Announcements

Principal Component Analysis

Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 8, 2018

Linear projections

Given $x_1, \dots, x_n \in \mathbb{R}^d$, for $q \ll d$ find a compressed representation with $\lambda_1, \dots, \lambda_n \in \mathbb{R}^q$ such that $x_i \approx \mu + \mathbf{V}_q \lambda_i$ and $\mathbf{V}_q^T \mathbf{V}_q = I$

$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^n \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

Linear projections

Given $x_1, \ldots, x_n \in \mathbb{R}^d$, for $q \ll d$ find a compressed representation with $\lambda_1, \ldots, \lambda_n \in \mathbb{R}^q$ such that $x_i \approx \mu + \mathbf{V}_q \lambda_i$ and $\mathbf{V}_q^T \mathbf{V}_q = I$

$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^n \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

Fix $\mathbf{V}_q$ and solve for μ, λ_i:

$$\mu = \bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$$

$$\lambda_i = \mathbf{V}_q^T (x_i - \bar{x})$$

Which gives us:

$$\min_{\mathbf{V}_q} \sum_{i=1}^N ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q

Linear projections

$z^T \Sigma z \geq 0 \quad \forall z$

$$\sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2$$

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2 = \min_{\mathbf{V}_q} Tr(\Sigma) - Tr(\mathbf{V}_q^T \Sigma \mathbf{V}_q)$$

Eigenvalue decomposition of Σ =

V_q : maximizes $Tr(V_q^T \Sigma V_q)$

Linear projections

$$\sum_{i=1}^N ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2$$

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Eigenvalue decomposition of $\sum$ =

$\mathbf{V}_q$ are the first q eigenvectors of Σ

Minimize reconstruction error and capture the most variance in your data.

Pictures

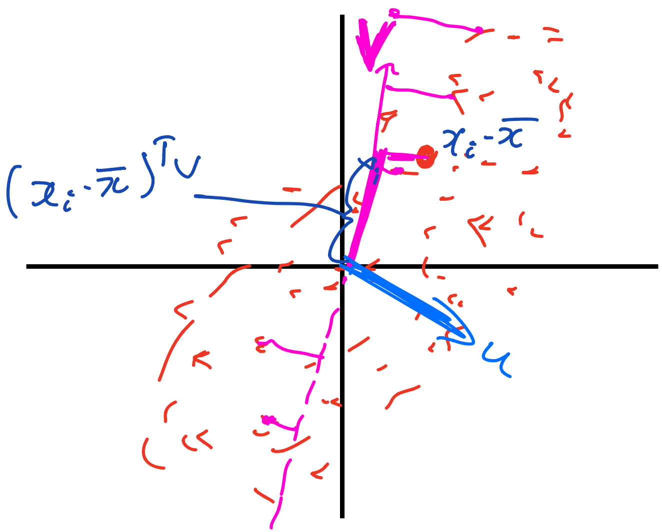
$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

$\mathbf{V}_q$ with $\mathbf{V}_q^T \mathbf{V}_q = I$ maximizes $Tr(\mathbf{V}_q^T \Sigma \mathbf{V}_q)$

