

# Some Essentials of Probability for Probabilistic Machine Learning

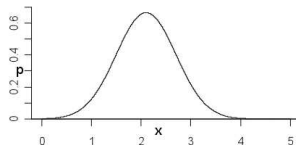
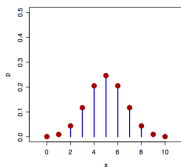
Piyush Rai  
IIT Kanpur

Probabilistic Machine Learning (CS772A)

Jan 4, 2016

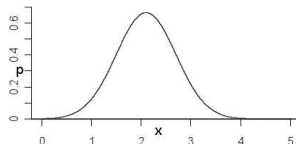
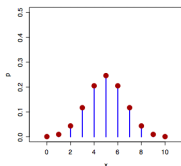
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- A random variable (r.v.)  $X$  denotes possible outcomes of an event
- Can be **discrete** (i.e., finite many possible outcomes) or **continuous**



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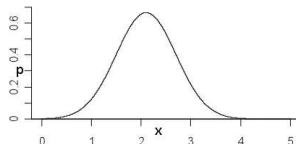
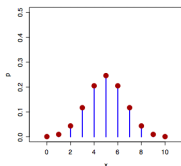
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  - A random variable  $X \in \{1, 2, \dots, 6\}$  denoting outcome of a dice roll

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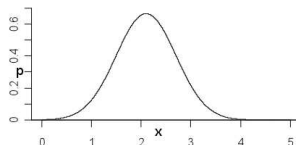
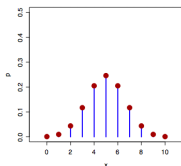
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- An r.v. is associated with a probability mass function or prob. distribution

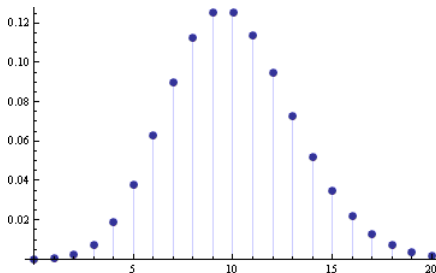
# Discrete Random Variables

- For a discrete r.v.  $X$ ,  $p(x)$  denotes the probability that  $p(X = x)$
- $p(x)$  is called the probability mass function (PMF)

$$p(x) \geq 0$$

$$p(x) \leq 1$$

$$\sum_x p(x) = 1$$



Picture courtesy: johndcook.com

# Continuous Random Variables

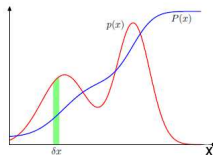
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$$p(x) \geq 0 \quad \text{and} \quad \int_{-\infty}^{\infty} p(x) dx = 1$$

- Probability that a cont. r.v.  $X \in (x, x + \delta x)$  is  $p(x)\delta x$  as  $\delta x \rightarrow 0$



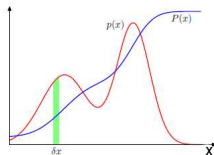


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- Probability that  $X$  lies between  $(-\infty, z)$  is given by the **cumulative distribution function** (CDF)  $P(z)$  where

$$P(z) = p(X \leq z) = \int_{-\infty}^z p(x) dx \quad \text{and} \quad p(x) = |P'(z)|_{z=x}$$

# A word about notation..

- $p(\cdot)$  can mean different things depending on the context
  - $p(X)$  denotes the PMF/PDF of an r.v.  $X$
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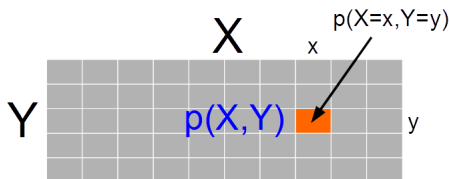
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- Actual meaning should be clear from the context (but be careful)
- Exercise the same care when  $p(\cdot)$  is a specific distribution (Bernoulli, Beta, Gaussian, etc.)
- The following means **drawing a sample** from the distribution  $p(X)$

$$x \sim p(X)$$

# Joint Probability

Joint probability  $p(X, Y)$  models probability of co-occurrence of two r.v.  $X, Y$   
For discrete r.v., the joint PMF  $p(X, Y)$  is like a table (that sums to 1)

