ENM 360: Introduction to Data-driven Modeling

Lecture #27: Principal component analysis

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December 8, 2020

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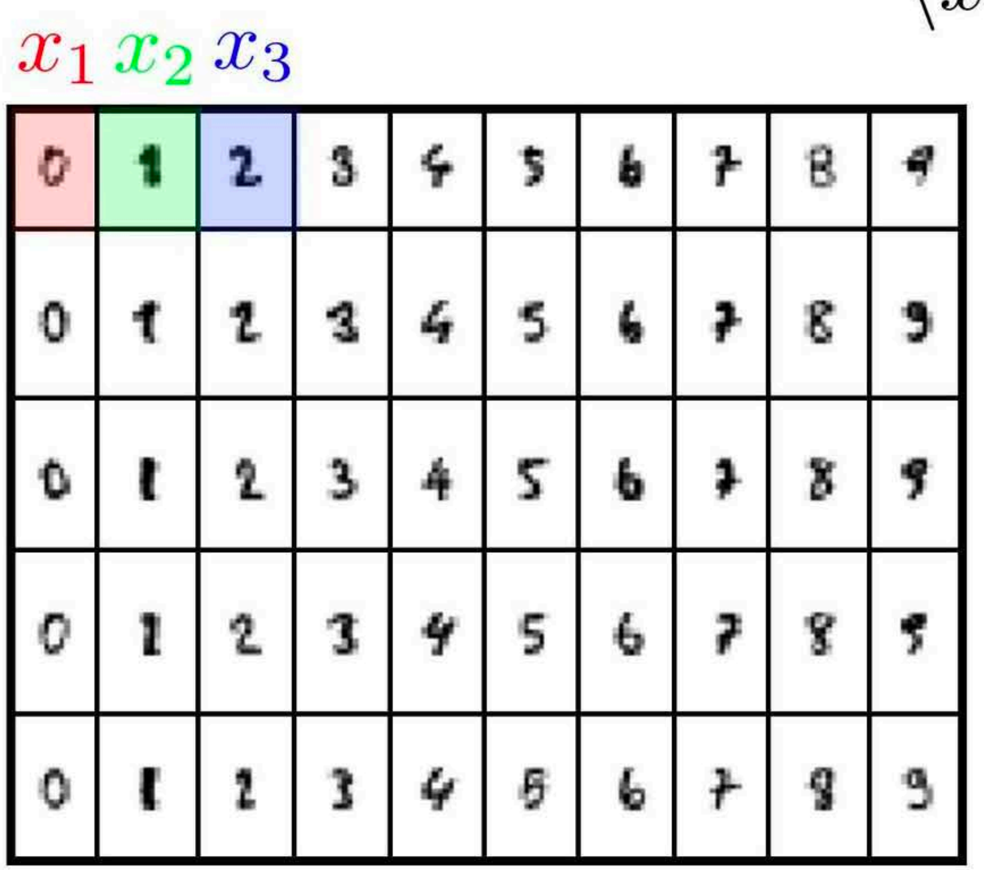
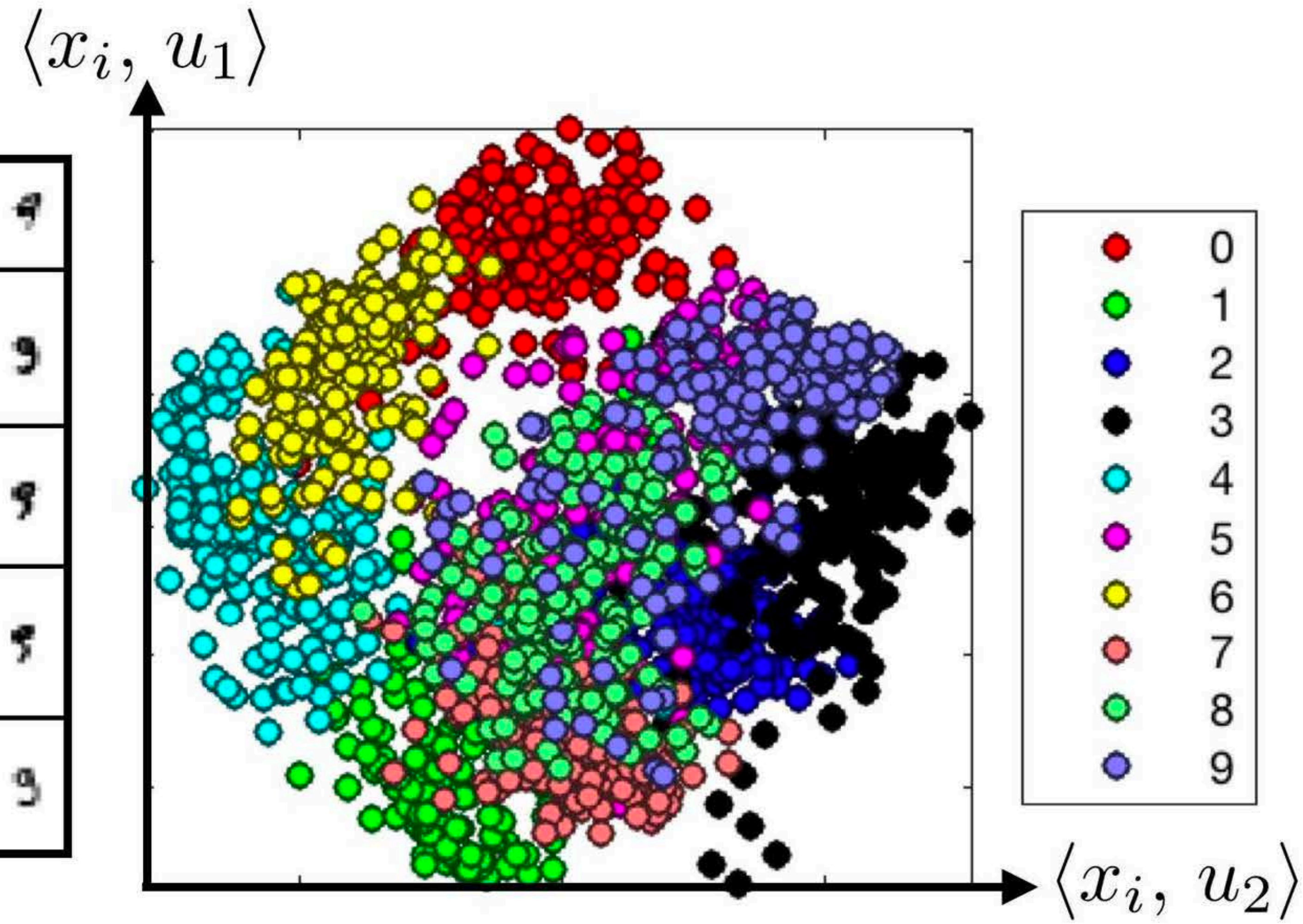
Principal component analysis