$x_i - \bar{x}$



$q = 1 \Rightarrow V_q \in \mathbb{R}^d$

$\sum_i v^T (x_i - \bar{x})(x_i - \bar{x})^T v = v^T \Sigma v$

$v^T \Sigma v > u^T \Sigma u$

Pictures

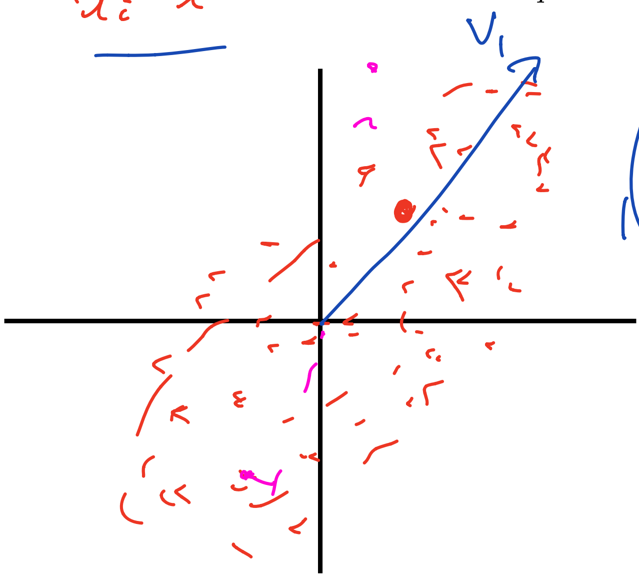
$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

$\mathbf{V}_q$ with $\mathbf{V}_q^T \mathbf{V}_q = I$ maximizes $Tr(\mathbf{V}_q^T \Sigma \mathbf{V}_q)$

$x_i - \bar{x}$



$q = 2 \Rightarrow V_q \in \mathbb{R}^{d \times 2}$

$(\quad) = \sum_i v_1^T (x_i - \bar{x})(x_i - \bar{x})^T v_1$

$+ \sum_i v_2^T (x_i - \bar{x})(x_i - \bar{x})^T v_2$

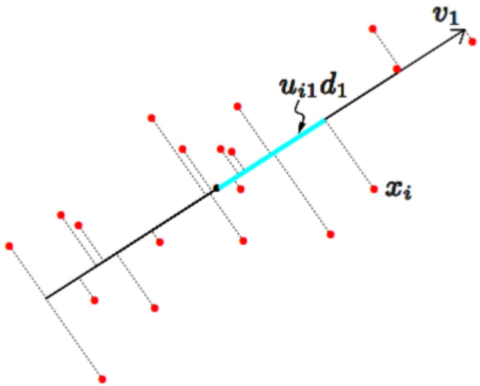
Linear projections

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

where $\mathbf{V}_q = [v_1, v_2, \dots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$



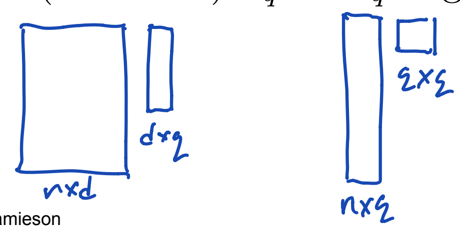
$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

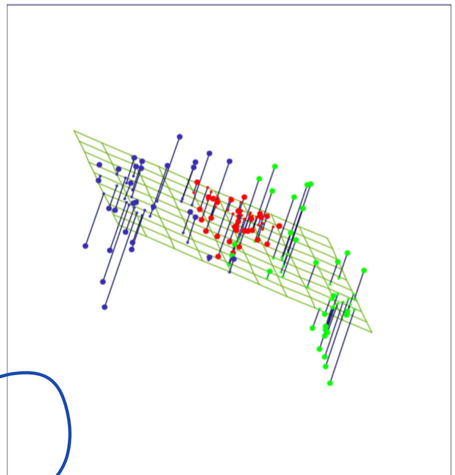
Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \text{diag}(d_1, \dots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$