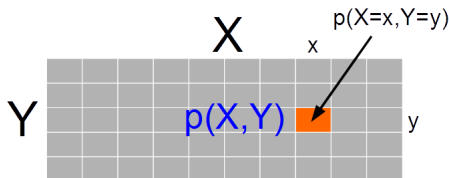
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For continuous r.v., we have joint PDF  $p(X, Y)$

$$\int_x \int_y p(X = x, Y = y) dx dy = 1$$

# Marginal Probability

- For discrete r.v.

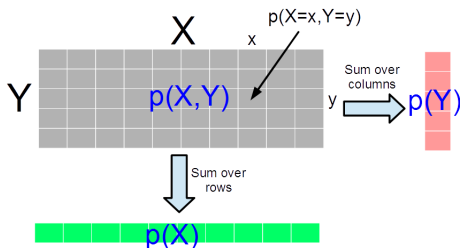
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- For discrete r.v. it is the sum of the PMF table along the rows/columns



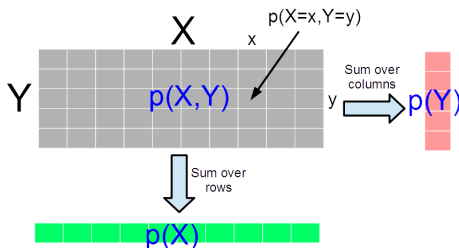


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# Conditional Probability

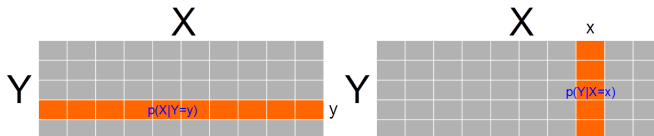
- Meaning: Probability of one event when we know the outcome of the other
- Conditional probability  $p(X|Y)$  or  $p(Y|X)$ : like taking a slice of  $p(X, Y)$

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<sup>1</sup>Picture courtesy: Computer vision: models, learning and inference (Simon Price)

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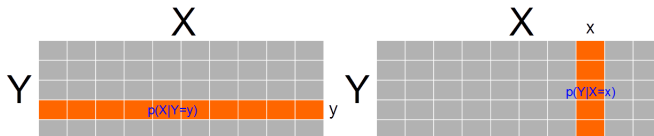
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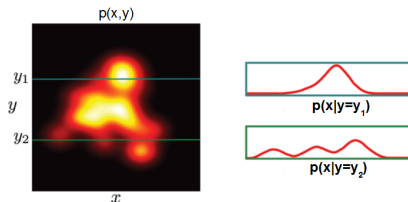
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# Some Basic Rules

- **Sum rule:** Gives the marginal probability
  - For discrete r.v.:  $p(X) = \sum_Y p(X, Y)$
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- Bayes rule is also central to parameter estimation (more on this later)
- Also remember the **chain rule**

$$p(X_1, X_2, \dots, X_N) = p(X_1)p(X_2|X_1) \dots p(X_N|X_1, \dots, X_{N-1})$$

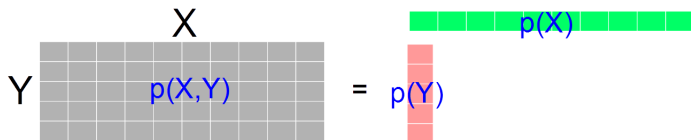
# Independence

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- $X \perp\!\!\!\perp Y$  is also called **marginal independence**