Input data:	$X = (x_i)_{i=1}^n \in \mathbb{R}^{n \times p}, x_i \in \mathbb{R}^p$
Remove mean:	$x_i \leftarrow x_i - \frac{1}{n} \sum_j x_j$
Covariance:	$C \overset{\text{def.}}{=} \frac{1}{n} X^\top X \in \mathbb{R}^{p \times p}$
Eigen-decomposition:	$C = U \operatorname{diag}(\sigma_k^2) U^\top, U = (u_k)_{k=1}^p$





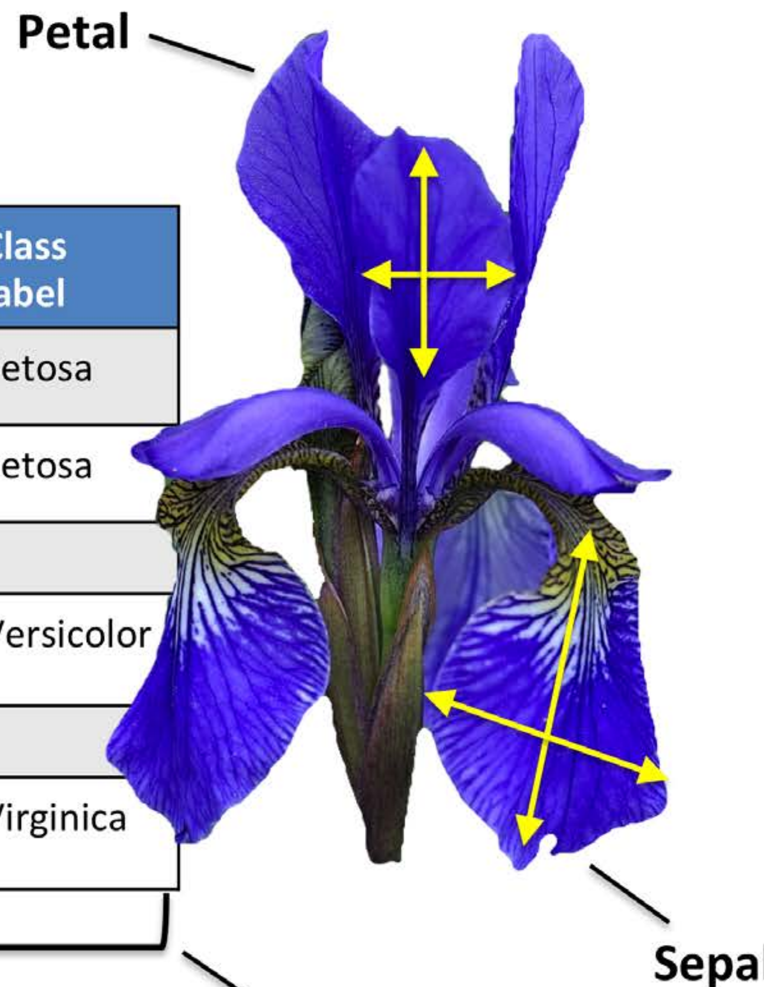
Example: the Iris data set

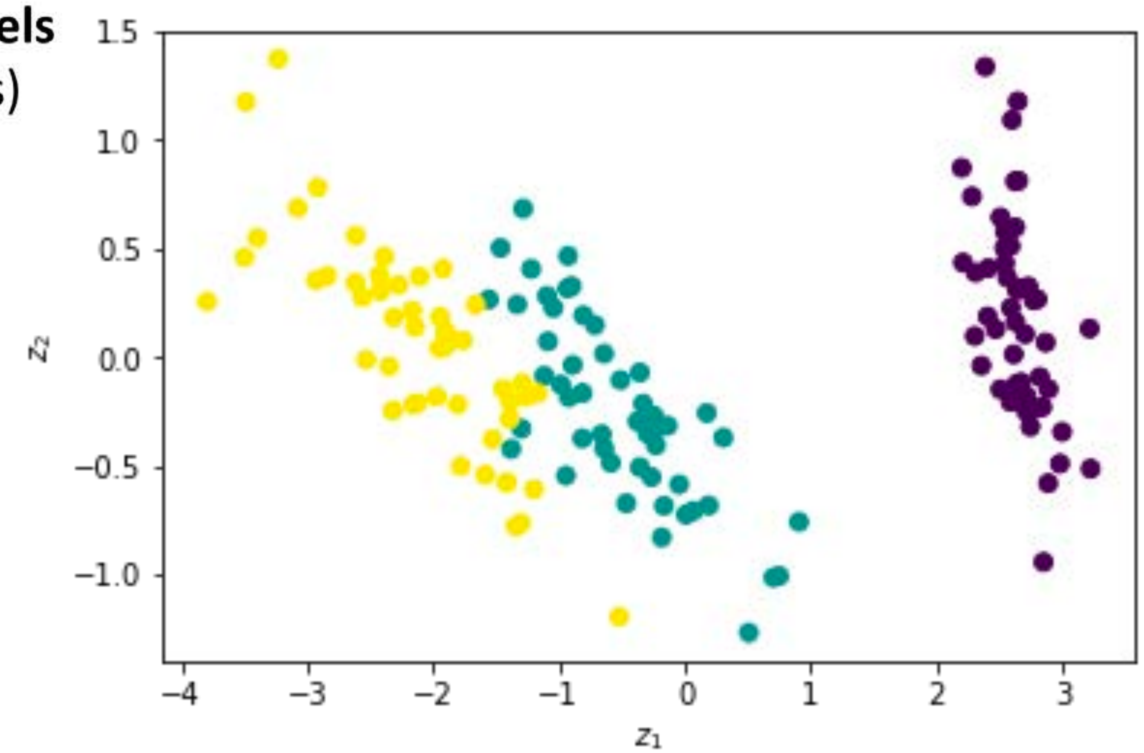
Samples
(instances, observations)