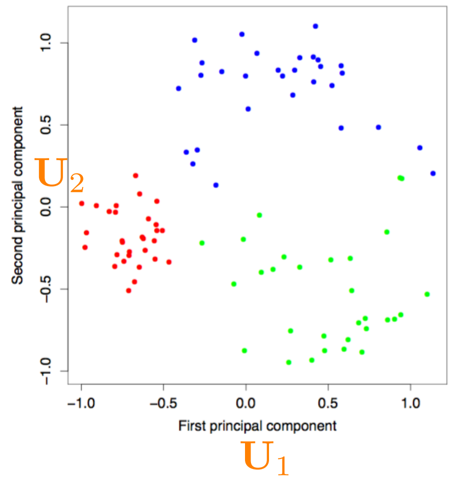


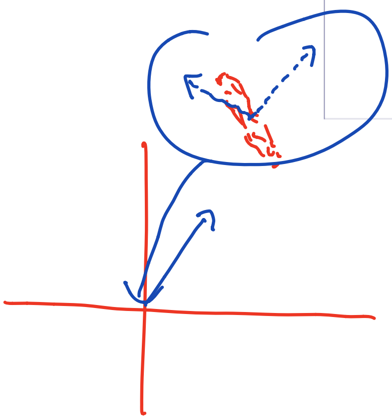
Dimensionality reduction

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD*



$$\mathbf{X} - \mathbf{1}\bar{x}^T$$





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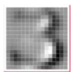
Dimensionality reduction

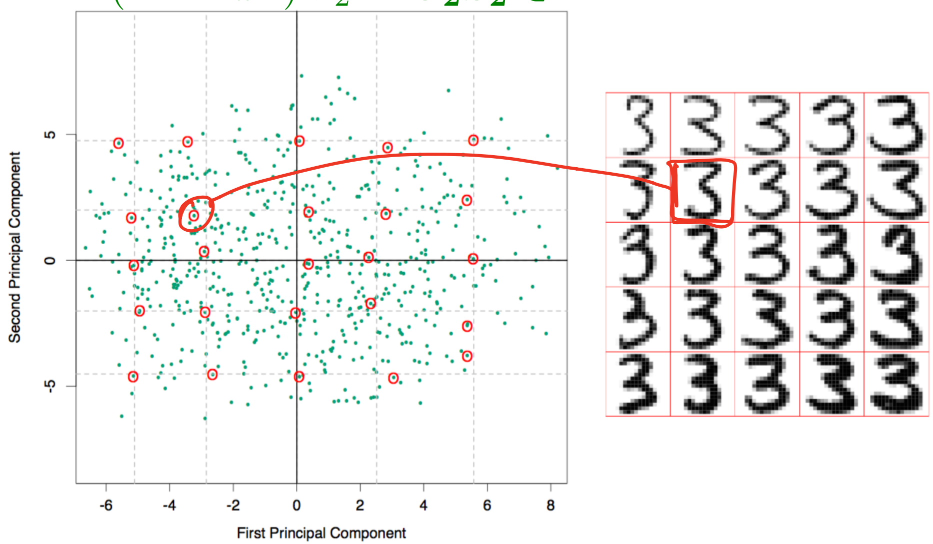
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T$

Handwritten 3's, 16x16 pixel image so that $x_i \in \mathbb{R}^{256}$

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

$=$  $+ \lambda_1 \cdot$  $+ \lambda_2 \cdot$ .

$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_2 = \mathbf{U_2 S_2} \in \mathbb{R}^{n \times 2}$



$\mathrm{diag}(\mathbf{S})$

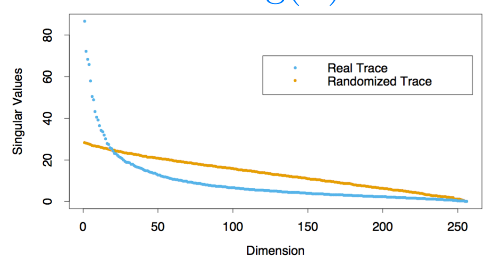


FIGURE 14.24. *The 256 singular values for the digitized threes, compared to those for a randomized version of the data (each column of* $\mathbf{X}$ *was scrambled).*

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Singular Value Decomposition (SVD)

$e_i = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i\text{th pos}$

Theorem (SVD): Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$ where $\mathbf{S} \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