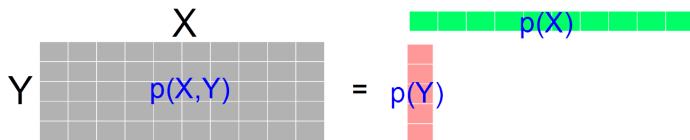
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- $X \perp\!\!\!\perp Y$  is also called **marginal independence**
- **Conditional independence** ( $X \perp\!\!\!\perp Y|Z$ ): independence when another event  $Z$  is observed

$$p(X, Y|Z) = p(X|Z)p(Y|Z)$$

# Expectation

- **Expectation** or **mean**  $\mu$  of an r.v. with PMF/PDF  $p(X)$

$$\mathbb{E}[X] = \sum_x xp(x) \quad (\text{for discrete distributions})$$

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- **Linearity of expectation** (very important/useful property)

$$\mathbb{E}[\alpha f(x) + \beta g(x)] = \alpha \mathbb{E}[f(x)] + \beta \mathbb{E}[g(x)]$$

# Variance and Covariance

- **Variance**  $\sigma^2$  (or “spread” around mean) of an r.v. with PMF/PDF  $p(X)$

$$\text{var}[X] = \mathbb{E}[(X - \mu)^2]$$

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- Cov. of components of a vector r.v.  $\mathbf{x}$  with each other:  $\text{cov}[\mathbf{x}] = \text{cov}[\mathbf{x}, \mathbf{x}]$

# Transformation of Random Variables

Suppose  $\mathbf{y} = f(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$  be a linear function of an r.v.  $\mathbf{x}$

Suppose  $\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}$  and  $\text{cov}[\mathbf{x}] = \boldsymbol{\Sigma}$

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Likewise if  $y = f(\mathbf{x}) = \mathbf{a}^T \mathbf{x} + b$  is a scalar-valued linear function of an r.v.  $\mathbf{x}$ :

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- Expectation of  $\mathbf{y}$

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# Common Probability Distributions

**Important:** We will use these extensively to model **data** as well as **parameters**

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Some **discrete distributions** and what they can model:

- **Bernoulli:** Binary numbers, e.g., outcome (head/tail, 0/1) of a coin toss
- **Binomial:** Bounded non-negative integers, e.g., # of heads in  $n$  coin tosses
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- .. and many others

Some **continuous distributions** and what they can model:

- **Uniform:** numbers defined over a fixed range
- **Beta:** numbers between 0 and 1, e.g., probability of head for a biased coin
- **Gamma:** Positive unbounded real numbers
- **Dirichlet:** vectors that sum of 1 (fraction of data points in different clusters)
- **Gaussian:** real-valued numbers or real-valued vectors
- .. and many others

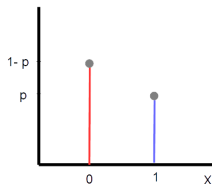
# Discrete Distributions

# Bernoulli Distribution

- Distribution over a binary r.v.  $x \in \{0, 1\}$ , like a coin-toss outcome
- Defined by a probability parameter  $p \in (0, 1)$

$$P(x = 1) = p$$

- Distribution defined as:  $\text{Bernoulli}(x; p) = p^x(1 - p)^{1-x}$



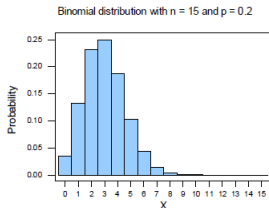
- Mean:  $\mathbb{E}[x] = p$
- Variance:  $\text{var}[x] = p(1 - p)$



# Binomial Distribution

- Distribution over number of successes  $m$  (an r.v.) in a number of trials
- Defined by two parameters: total number of trials ( $N$ ) and probability of each success  $p \in (0, 1)$
- Can think of Binomial as multiple independent Bernoulli trials
- Distribution defined as

$$\text{Binomial}(m; N, p) = \binom{N}{m} p^m (1 - p)^{N-m}$$



- Mean:  $\mathbb{E}[m] = Np$
- Variance:  $\text{var}[m] = Np(1 - p)$

# Multinoulli Distribution

- Also known as the **categorical distribution** (models categorical variables)
- Think of a random assignment of an item to one of  $K$  bins - a  $K$  dim. binary r.v.  $\mathbf{x}$  with single 1 (i.e.,  $\sum_{k=1}^K x_k = 1$ ): **Modeled by a multinoulli**

