Probability & Information Theory

Shan-Hung Wu
shwu@cs.nthu.edu.tw

Department of Computer Science,
National Tsing Hua University, Taiwan

Machine Learning

Outline

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Random Variables

- A ***random variable*** x is a variable that can take on different values randomly
  - E.g., $\Pr(\mathrm{x} = x_1) = 0.1$, $\Pr(\mathrm{x} = x_2) = 0.3$, etc.
  - Technically, x is a function that maps events to a real values
- Must be coupled with a ***probability distribution*** P that specifies how likely each value is
  - $\mathrm{x} \sim \mathrm{P}(\theta)$ means "x has distribution P parametrized by θ"

Probability Mass and Density Functions

- If x is discrete, $\mathrm{P}(\mathrm{x} = x)$ denotes a ***probability mass function*** $P_{\mathrm{x}}(x) = \mathrm{Pr}(\mathrm{x} = x)$
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  - $p_{\mathrm{x}}(x)$ can be greater than 1
  - E.g., a continuous uniform distribution within $[a, b]$ has $p(x) = 1/b-a$ if $x \in [a, b]$; 0 otherwise

Marginal Probability

- Consider a probability distribution over a set of variables, e.g., $\mathrm{P}(\mathrm{x}, \mathrm{y})$
- The probability distribution over the subset of random variables called the ***marginal probability*** distribution:

$$\mathrm{P}(\mathrm{x} = x) = \sum_y P(x, y) \quad \text{or} \quad \int p(x, y) dy$$

  - Also called the sum rule of probability

Conditional Probability

- Conditional density function:

$$\mathrm{P}(\mathrm{x} = x \,|\, \mathrm{y} = y) = \frac{\mathrm{P}(\mathrm{x} = x, \mathrm{y} = y)}{\mathrm{P}(\mathrm{y} = y)}$$

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- Product rule of probability:

$$\mathrm{P}(\mathrm{x}^{(1)}, \cdots, \mathrm{x}^{(n)}) = \mathrm{P}(\mathrm{x}^{(1)}) \Pi_{i=2}^{n} \mathrm{P}(\mathrm{x}^{(i)} \,|\, \mathrm{x}^{(1)}, \cdots, \mathrm{x}^{(i-1)})$$

  - E.g., $\mathrm{P}(\mathrm{a}, \mathrm{b}, \mathrm{c}) = \mathrm{P}(\mathrm{a} \,|\, \mathrm{b}, \mathrm{c}) \mathrm{P}(\mathrm{b} \,|\, \mathrm{c}) \mathrm{P}(\mathrm{c})$

Independence and Conditional Independence

- We say random variables x is ***independent*** with y iff

$$\mathrm{P}(\mathrm{x} \,|\, \mathrm{y}) = \mathrm{P}(\mathrm{x})$$

  - Implies $\mathrm{P}(\mathrm{x}, \mathrm{y}) = \mathrm{P}(\mathrm{x})\mathrm{P}(\mathrm{y})$
  - Denoted by $\mathrm{x} \perp \mathrm{y}$

Independence and Conditional Independence

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$$P(x|y) = P(x)$$

  - Implies $P(x,y) = P(x)P(y)$
  - Denoted by $x \perp y$
- We say random variables x is ***conditionally independent*** with y given z iff

$$P(x|y,z) = P(x|z)$$

  - Implies $P(x,y|z) = P(x|z)P(y|z)$
  - Denoted by $x \perp y|z$

Expectation

- The ***expectation*** (or ***expected value*** or ***mean***) of some function f with respect to x is the "average" value that f takes on:[1]

$$\mathrm{E}_{\mathrm{x}\sim\mathrm{P}}[\mathrm{f}(\mathrm{x})] = \sum_x P_{\mathrm{x}}(x) f(x) \quad \text{or} \quad \int p_{\mathrm{x}}(x) f(x) dx = \mu_{\mathrm{f}(\mathrm{x})}$$

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- Expectation is linear: $\mathrm{E}[a\mathrm{f}(\mathrm{x}) + b] = a\mathrm{E}[\mathrm{f}(\mathrm{x})] + b$ for deterministic a and b

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- Expectation is linear: $\mathrm{E}[a\mathrm{f}(\mathrm{x}) + b] = a\mathrm{E}[\mathrm{f}(\mathrm{x})] + b$ for deterministic a and b
- $\mathrm{E}[\mathrm{E}[\mathrm{f}(\mathrm{x})]] = \mathrm{E}[\mathrm{f}(\mathrm{x})]$, as $\mathrm{E}[\mathrm{f}(\mathrm{x})]$ is deterministic

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Expectation over Multiple Variables

- Defined over the join probability distribution, e.g.,

$$\mathrm{E}[\mathrm{f}(\mathrm{x},\mathrm{y})] = \sum_{x,y} P_{\mathrm{x,y}}(x,y) f(x,y) \quad \text{or} \quad \int_{x,y} p_{\mathrm{x,y}}(x,y) f(x,y) dx dy$$