$V = [v_1, \dots, v_n]$

$[V^TV]_{i,j} = v_i^T v_j$

$$\mathbf{A}^T\mathbf{A}v_i = (USV^T)^T(USV^T)v_i = VS\cancel{U^TU}SV^Tv_i = VS^2V^Tv_i$$

$$= VS^2e_i$$

$$= S_{ii}^2 Ve_i$$

$$= S_{ii}^2 v_i$$

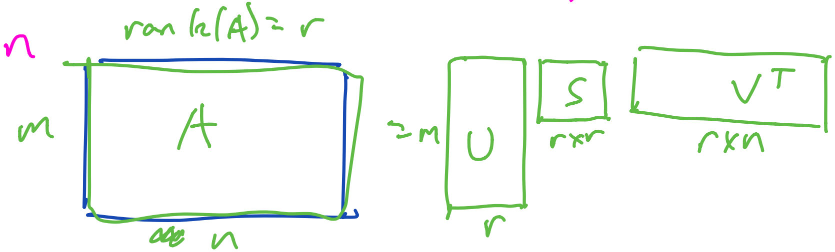
$U = [u_1, \dots, u_n]$

$$\mathbf{A}\mathbf{A}^T u_i = USV^T(USV^T)^T u_i = US^2U^Tu_i$$

$$= S_{ii}^2 u_i$$

$mr + rr + rn$

mn



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$$\mathbf{A}^T\mathbf{A}v_i = \mathbf{S}_{i,i}^2 v_i$$

$$\mathbf{A}\mathbf{A}^T u_i = \mathbf{S}_{i,i}^2 u_i$$

$\mathbf{V}$ are the first r eigenvectors of $\mathbf{A}^T\mathbf{A}$ with eigenvalues $\text{diag}(\mathbf{S})$
$\mathbf{U}$ are the first r eigenvectors of $\mathbf{A}\mathbf{A}^T$ with eigenvalues $\text{diag}(\mathbf{S})$

Linear projections

$\mathbf{V}_q$ are the first q eigenvectors of Σ

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$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

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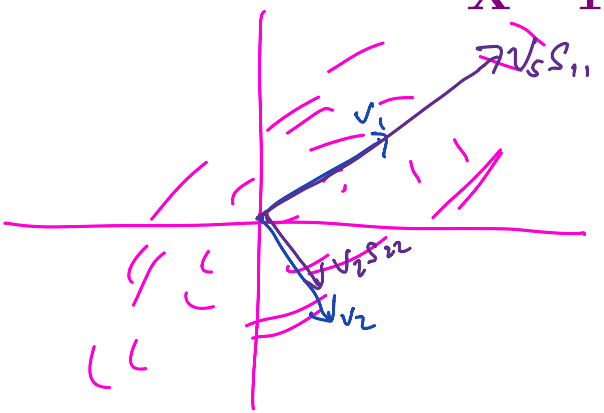
Singular Value Decomposition defined as

$$\overbrace{\mathbf{X} - \mathbf{1}\bar{x}^T}^{n\times d} = \overset{n\times 2}{\mathbf{U}}\,\overset{2\times 2}{\mathbf{S}}\,\overset{2\times d}{\mathbf{V}}{}^T$$

PCA



Pictures, intuition!

$JX = X - \mathbf{1}\underbrace{\mathbf{1}^T X/n}_{= \sum_{i=1}^{n} x_i^T / n}$ $\quad \mathbf{1}^T \boxed{X}$

