CS189/CS289A
Introduction to Machine Learning
Lecture 7: The Multivariate Normal Distribution

Peter Bartlett

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Outline

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- Probability density function.

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- 2-D Gaussian

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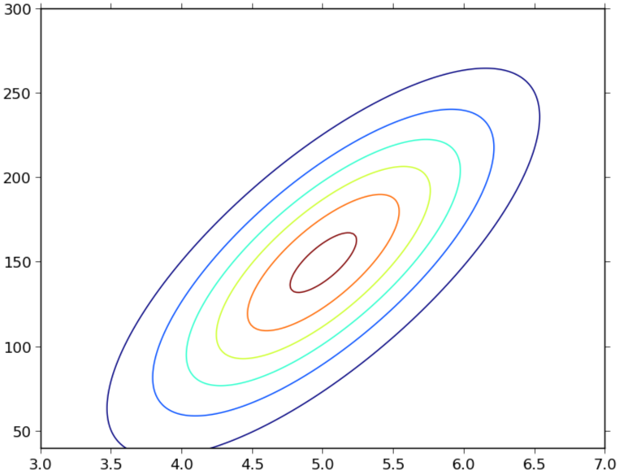

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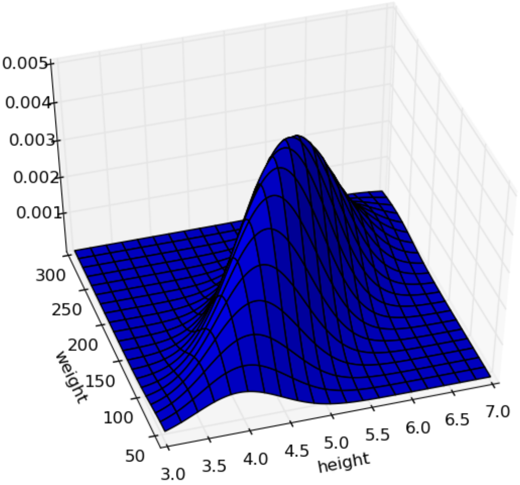

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- Suppose we project height and weight in a particular direction. What is the direction of maximum variance? minimum variance?

2-D Gaussian distribution

Consider independent Gaussian random variables X and Y:

$$p_X(x) = \frac{1}{\sqrt{2\pi\sigma_X^2}} \exp\left(-\frac{(x-\mu_X)^2}{2\sigma_X^2}\right).$$

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$$\begin{aligned} p(x,y) &= p_X(x)p_Y(y) \\ &= \frac{1}{\sqrt{(2\pi)^2\sigma_X^2\sigma_Y^2}} \exp\left(-\frac{(x-\mu_X)^2}{2\sigma_X^2} - \frac{(y-\mu_Y)^2}{2\sigma_Y^2}\right) \\ &= \frac{1}{\sqrt{(2\pi)^2|\Sigma|}} \exp\left(-\frac{1}{2}\left(\begin{bmatrix} x-\mu_X & y-\mu_Y \end{bmatrix} \begin{bmatrix} \sigma_X^2 & 0 \\ 0 & \sigma_Y^2 \end{bmatrix}^{-1} \begin{bmatrix} x-\mu_X \\ y-\mu_Y \end{bmatrix}\right)\right). \end{aligned}$$

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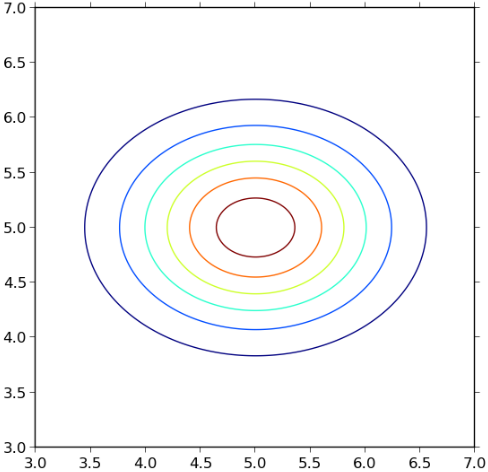
2-D Gaussian distribution

$$\mu = \begin{bmatrix} 5.0 \\ 5.0 \end{bmatrix} \qquad \Sigma = \begin{bmatrix} 0.8 & 0.0 \\ 0.0 & 0.6 \end{bmatrix}$$



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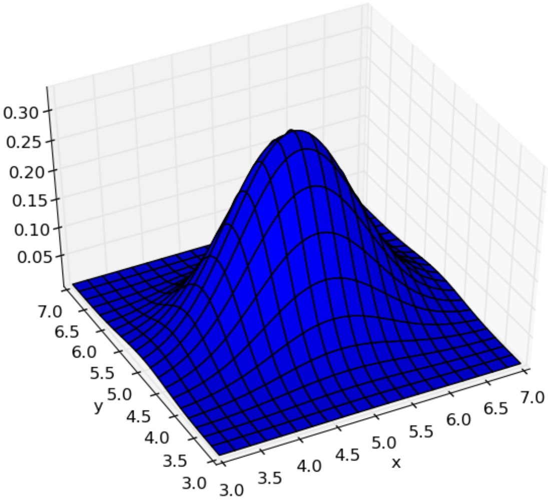

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What is $\mathbb{E}\left[(v'(X-\mu))^2\right]$?