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- Let vector  $\mathbf{p} = [p_1, p_2, \dots, p_K]$  define the probability of going to each bin
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- Think of repeating the Multinoulli  $N$  times
- Like distributing  $N$  items to  $K$  bins. Suppose  $x_k$  is count in bin  $k$

$$0 \leq x_k \leq N \quad \forall k = 1, \dots, K, \quad \sum_{k=1}^K x_k = N$$

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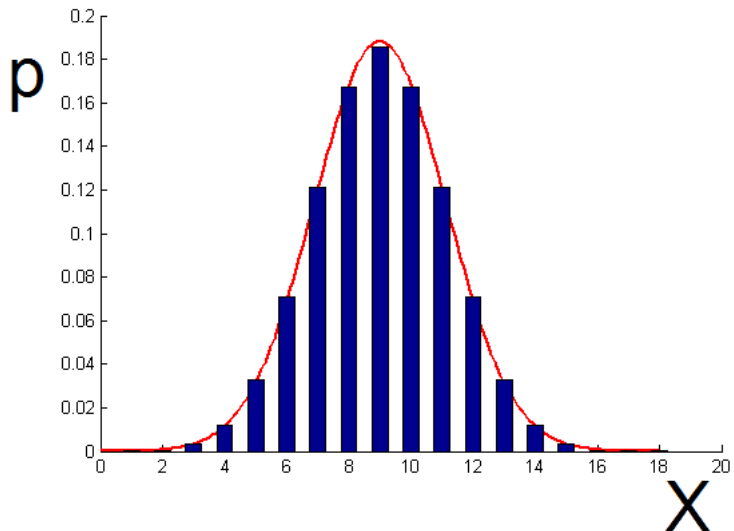
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- Variance:  $\text{var}[x_k] = Np_k(1 - p_k)$
- Note: For  $N = 1$ , multinomial is the same as multinoulli

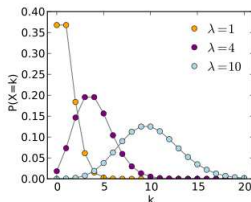
# Multinoulli/Multinomial: Pictorially



# Poisson Distribution

- Used to model a non-negative integer (count) r.v.  $k$
- Examples: number of words in a document, number of events in a fixed interval of time, etc.
- Defined by a positive rate parameter  $\lambda$
- Distribution defined as

$$\text{Poisson}(k; \lambda) = \frac{\lambda^k e^{-\lambda}}{k!} \quad k = 0, 1, 2, \dots$$



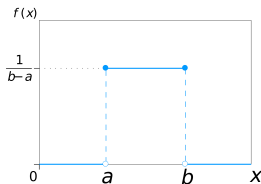
- Mean:  $\mathbb{E}[k] = \lambda$
- Variance:  $\text{var}[k] = \lambda$

# Continuous Distributions

# Uniform Distribution

- Models a continuous r.v.  $x$  distributed uniformly over a finite interval  $[a, b]$

$$\text{Uniform}(x; a, b) = \frac{1}{b - a}$$

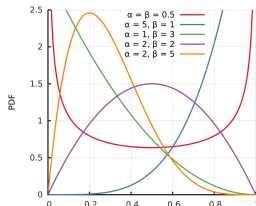


- Mean:  $\mathbb{E}[x] = \frac{(b+a)}{2}$
- Variance:  $\text{var}[x] = \frac{(b-a)^2}{12}$

# Beta Distribution

- Used to model an r.v.  $p$  between 0 and 1 (e.g., a probability)
- Defined by two **shape parameters**  $\alpha$  and  $\beta$

$$\text{Beta}(p; \alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1} (1-p)^{\beta-1}$$