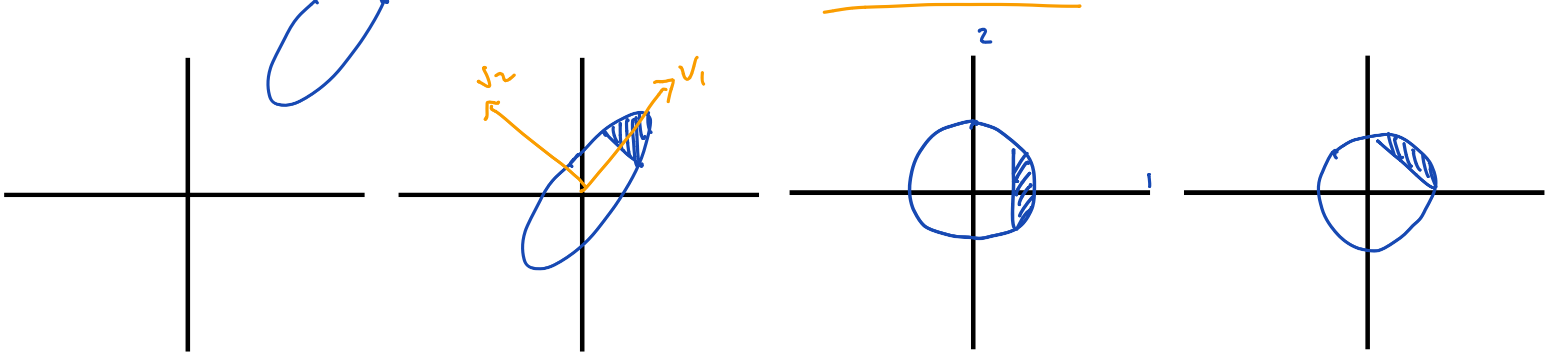
$= X - \mathbf{1}\bar{x}$

- Fill in the missing plots: $\mathbf{U}, \mathbf{S}, \mathbf{V} = \text{svd}(\mathbf{JX})$

$\mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n \qquad \mathbf{JX} = \mathbf{USV}^T$

$V = [v_1, v_2]$ $\qquad = U S \cancel{V^T V} S^{-1} = U$

$\mathbf{X} \qquad \mathbf{JX} \qquad \mathbf{JXVS}^{-1} \qquad \mathbf{JXVS}^{-1}\mathbf{V}^T$



$(JXV)_{i,1} = (x_i - \bar{x})^T v_1$

Kernel PCA

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q S_q} \in \mathbb{R}^{n \times q}$$

$$\mathbf{JX} = \mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T \qquad \mathbf{J} = I - \mathbf{11}^T/n$$

$$(\mathbf{JX})(\mathbf{JX})^T = USV^TVSU^T = US^2U^T \in \mathbb{R}^{n \times n}$$

$$(JX)^T(JX) = VSU^TUSV^T = VS^2V^T \in \mathbb{R}^{d \times d}$$

$$X \in \mathbb{R}^{n \times d}$$

PCA Algorithm

PCA

input
A matrix of m examples $X \in \mathbb{R}^{m,d}$
number of components n
if $(m > d)$
$A = X^\top X$
Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be the eigenvectors of A with largest eigenvalues
else
$B = X X^\top$
Let $\mathbf{v}_1, \ldots, \mathbf{v}_n$ be the eigenvectors of B with largest eigenvalues
for $i = 1, \ldots, n$ set $\mathbf{u}_i = \frac{1}{\|X^\top \mathbf{v}_i\|} X^\top \mathbf{v}_i$
output: $\mathbf{u}_1, \ldots, \mathbf{u}_n$

Cool tricks with SVD

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Ridge Regression revisited

$$\widehat{w}_{ridge} = \arg\min_w ||\mathbf{X}w - \mathbf{y}||_2^2 + \lambda||w||_2^2$$

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$ (Assume data centered)

Singular vector decomposition (SVD): $\mathbf{X} \cancel{- \mathbf{1}\bar{x}^T} = \underline{\mathbf{USV}^T}$

$$\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

Ridge Regression revisited

$$\widehat{w}_{ridge} = \arg\min_w ||\mathbf{X}w - \mathbf{y}||_2^2 + \lambda||w||_2^2$$

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

Singular vector decomposition (SVD): $\mathbf{X} \cancel{- \mathbf{1}\bar{x}^T} = \mathbf{U}\mathbf{S}\mathbf{V}^T$

$$\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

$$\hat{\mathbf{y}} = \sum_{i=1}^{d} u_i u_i^T \underbrace{\frac{s_i^2}{s_i^2 + \lambda}}_{\approx \begin{cases} 0 & s_i^2 << \lambda \\ 1 & s_i^2 >> \lambda \end{cases}} y_i$$

$$\mathbf{U} = [u_1, \ldots, u_d]$$

$$\mathbf{S} = \mathrm{diag}(s_1, \ldots, s_d)$$