} - P\mathbf{x} \stackrel{(*)}{=} \mathbf{x} - \mathbf{x}_U \stackrel{(**)}{=} \mathbf{x}_{U^{\perp}},$$

where (*) follows from the fact that P is the standard matrix of proj_U, and (**) follows from Corollary 6.5.3. So, $I_n - P$ is indeed the standard matrix of proj_{U[⊥]}. \Box

Corollary 6.6.6

Let $A \in \mathbb{R}^{n \times m}$ be a matrix of rank n (i.e. A is a matrix of full row rank). Then the matrix $I_m - A^T (AA^T)^{-1}A$ is the standard matrix of orthogonal projection onto N := Nul(A), that is, for all $\mathbf{x} \in \mathbb{R}^m$, the orthogonal projection of \mathbf{x} onto N is given by $\mathbf{x}_N = (I_m - A^T (AA^T)^{-1}A)\mathbf{x}$.

Proof.

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Proof. First, note that

$$\operatorname{Nul}(A) \stackrel{(*)}{=} \operatorname{Row}(A)^{\perp} = \operatorname{Col}(A^{\mathcal{T}})^{\perp}.$$

where (*) follows from Theorem 6.6.1.

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Proof. First, note that

$$\operatorname{Nul}(A) \stackrel{(*)}{=} \operatorname{Row}(A)^{\perp} = \operatorname{Col}(A^{T})^{\perp}.$$

where (*) follows from Theorem 6.6.1. Note further that $A^T \in \mathbb{R}^{m \times n}$ and that $\operatorname{rank}(A^T) = \operatorname{rank}(A) = n$, i.e. A^T has full column rank.

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Proof. First, note that

$$\operatorname{Nul}(A) \stackrel{(*)}{=} \operatorname{Row}(A)^{\perp} = \operatorname{Col}(A^{\mathcal{T}})^{\perp}.$$

where (*) follows from Theorem 6.6.1. Note further that $A^T \in \mathbb{R}^{m \times n}$ and that rank $(A^T) = \operatorname{rank}(A) = n$, i.e. A^T has full column rank. So, by Theorem 6.6.3, the standard matrix of orthogonal projection onto $\operatorname{Col}(A^T)$ is $A^T(AA^T)^{-1}A$.

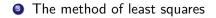
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where (*) follows from Theorem 6.6.1. Note further that $A^T \in \mathbb{R}^{m \times n}$ and that rank $(A^T) = \operatorname{rank}(A) = n$, i.e. A^T has full column rank. So, by Theorem 6.6.3, the standard matrix of orthogonal projection onto $\operatorname{Col}(A^T)$ is $A^T(AA^T)^{-1}A$. Finally, by Theorem 6.6.5, the standard matrix of orthogonal projection onto $\operatorname{Col}(A^T)^{\perp} = \operatorname{Nul}(A)$ is $I_m - A^T(AA^T)^{-1}A$. \Box



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- However, what if the equation $A\mathbf{x} = \mathbf{b}$ is inconsistent?
- Then the answer will obviously depend on which norm that we are using.

 In what follows, we will work only with the norm induced by the standard scalar product in Rⁿ, i.e. the standard Euclidean norm.

• Recall that this is the norm $||\cdot||$ given by

$$||\mathbf{x}|| = \sqrt{\mathbf{x} \cdot \mathbf{x}} = \sqrt{x_1^2 + \dots + x_n^2}$$
for all vectors $\mathbf{x} = \begin{bmatrix} x_1 & \dots & x_n \end{bmatrix}^T$ in \mathbb{R}^n .

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

$$A^T A \mathbf{x} = A^T \mathbf{b}$$

is consistent, and moreover, its solution set is precisely the set of vectors **x** in \mathbb{R}^m that minimize the expression

$$||A\mathbf{x} - \mathbf{b}||.$$

- **Terminology:** Suppose we are given a matrix $A \in \mathbb{R}^{n \times m}$ and a vector $\mathbf{b} \in \mathbb{R}^{n}$.
 - Vectors x ∈ ℝ^m that minimize the expression ||Ax − b|| are called the *least-squares solutions* of the equation Ax = b (such solutions are often denoted by x̂), whereas the number

$$\min_{\mathbf{x}\in\mathbb{R}^m}||A\mathbf{x}-\mathbf{b}||$$

is called the *least-squares error* for the equation $A\mathbf{x} = \mathbf{b}$.