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Diagonal covariance

Consider $X \sim N(\mu, \Sigma)$ where Σ is diagonal:

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_d^2 \end{bmatrix}.$$

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Consider the super-level sets of the pdf:

$$\mathcal{E}_r = \left\{ x \in \mathbb{R}^d : (x-\mu)'\Sigma^{-1}(x-\mu) \leq r^2 \right\}$$

Diagonal covariance

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\begin{aligned}
& (x-\mu)'\Sigma^{-1}(x-\mu) \leq r^2 \\
\Leftrightarrow \quad & \sum_{i=1}^{d} \frac{(x_i-\mu_i)^2}{\sigma_i^2} \leq r^2.
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Thus, the $\mathcal{E}_r$ correspond to *axis-aligned ellipsoids* in $\mathbb{R}^d$.
For instance, if $x_2 = \mu_2, \ldots, x_d = \mu_d$, then $x \in \mathcal{E}_r$ when

$$
(x_1-\mu_1)^2 \le r^2\sigma_1^2 \qquad \Leftrightarrow \qquad |x_1-\mu_1| \le r\sigma_1.
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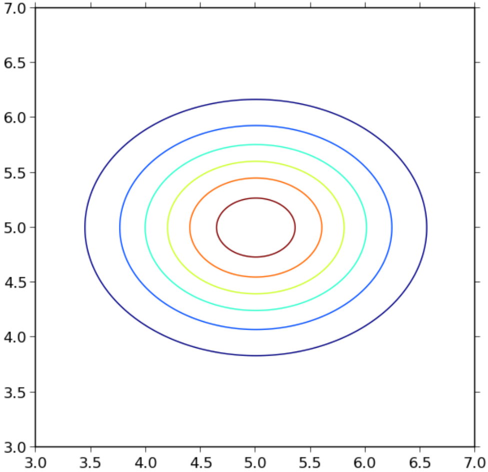

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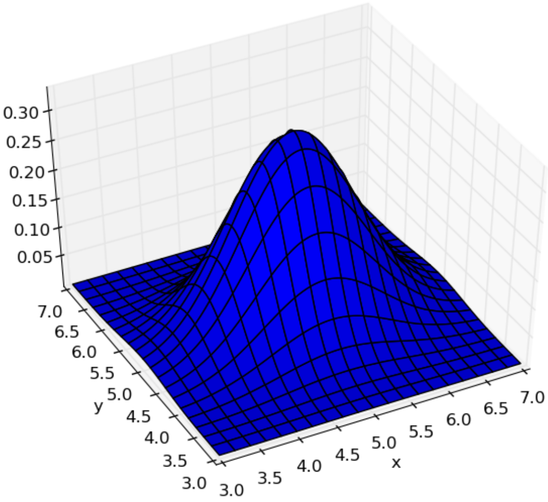

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- This explains the appearance of $1/\sqrt{|\Sigma|}$ in the normalization factor.
- It also shows that, for a fixed r, $\Pr(\mathcal{E}_r)$ is the same, for all μ and Σ (but depends on d).

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$$\text{e.g.} \qquad Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

Non-diagonal covariance

This leaves the mean unchanged:

$$\mathbb{E}Y = \mu_X + \mathbb{E}\left[Q(X - \mu_X)\right] = \mu_X + Q(\mathbb{E}\left[X\right] - \mu_X) = \mu_X.$$

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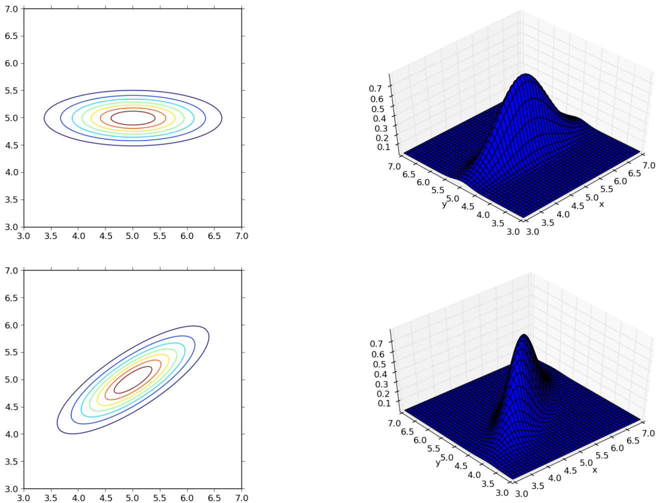
&= Q\mathbb{E}\left[(X - \mu_X)(X - \mu_X)'\right] Q' \\
&= Q\Sigma_X Q'.
\end{aligned}$$

It is no longer diagonal.