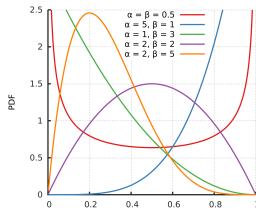


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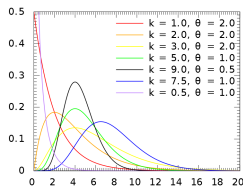
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- Variance:  $\text{var}[p] = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}$
- Often used to model the probability parameter of a Bernoulli or Binomial (also **conjugate** to these distributions)



# Gamma Distribution

- Used to model positive real-valued r.v.  $x$
- Defined by a **shape parameters**  $k$  and a **scale parameter**  $\theta$

$$\text{Gamma}(x; k, \theta) = \frac{x^{k-1} e^{-\frac{x}{\theta}}}{\theta^k \Gamma(k)}$$



- Mean:  $\mathbb{E}[x] = k\theta$
- Variance:  $\text{var}[x] = k\theta^2$
- Often used to model the rate parameter of Poisson or exponential distribution, or to model the inverse variance of a Gaussian

# Dirichlet Distribution

- Used to model non-negative r.v. vectors  $\mathbf{p} = [p_1, \dots, p_K]$  that sum to 1

$$0 \leq p_k \leq 1, \quad \forall k = 1, \dots, K \quad \text{and} \quad \sum_{k=1}^K p_k = 1$$

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- Equivalent to a distribution over the  $K - 1$  dimensional simplex
- Defined by a  $K$  size vector  $\alpha = [\alpha_1, \dots, \alpha_K]$  of positive reals
- Distribution defined as

$$\text{Dirichlet}(\mathbf{p}; \alpha) = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K p_k^{\alpha_k - 1}$$

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- Often used to model parameters of Multinoulli/Multinomial
- Dirichlet is conjugate to Multinoulli/Multinomial
- Note:** Dirichlet can be seen as a generalization of the Beta distribution. Normalizing a bunch of Gamma r.v.'s gives an r.v. that is Dirichlet distributed.

# Dirichlet Distribution

- For  $\mathbf{p} = [p_1, p_2, \dots, p_K]$  drawn from  $\text{Dirichlet}(\alpha_1, \alpha_2, \dots, \alpha_K)$

- Mean:  $\mathbb{E}[p_k] = \frac{\alpha_k}{\sum_{k=1}^K \alpha_k}$

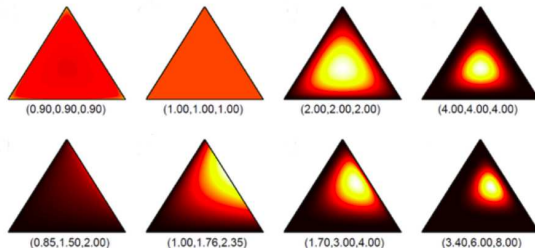
- Variance:  $\text{var}[p_k] = \frac{\alpha_k(\alpha_0 - \alpha_k)}{\alpha_0^2(\alpha_0 + 1)}$  where  $\alpha_0 = \sum_{k=1}^K \alpha_k$

- Note:  $\mathbf{p}$  is a point on  $(K - 1)$ -simplex

- Note:  $\alpha_0 = \sum_{k=1}^K \alpha_k$  controls how peaked the distribution is

- Note:  $\alpha_k$ 's control where the peak(s) occur

Plot of a 3 dim. Dirichlet (2 dim. simplex) for various values of  $\alpha$ :



Picture courtesy: Computer vision: models, learning and inference (Simon Price)

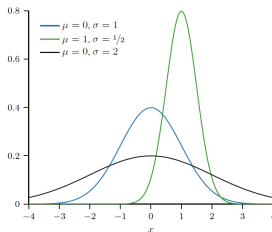
Now comes the  
Gaussian (Normal) distribution..