 By Theorem 6.7.1, the equation Ax = b has at least one least-squares solution x̂, and consequently, the least-squares error is defined and is equal to ||Ax̂ - b||.

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

$$A^T A \mathbf{x} = A^T \mathbf{b}$$

is consistent, and moreover, its solution set is precisely the set of vectors **x** in \mathbb{R}^m that minimize the expression

$$|A\mathbf{x} - \mathbf{b}||.$$

Remark: Obviously, if Ax = b is consistent, then the least-squares solutions of Ax = b are precisely the solutions of the equation Ax = b itself.

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

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- Remark: Obviously, if Ax = b is consistent, then the least-squares solutions of Ax = b are precisely the solutions of the equation Ax = b itself.
 - This is because if $A\mathbf{x} = \mathbf{b}$ is consistent, then the solutions of that equation minimize the expression $||A\mathbf{x} \mathbf{b}||$ (indeed, $||A\mathbf{x} \mathbf{b}|| = 0$ iff $A\mathbf{x} = \mathbf{b}$).

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

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- Remark: Obviously, if Ax = b is consistent, then the least-squares solutions of Ax = b are precisely the solutions of the equation Ax = b itself.
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 - Moreover, the matrix-vector equation Ax = b is consistent iff the least-squares error of this equation is zero.

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

$$A^T A \mathbf{x} = A^T \mathbf{b}$$

is consistent, and moreover, its solution set is precisely the set of vectors ${\bf x}$ in \mathbb{R}^m that minimize the expression

$$||A\mathbf{x} - \mathbf{b}||.$$

• First an example, then a proof.

Let

$$A = \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix},$$

with entries understood to be in \mathbb{R} . Find all least-squares solutions $\hat{\mathbf{x}}$ of $A\mathbf{x} = \mathbf{b}$, as well as the least-squares error. Is the equation $A\mathbf{x} = \mathbf{b}$ consistent?

Solution.

Let

$$A = \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix},$$

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Solution. We apply Theorem 6.7.1.

Let

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Solution. We apply Theorem 6.7.1. So, we need to find the solutions of the equation $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$.

Let

$$A = \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix}$$

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Solution. We apply Theorem 6.7.1. So, we need to find the solutions of the equation $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$. We first compute

$$A^{T}A = \begin{bmatrix} 6 & 6 \\ 6 & 42 \end{bmatrix}$$
 and $A^{T}\mathbf{b} = \begin{bmatrix} 6 \\ -6 \end{bmatrix}$,

Let

$$A = \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix},$$

with entries understood to be in \mathbb{R} . Find all least-squares solutions $\hat{\mathbf{x}}$ of $A\mathbf{x} = \mathbf{b}$, as well as the least-squares error. Is the equation $A\mathbf{x} = \mathbf{b}$ consistent?

Solution. We apply Theorem 6.7.1. So, we need to find the solutions of the equation $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$. We first compute

$$A^{\mathsf{T}}A = \begin{bmatrix} 6 & 6 \\ 6 & 42 \end{bmatrix}$$
 and $A^{\mathsf{T}}\mathbf{b} = \begin{bmatrix} 6 \\ -6 \end{bmatrix}$,

and then we compute

$$\mathsf{RREF}\left(\left[\begin{array}{ccc}A^{\mathsf{T}}A & A^{\mathsf{T}}\mathbf{b}\end{array}\right]\right) = \left[\begin{array}{cccc}1 & 0 & 4/3\\0 & 1 & -1/3\end{array}\right].$$

It follows that

$$\hat{\mathbf{x}} = \begin{bmatrix} 4/3 \\ -1/3 \end{bmatrix}$$

is the unique solution of the matrix-vector equation $A^T A \hat{\mathbf{x}} = A^T \mathbf{b}$, and consequently, the unique least-squares solution of the matrix-vector equation $A \mathbf{x} = \mathbf{b}$.