Non-diagonal covariance



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(Eigenvalues are roots of the *characteristic polynomial*, $\det(A - \lambda I)$.)

Non-diagonal covariance

Spectral Theorem

Non-diagonal covariance

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For a symmetric real matrix $A \in \mathbb{R}^{n \times n}$, we can find n orthonormal eigenvectors of A $(v_1, \ldots, v_n)$, and the eigenvalues $(\lambda_1, \ldots, \lambda_n)$ are real.

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$$AU = U\Lambda, \qquad A = U\Lambda U',$$

where

$$U = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix}, \qquad \Lambda = \operatorname{diag}\left(\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \ldots \\ \lambda_n \end{bmatrix}\right).$$

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(Why "hence"? $U'U = I$, so $UU' = I$.)

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Also, the *precision matrix* can be written

$$\Sigma^{-1} = U \Lambda^{-1} U'.$$

(Check!)

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In this new basis, the covariance is the diagonal matrix Λ^{-1}.

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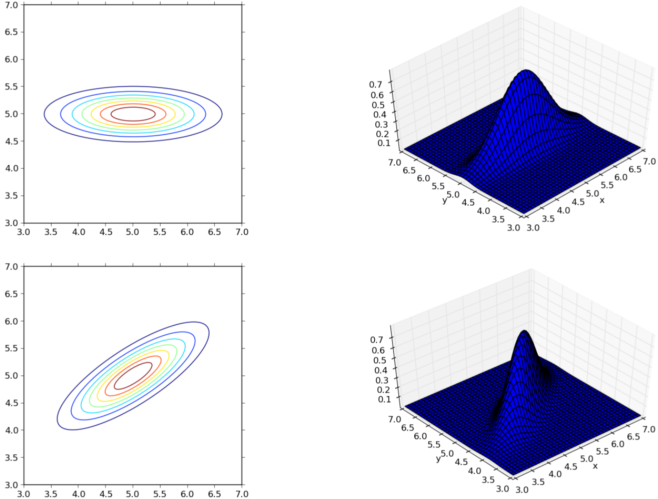
This is the same as the diagonal case, but with a new coordinate system, defined by the eigenvectors.

Non-diagonal covariance



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(As in the diagonal case.)

Outline

- Probability density function.
- 2-D Gaussian
- Covariance matrix.
- Diagonal covariance.
- Non-diagonal covariance and diagonalization.
- **Properties of multivariate Gaussians.**

Properties of multivariate Gaussians

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- If we accept that $X + Y$ is Gaussian, let's calculate its mean and covariance.

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- The mean and covariance of Y are immediate from the definitions.
- To show that Y has a Gaussian distribution, we write its density as an integral (integrating out the Z variables), *complete the squares* to compute the integral, and recognize the answer as a $\mathcal{N}(\mu_Y, \Sigma_{YY})$ density.

Properties of multivariate Gaussians

Affine transformations

Given a d-dimensional Gaussian $X \sim \mathcal{N}(\mu, \Sigma^2)$, matrix $A \in \mathbb{R}^{m \times d}$ and vector $b \in \mathbb{R}^m$, define

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Given a d-dimensional standard normal $X \sim \mathcal{N}(0, I)$, we have

$$Y = AX + \mu \sim \mathcal{N}(\mu, AA').$$

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Given a d-dimensional normal $X \sim \mathcal{N}(\mu, \Sigma)$ with Σ positive definite,

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What is $\Sigma^{-1/2}$? We can write $\Sigma = U\Lambda U'$ for U with orthonormal columns and Λ diagonal. Then defining $\Sigma^{-1/2} = U\Lambda^{-1/2}U'$, we have

$$\Sigma^{-1/2}\Sigma^{-1/2} = U\Lambda^{-1/2}U'U\Lambda^{-1/2}U' = U\Lambda^{-1}U' = \Sigma^{-1}.$$

Outline

- Probability density function.
- 2-D Gaussian
- Covariance matrix.
- Diagonal covariance.
- Non-diagonal covariance and diagonalization.
- Properties of multivariate Gaussians.