# Univariate Gaussian Distribution

- Distribution over real-valued scalar r.v.  $x$
- Defined by a scalar **mean**  $\mu$  and a scalar **variance**  $\sigma^2$
- Distribution defined as

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

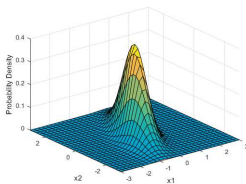


- Mean:  $\mathbb{E}[x] = \mu$
- Variance:  $\text{var}[x] = \sigma^2$
- Precision (inverse variance)  $\beta = 1/\sigma^2$

# Multivariate Gaussian Distribution

- Distribution over a multivariate r.v. vector  $\mathbf{x} \in \mathbb{R}^D$  of real numbers
- Defined by a **mean vector**  $\boldsymbol{\mu} \in \mathbb{R}^D$  and a  $D \times D$  **covariance matrix**  $\boldsymbol{\Sigma}$

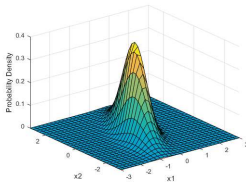
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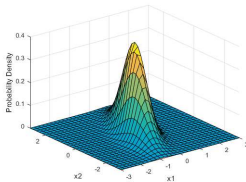


- The covariance matrix  $\boldsymbol{\Sigma}$  must be symmetric and positive definite
  - All eigenvalues are positive
  - $\mathbf{z}^\top \boldsymbol{\Sigma} \mathbf{z} > 0$  for any real vector  $\mathbf{z}$

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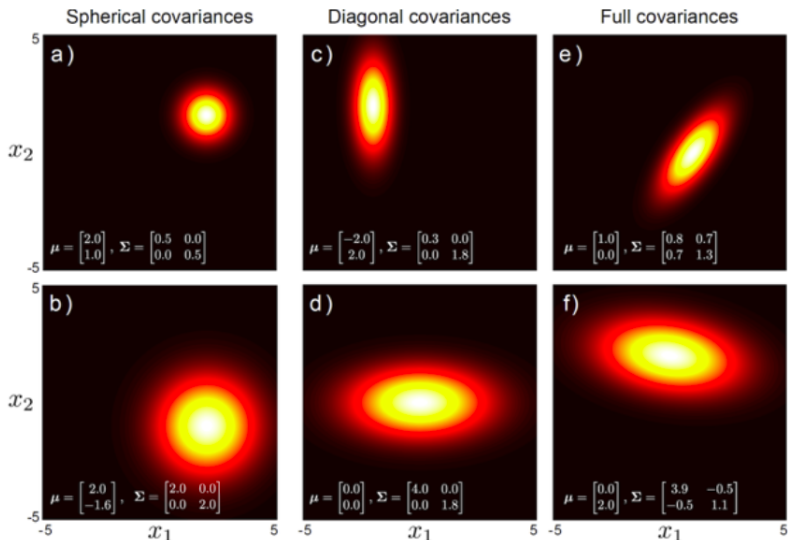
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  - All eigenvalues are positive
  - $\mathbf{z}^\top \boldsymbol{\Sigma} \mathbf{z} > 0$  for any real vector  $\mathbf{z}$
- Often we parameterize a multivariate Gaussian using the inverse of the covariance matrix, i.e., the **precision matrix**  $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$

# Multivariate Gaussian: The Covariance Matrix

The covariance matrix can be spherical, diagonal, or full



Picture courtesy: Computer vision: models, learning and inference (Simon Price)

# Some nice properties of the Gaussian distribution..

# Multivariate Gaussian: Marginals and Conditionals

- Given jointly Gaussian distribution  $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with  $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$  with

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix}, \quad \boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}, \quad \boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}$$

# Multivariate Gaussian: Marginals and Conditionals

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**Thus marginals and conditionals  
of Gaussians are Gaussians**

# Multivariate Gaussian: Marginals and Conditionals

- Given the conditional and marginal of r.v. being conditioned on

$$\begin{aligned}p(\mathbf{y}|\mathbf{x}) &= \mathcal{N}(\mathbf{y}|\mathbf{Ax} + \mathbf{b}, \mathbf{L}^{-1}) \\p(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})\end{aligned}$$

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$$\begin{aligned}p(\mathbf{y}) &= \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^T) \\p(\mathbf{x}|\mathbf{y}) &= \mathcal{N}(\mathbf{x}|\boldsymbol{\Sigma}\{\mathbf{A}^T\mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\}, \boldsymbol{\Sigma})\end{aligned}$$

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- Very useful property for probabilistic models with Gaussian likelihoods and/or priors. Also very handy for computing **marginal likelihoods**.