	Sepal length	Sepal width	Petal length	Petal width	Class label
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
			...		
50	6.4	3.5	4.5	1.2	Versicolor
			...		
150	5.9	3.0	5.0	1.8	Virginica

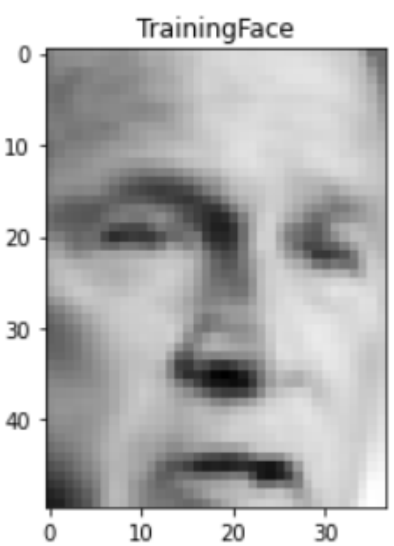
Features
(attributes, measurements, dimensions)

Class labels
(targets)





Example: Eigenfaces



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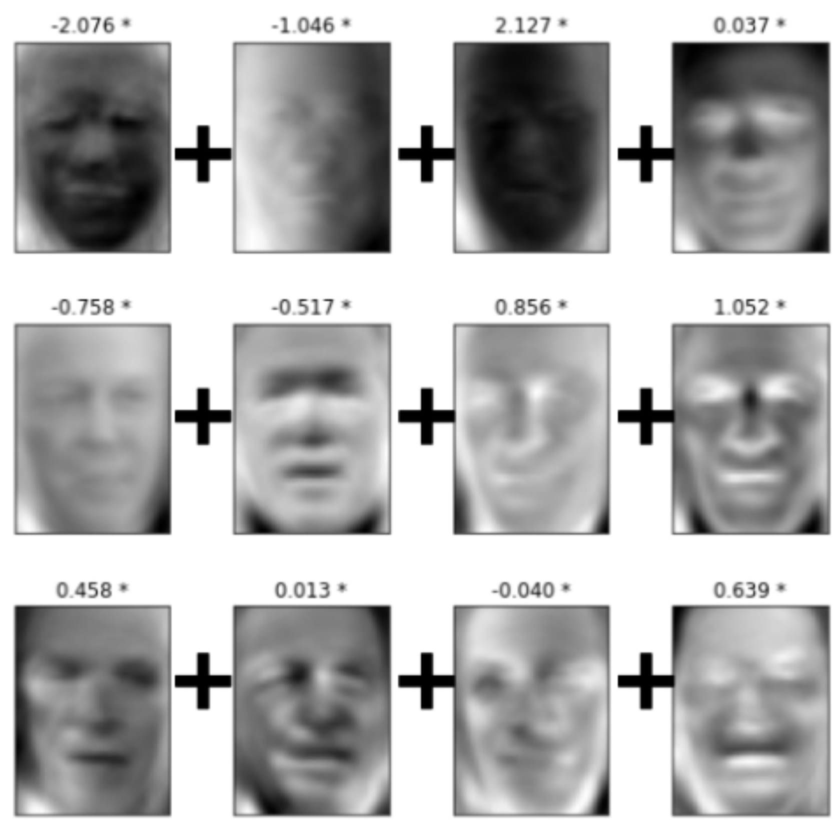
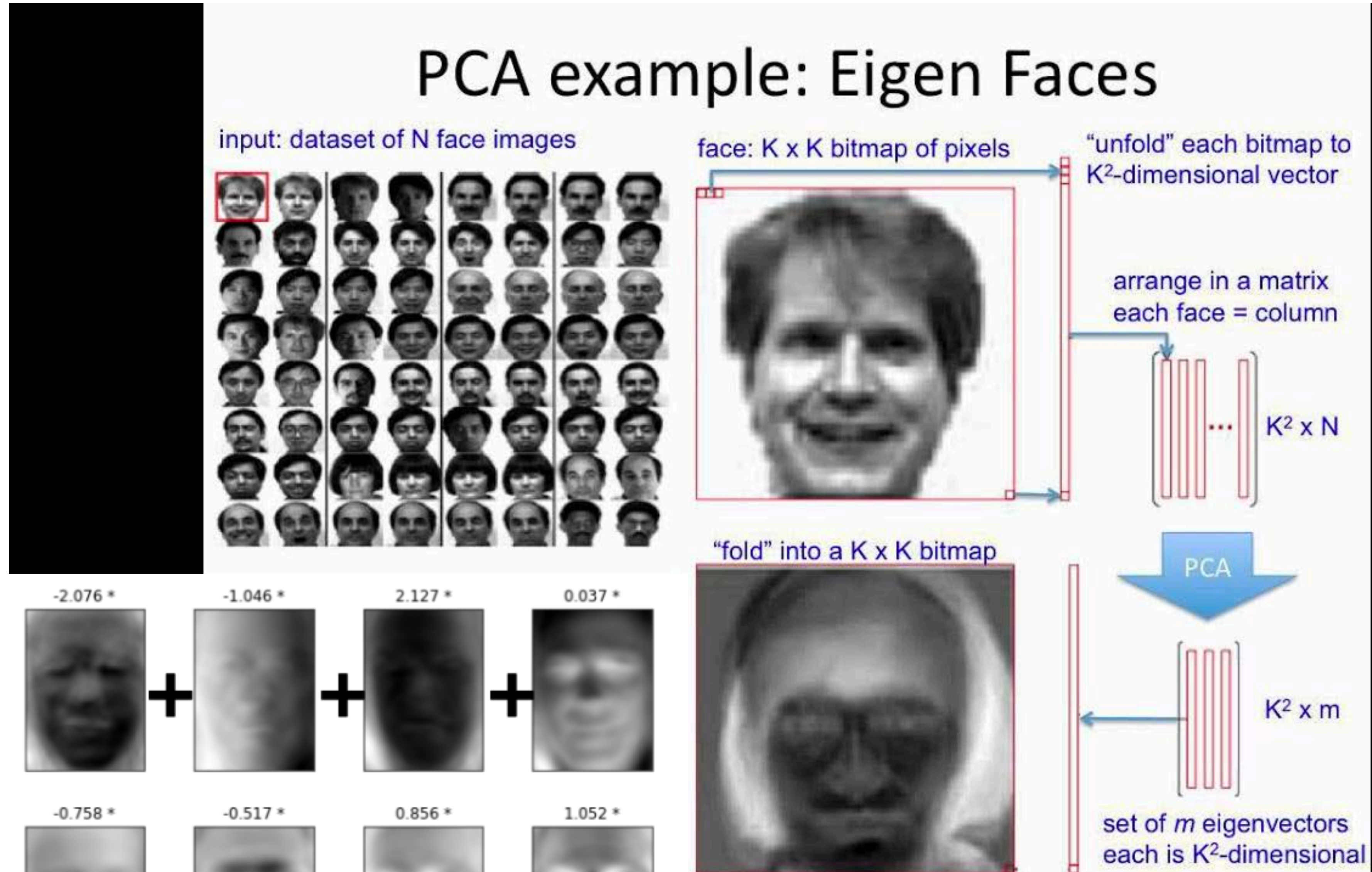
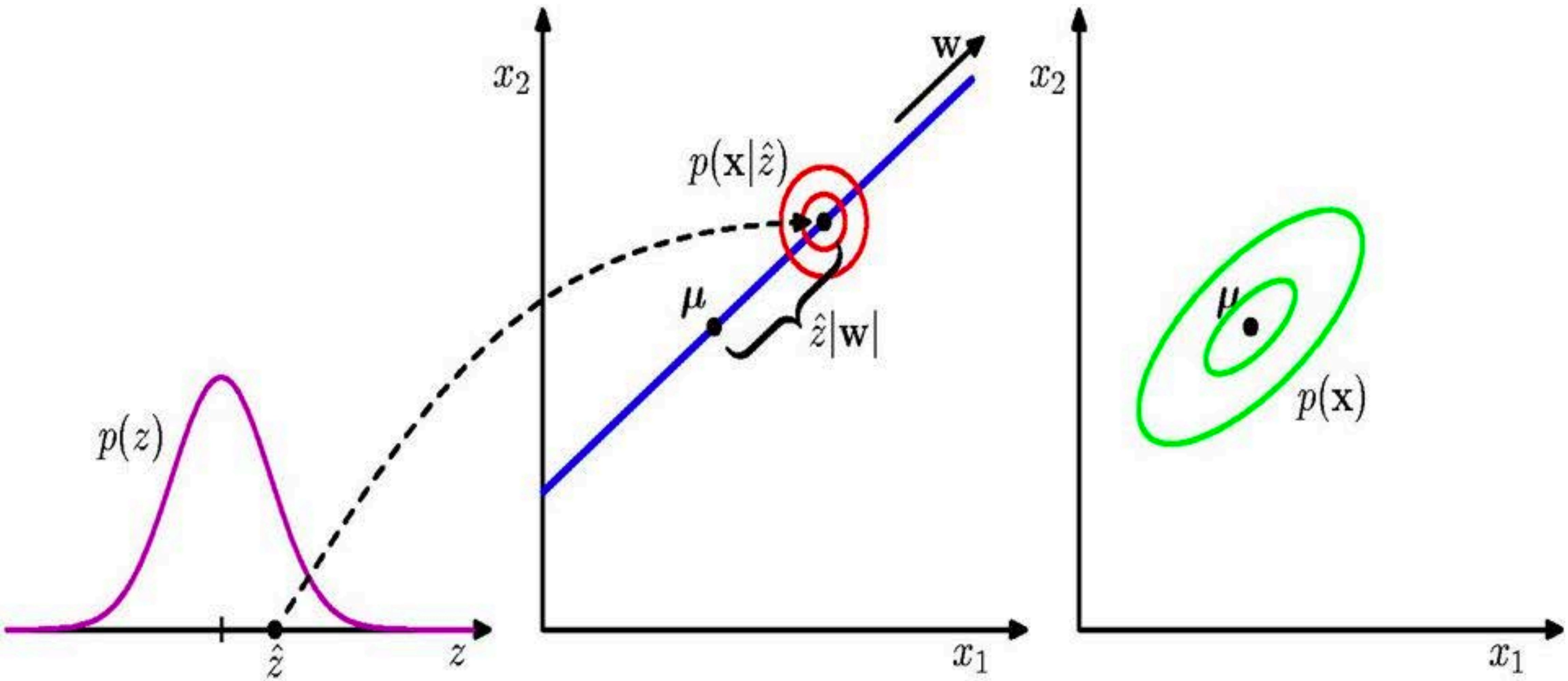




Example: Probabilistic PCA



data space: 2-dimensional latent space: 1-dimensional

- get a value $\hat{z}$ for the latent variable z
- get a value for x from an isotropic Gaussian distribution

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$

- green ellipses: density contours for the marginal distribution p(x)