CS189/CS289A
Introduction to Machine Learning
Lecture 8: More on the Multivariate Normal Distribution

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February 12, 2015

Outline

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- Review: Diagonal covariance matrices.

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- Non-diagonal covariance and diagonalization.

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- Symmetric: $\Sigma_{i,j} = \Sigma_{j,i}$.
- Non-negative diagonal entries: $\Sigma_{i,i} \geq 0$.
- Positive semidefinite: for all $v \in \mathbb{R}^d$, $v'\Sigma v \geq 0$.

Review: 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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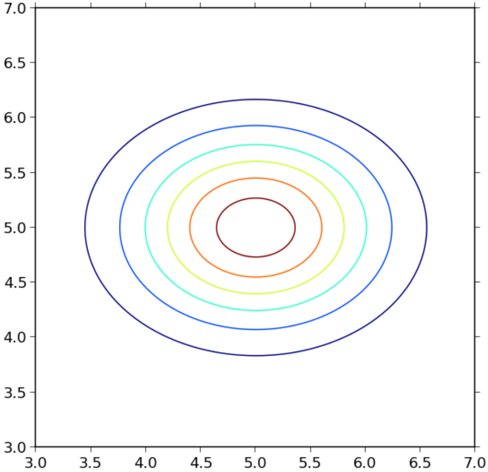
$$= \left\{ x \in \mathbb{R}^d : \sum_{i=1}^{d} \frac{(x_i - \mu_i)^2}{\sigma_i^2} \le r^2 \right\},$$

correspond to *axis-aligned ellipsoids* in $\mathbb{R}^d$, of length $2r\sigma_i$ in the x_i direction.
The volume of $\mathcal{E}_r$ is proportional to $\prod_{i=1}^d \sigma_i = \sqrt{|\Sigma|}$.
Hence, for a fixed r, $\Pr(\mathcal{E}_r)$ does not depend on μ and Σ (but does depend on d).

Review: Diagonal covariance

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



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

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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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It is no longer diagonal.

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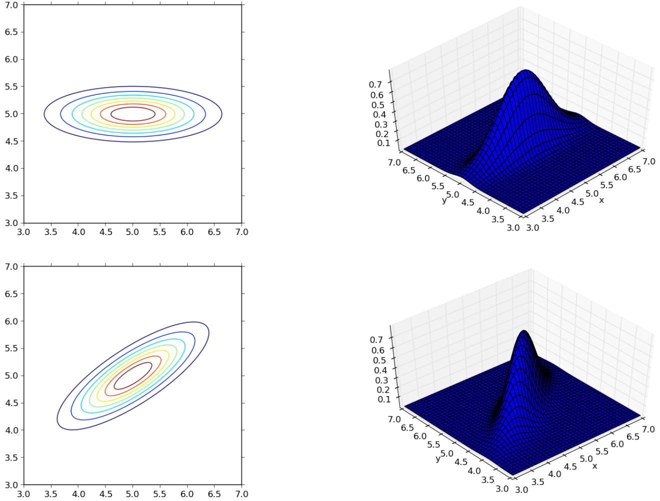

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Eigenvalues and eigenvectors

For a square matrix A, λ is an *eigenvalue* and x is an *eigenvector* if

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

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Spectral Theorem

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

(this is called *diagonalization*), where

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

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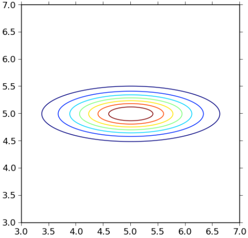
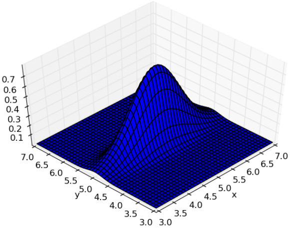
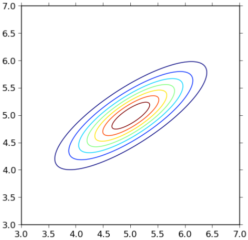
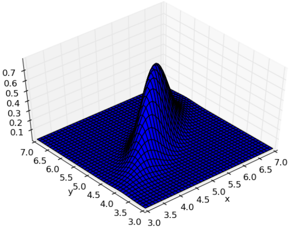
This is the same as the diagonal case, but with a new coordinate system, defined by the eigenvectors.

Non-diagonal covariance









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(As in the diagonal case.)

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Probability measure

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Expectation

$$\mathbb{E}[X] = \begin{bmatrix} \mathbb{E}[X_1] \\ \vdots \\ \mathbb{E}[X_d] \end{bmatrix} = \int_{\mathbb{R}^d} x p(x; \mu, \Sigma)\, dx = \mu.$$

Properties of multivariate Gaussians

Probability measure

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Covariance

$$\mathrm{Cov}[X] = \mathbb{E}\left[(X - \mu)(X - \mu)'\right] = \int_{\mathbb{R}^d} (x - \mu)(x - \mu)' p(x; \mu, \Sigma)\, dx = \Sigma.$$

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Sums of independent Gaussians

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  This corresponds to *convolving* the densities.
  The family of Gaussian densities is closed under convolutions.

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  The family of Gaussian densities is closed under convolutions.
- Since $X + Y$ is Gaussian, we only need its mean and covariance.