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The least-squares error of $A\mathbf{x} = \mathbf{b}$ is

$$||A\hat{\mathbf{x}} - \mathbf{b}|| = || \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} 4/3 \\ -1/3 \end{bmatrix} - \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix} || = || \begin{bmatrix} -1 \\ -3 \\ 3 \\ -1 \end{bmatrix} || = 2\sqrt{5}.$$

It follows that

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The least-squares error of $A\mathbf{x} = \mathbf{b}$ is

$$||A\hat{\mathbf{x}} - \mathbf{b}|| = || \begin{bmatrix} 1 & -2 \\ -1 & 2 \\ 0 & 3 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} 4/3 \\ -1/3 \end{bmatrix} - \begin{bmatrix} 3 \\ 1 \\ -4 \\ 2 \end{bmatrix} || = || \begin{bmatrix} -1 \\ -3 \\ 3 \\ -1 \end{bmatrix} || = 2\sqrt{5}.$$

Since the least-squares error of the equation $A\mathbf{x} = \mathbf{b}$ is strictly positive, we see that the equation is inconsistent. \Box

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

 $A^T A \mathbf{x} = A^T \mathbf{b}$

is consistent, and moreover, its solution set is precisely the set of vectors ${\bf x}$ in \mathbb{R}^m that minimize the expression

 $||A\mathbf{x} - \mathbf{b}||.$

Proof.

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

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Proof. We are looking for vectors $\mathbf{x} \in \mathbb{R}^m$ that minimize the expression $||A\mathbf{x} - \mathbf{b}||$.

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation

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Proof. We are looking for vectors $\mathbf{x} \in \mathbb{R}^m$ that minimize the expression $||A\mathbf{x} - \mathbf{b}||$. Our goal is to show is that the vectors we are looking for are precisely those that satisfy $A^T A \mathbf{x} = A^T \mathbf{b}$.

Proof (continued). By Proposition 3.3.2(a), we have that $C := \text{Col}(A) = \{A\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^m\}.$

Moreover, by Corollary 6.5.3, $\mathbf{b} = \mathbf{b}_C + \mathbf{b}_{C^{\perp}}$ is the only way to decompose **b** as a sum of a vector in *C* and a vector in C^{\perp} .

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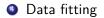
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Theorem 6.7.1

Let $A \in \mathbb{R}^{n \times m}$ and $\mathbf{b} \in \mathbb{R}^n$. Then the matrix-vector equation $A^T A \mathbf{x} = A^T \mathbf{b}$ is consistent, and moreover, its solution set is precisely the set of vectors \mathbf{x} in \mathbb{R}^m that minimize the expression $||A\mathbf{x} - \mathbf{b}||.$



Oata fitting

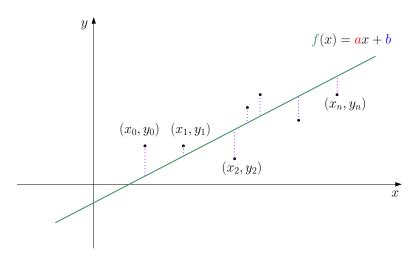
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- Suppose we are given a collection of two or more data points, and we wish to find a line that best fits them. How would we do this?
 - We will be plotting our data points, say $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$, in \mathbb{R}^2 .
 - Most commonly, the x-axis is time (measured in whatever time units happen to be convenient for the problem that we are studying), whereas the y-axis is the quantity that we are measuring, such as population size, the average global temperature, the number of products of a certain type produced or consumed in a given region, etc.
 - We are looking for a line f(x) = ax + b that best fits our data points (picture: next slide).