# Gaussians: Product of Gaussians

- Pointwise multiplication of two Gaussians is another (unnormalized) Gaussian

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) \mathcal{N}(\mathbf{x}; \boldsymbol{\nu}, \mathbf{P}) = \frac{1}{Z} \mathcal{N}(\mathbf{x}; \boldsymbol{\omega}, \mathbf{T}),$$

where

$$\mathbf{T} = (\boldsymbol{\Sigma}^{-1} + \mathbf{P}^{-1})^{-1}$$

$$\boldsymbol{\omega} = \mathbf{T}(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \mathbf{P}^{-1}\boldsymbol{\nu})$$

$$Z^{-1} = \mathcal{N}(\boldsymbol{\mu}; \boldsymbol{\nu}, \boldsymbol{\Sigma} + \mathbf{P}) = \mathcal{N}(\boldsymbol{\nu}; \boldsymbol{\mu}, \boldsymbol{\Sigma} + \mathbf{P})$$

# Multivariate Gaussian: Affine Transforms

- Given a  $\mathbf{x} \in \mathbb{R}^d$  with a multivariate Gaussian distribution

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Consider an affine transform of  $\mathbf{x}$  into  $\mathbb{R}^D$

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$$

where  $\mathbf{A}$  is  $D \times d$  and  $\mathbf{b} \in \mathbb{R}^D$

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- $\mathbf{y} \in \mathbb{R}^D$  will have a multivariate Gaussian distribution

$$\mathcal{N}(\mathbf{y}; \mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top)$$



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Many well-known distribution (Bernoulli, Binomial, categorical, beta, gamma, Gaussian, etc.) are exponential family distributions

[https://en.wikipedia.org/wiki/Exponential\\_family](https://en.wikipedia.org/wiki/Exponential_family)

# Binomial as Exponential Family

- Recall the exponential family distribution

$$p(x; \theta) = h(x)e^{\eta(\theta)T(x) - A(\theta)}$$

- Binomial in the usual form:

$$\text{Binomial}(x; n, p) = \binom{n}{x} p^x (1 - p)^{n-x}$$

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- Can re-express it as

$$\binom{n}{x} e^{(x \log(\frac{p}{1-p}) + n \log(1-p))}$$

- $h(x) = \binom{n}{x}$
- $\eta(\theta) = \log\left(\frac{p}{1-p}\right)$
- $T(x) = x$
- $A(\theta) = -n \log(1-p)$

# Gaussian as Exponential Family

- Recall the exponential family distribution

$$p(x; \theta) = h(x)e^{\eta(\theta)T(x) - A(\theta)}$$

- Gaussian in the usual form:

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



# Gaussian as Exponential Family

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- Can re-express it as  $p(x; \theta) = h(x)e^{\eta(\theta)T(x) - A(\theta)}$  where
  - $h(x) = \frac{1}{\sqrt{2\pi}}$
  - $\eta(\theta) = \left(\frac{\mu}{\sigma^2}, -\frac{1}{2\sigma^2}\right)^T$
  - $T(x) = (x, x^2)^T$
  - $A(\theta) = \frac{\mu^2}{2\sigma^2} + \log \sigma$

# Conjugate Priors

- Given a distribution  $p(x|\theta)$
- We say  $p(\theta)$  is conjugate to  $p(x|\theta)$  if

$$p(\theta|x) \propto p(x|\theta)p(\theta)$$

has the same form as  $p(\theta)$

- Many pairs of distributions are conjugate to each other, e.g.,
  - Gaussian-Gaussian
  - Bernoulli-Beta
  - Poisson-Gamma
  - .. and many others
- More on this in the next class..

# Next class: Parameter estimation in probabilistic models