Properties of multivariate Gaussians

Sum of two scalar standard normals: completing the square

$$
\begin{aligned}
p_{X+Y}(z) &= \int p_X(x) p_Y(z-x)\, dx = (p_X * p_Y)(z) \\
&= \frac{1}{2\pi} \int \exp\left(-\frac{1}{2} \left(2x^2 - 2xz + z^2 \right) \right) dx \\
&= \frac{1}{2\pi} \int \exp\left(-\frac{1}{2} \left(2(x - z/2)^2 - z^2/2 + z^2 \right) \right) dx \\
&= \frac{\exp(-z^2/4)}{\sqrt{2\pi \cdot 2}} \frac{1}{\sqrt{2\pi/2}} \int \exp\left(-\frac{1}{2} \left(\frac{(x - z/2)^2}{1/2} \right) \right) dx \\
&= \frac{\exp(-z^2/4)}{\sqrt{2\pi \cdot 2}} \qquad \text{i.e., } \mathcal{N}(0, 2).
\end{aligned}
$$

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But (X, Y) is not jointly Gaussian. (Check!)
And $X + Y$ is not Gaussian. (Check!)
And, replacing the threshold 1 with a suitable constant, we can ensure that X, Y are uncorrelated but dependent. (Check!)

Properties of multivariate Gaussians

Marginals

Given a d-dimensional Gaussian $X \sim \mathcal{N}(\mu, \Sigma)$, write

$$X = \begin{bmatrix} Y \\ Z \end{bmatrix}, \qquad \mu = \begin{bmatrix} \mu_Y \\ \mu_Z \end{bmatrix}, \qquad \Sigma = \begin{bmatrix} \Sigma_{YY} & \Sigma_{YZ} \\ \Sigma_{ZY} & \Sigma_{ZZ} \end{bmatrix},$$

where $Y \in \mathbb{R}^m$ and $Z \in \mathbb{R}^{d-m}$.

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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 normal density. (And necessarily it's 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

$$Y = AX + b.$$

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- $\mathrm{Cov}(Y) = \mathbb{E}\left[(Y - \mathbb{E}Y)(Y - \mathbb{E}Y)'\right] = \mathbb{E}\left[(A(X - \mu))(A(X - \mu))'\right] = A\mathbb{E}[(X - \mu)(X - \mu)']A' = A\Sigma A'$.

Properties of multivariate Gaussians

Example

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

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This is called *whitening* X.

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

- Review: Diagonal covariance matrices.
- Non-diagonal covariance and diagonalization.
- Properties of multivariate Gaussians.
- **Estimating Gaussians.**

Maximum likelihood

Gaussian Estimation

- Work with the log likelihood:

$$\ell(\mu, \sigma^2) = \log\left(\prod_{i=1}^{n}\left(\frac{1}{(2\pi\sigma^2)^{1/2}}\exp\left(-\frac{(x_i-\mu)^2}{2\sigma^2}\right)\right)\right)$$

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$$= -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2.$$

Set $\nabla\ell(\theta) = 0$ and solve.

Maximum likelihood

Gaussian maximum likelihood estimation

$\nabla \ell(\theta) = 0$ for

$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i, \qquad \frac{n}{2\sigma^2} = \frac{1}{2\sigma^4} \sum_{i=1}^{n} (x_i - \mu)^2$$

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)^2.$$

Other estimators for Gaussian parameters

Gaussian Estimation

Other estimators for Gaussian parameters

Gaussian Estimation

- We can also use penalized maximum likelihood estimators:

$$\ell(\mu, \sigma^2) - \text{penalty}(\mu, \sigma^2)$$
$$= \log \left(\prod_{i=1}^{n} \left(\frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left(-\frac{(x_i - \mu)^2}{2\sigma^2} \right) \right) \right) - \text{penalty}(\mu, \sigma^2)$$

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- And Bayesian estimators:

$$\begin{aligned} \text{prior distribution:} \quad & \pi(\theta) = 1 \\ \text{posterior distribution:} \quad & p(\theta | X_1 = x_1) \propto \underbrace{p(X_1 = x_1 | \theta)}_{\text{likelihood}} \underbrace{\pi(\theta)}_{\text{prior}} \\ & = \frac{p(X_1 = x_1|\theta)\pi(\theta)}{\int p(X_1 = x_1 | q)\, d\pi(q)} \end{aligned}$$

Other estimators for Gaussian parameters

Gaussian Estimation

- Penalized maximum likelihood estimators and Bayesian estimators are particularly effective in the high-dimensional setting, when the number of parameters is large compared to the amount of data.

Maximum likelihood

Multivariate Gaussian Estimation

- Log likelihood:

$$\ell(\mu, \Sigma) = \log\left(\prod_{i=1}^{n}\left(\frac{1}{(2\pi)^{d/2}\left|\Sigma\right|^{1/2}}\exp\left(-\frac{1}{2}(x_i-\mu)'\Sigma^{-1}(x_i-\mu)\right)\right)\right)$$

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Set $\nabla \ell(\theta) = 0$ and solve.

Maximum likelihood

Gaussian maximum likelihood estimation

$\nabla_\mu \ell(\mu, \Sigma) = 0$ for

$$\sum_{i=1}^{n} \Sigma^{-1}(\mu - x_i) = 0 \qquad \text{check: } \nabla_\mu^2 \ell = -\frac{n}{2}\Sigma^{-1}$$

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i. \qquad \text{(sample mean)}$$

And it's possible to show that the maximum of $\ell(\mu, \Sigma)$ occurs at

$$\hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})(x_i - \hat{\mu})'. \qquad \text{(sample covariance)}$$

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