$$ax_0 + b = y_0$$

$$ax_1 + b = y_1$$

$$\vdots$$

$$ax_n + b = y_n$$

$$ax_0 + b = y_0$$

$$ax_1 + b = y_1$$

$$\vdots$$

$$ax_n + b = y_n$$

This linear system can be rewritten as the matrix-vector equation below, where the vector [a b]^T is the unknown.

$$\begin{bmatrix} x_0 & 1 \\ x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix}$$

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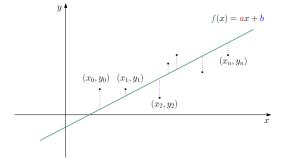
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- Except in rare cases, the system above will be inconsistent.
- For this reason, we will look for the least-squares solution(s) $\begin{bmatrix} \hat{a} & \hat{b} \end{bmatrix}^T$ of the system, which yields the line $\hat{f}(x) = \hat{a}x + \hat{b}$.

• This (approximate) solution minimizes the following quantity:

$$|| \begin{bmatrix} x_0 & 1 \\ x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} - \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix} || = || \begin{bmatrix} ax_0 + b - y_0 \\ ax_1 + b - y_1 \\ \vdots \\ ax_n + b - y_n \end{bmatrix} || = || \begin{bmatrix} f(x_0) - y_0 \\ f(x_1) - y_1 \\ \vdots \\ f(x_n) - y_n \end{bmatrix} || = \sqrt{\sum_{i=0}^n \left(f(x_i) - y_i \right)^2}.$$

• So, we are effectively minimizing the sum of squares of the vertical distances between our data points and the line.



Using the method of least squares, find the line that best fits the data points (1, 2), (2, 3), (3, 3), (5, 6).

Solution.

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Solution. We are looking for the function f(x) = ax + b that best fits these four data points.

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At a glance, we can see that this system is inconsistent;

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At a glance, we can see that this system is inconsistent; so, we will not be able to find an exact solution and will instead have to settle for an approximate one.

Using the method of least squares, find the line that best fits the data points (1, 2), (2, 3), (3, 3), (5, 6).

Solution (continued). This system can be rewritten as a matrix-vector equation below, where $\begin{bmatrix} a & b \end{bmatrix}^T$ is the unknown.

$$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 3 \\ 6 \end{bmatrix}$$

Using the method of least squares, find the line that best fits the data points (1, 2), (2, 3), (3, 3), (5, 6).

Solution (continued). This system can be rewritten as a matrix-vector equation below, where $\begin{bmatrix} a & b \end{bmatrix}^T$ is the unknown.

$$\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 3 \\ 6 \end{bmatrix}$$

We multiply both sides by the transpose of the matrix on the left, and we get the following (where *a* and *b* became \hat{a} and \hat{b} , respectively, because we are now approximating):

$$\begin{bmatrix} 1 & 2 & 3 & 5 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 5 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \\ 3 \\ 6 \end{bmatrix}$$

Using the method of least squares, find the line that best fits the data points (1, 2), (2, 3), (3, 3), (5, 6).

Solution (continued). After performing matrix multiplication, we obtain

$$\begin{bmatrix} 39 & 11 \\ 11 & 5 \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \begin{bmatrix} 47 \\ 14 \end{bmatrix}.$$

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We now form the augmented matrix of the matrix-vector equation above, and we row reduce to obtain:

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$$\mathsf{RREF}\Big(\left[\begin{array}{rrrrr} 39 & 11 & 47 \\ 11 & 5 & 14 \end{array}\right]\Big) = \left[\begin{array}{rrrrr} 1 & 0 & 81/74 \\ 0 & 1 & 29/74 \end{array}\right]$$

This yields the least-squares solution

$$\left[\begin{array}{c} \hat{a} \\ \hat{b} \end{array}\right] = \left[\begin{array}{c} 81/74 \\ 29/74 \end{array}\right].$$

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$$\left[\begin{array}{c} \hat{a} \\ \hat{b} \end{array}\right] = \left[\begin{array}{c} 81/74 \\ 29/74 \end{array}\right].$$

So, the line that best fits our data points is

$$\hat{f}(x) = \frac{81}{74}x + \frac{29}{74}.$$