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- $\mathrm{E}[\mathrm{f}(\mathrm{x}) \,|\, \mathrm{y} = y] = \int p_{\mathrm{x}\,|\,\mathrm{y}}(x\,|\,y) f(x) dx$ is called the ***conditional expectation***
- $\mathrm{E}[\mathrm{f}(\mathrm{x})\mathrm{g}(\mathrm{y})] = \mathrm{E}[\mathrm{f}(\mathrm{x})]\mathrm{E}[\mathrm{g}(\mathrm{y})]$ if x and y are independent [Proof]

Variance

- The ***variance*** measures how much the values of f deviate from its expected value when seeing different values of x:

$$\mathrm{Var}[\mathrm{f}(\mathrm{x})] = \mathrm{E}\left[(\mathrm{f}(\mathrm{x}) - \mathrm{E}[\mathrm{f}(\mathrm{x})])^2\right] = \sigma^2_{\mathrm{f}(\mathrm{x})}$$

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  - $\sigma_{\mathrm{f}(\mathrm{x})}$ is called the ***standard deviation***
- $\mathrm{Var}[\mathrm{f}(\mathrm{x})] = \mathrm{E}[\mathrm{f}(\mathrm{x})^2] - \mathrm{E}[\mathrm{f}(\mathrm{x})]^2$ [Proof]
- $\mathrm{Var}[af(\mathrm{x}) + b] = a^2\mathrm{Var}[\mathrm{f}(\mathrm{x})]$ for deterministic a and b [Proof]

Covariance I

- ***Covariance*** gives some sense of how much two values are ***linearly*** related to each other

$$\mathrm{Cov}[\mathrm{f}(\mathrm{x}), \mathrm{g}(\mathrm{y})] = \mathrm{E}\left[(\mathrm{f}(\mathrm{x}) - \mathrm{E}[\mathrm{f}(\mathrm{x})])(\mathrm{g}(\mathrm{y}) - \mathrm{E}[\mathrm{g}(\mathrm{y})])\right]$$

  - If sign positive, both variables tend to take on high values simultaneously
  - If sign negative, one variable tend to take on high value while the other taking on low one

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  - If sign positive, both variables tend to take on high values simultaneously
  - If sign negative, one variable tend to take on high value while the other taking on low one
- If x and y are independent, then $\mathrm{Cov}(\mathrm{x}, \mathrm{y}) = 0$ [Proof]
  - The converse is ***not*** true as X and Y may be related in a nonlinear way
  - E.g., $\mathrm{y} = \sin(\mathrm{x})$ and $\mathrm{x} \sim \mathrm{Uniform}(-\pi, \pi)$

Covariance II

- $\mathrm{Var}(a\mathrm{x}+b\mathrm{y}) = a^2\mathrm{Var}(\mathrm{x}) + b^2\mathrm{Var}(\mathrm{y}) + 2ab\mathrm{Cov}(\mathrm{x},\mathrm{y})$ [Proof]

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  - $\mathrm{Var}(\mathrm{x}+\mathrm{y}) = \mathrm{Var}(\mathrm{x}) + \mathrm{Var}(\mathrm{y})$ if x and y are independent
- $\mathrm{Cov}(a\mathrm{x}+b, c\mathrm{y}+d) = ac\mathrm{Cov}(\mathrm{x},\mathrm{y})$ [Proof]

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- $\mathrm{Var}(ax+by) = a^2\mathrm{Var}(x) + b^2\mathrm{Var}(y) + 2ab\mathrm{Cov}(x,y)$ [Proof]
  - $\mathrm{Var}(x+y) = \mathrm{Var}(x) + \mathrm{Var}(y)$ if x and y are independent
- $\mathrm{Cov}(ax+b, cy+d) = ac\mathrm{Cov}(x,y)$ [Proof]
- $\mathrm{Cov}(ax+by, cw+dv) =$
  $ac\mathrm{Cov}(x,w) + ad\mathrm{Cov}(x,v) + bc\mathrm{Cov}(y,w) + bd\mathrm{Cov}(y,v)$ [Proof]

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Multivariate Random Variables I

- A multivariate random variable is denoted by $\mathbf{x} = [\mathrm{x}_1, \cdots, \mathrm{x}_d]^\top$
  - Normally, x_i's (***attributes*** or ***variables*** or ***features***) are dependent with each other
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$$\Sigma_{\mathbf{x}} = \begin{bmatrix} \sigma^2_{\mathrm{x}_1} & \sigma_{\mathrm{x}_1,\mathrm{x}_2} & \cdots & \sigma_{\mathrm{x}_1,\mathrm{x}_d} \\ \sigma_{\mathrm{x}_2,\mathrm{x}_1} & \sigma^2_{\mathrm{x}_2} & \cdots & \sigma_{\mathrm{x}_2,\mathrm{x}_d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{\mathrm{x}_d,\mathrm{x}_1} & \sigma_{\mathrm{x}_d,\mathrm{x}_2} & \cdots & \sigma^2_{\mathrm{x}_d} \end{bmatrix}$$

  - $\sigma_{\mathrm{x}_i,\mathrm{x}_j} = \mathrm{Cov}(\mathrm{x}_i, \mathrm{x}_j) = \mathrm{E}[(\mathrm{x}_i - \mu_{\mathrm{x}_i})(\mathrm{x}_j - \mu_{\mathrm{x}_j})] = \mathrm{E}(\mathrm{x}_i \mathrm{x}_j) - \mu_{\mathrm{x}_i}\mu_{\mathrm{x}_j}$

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- $\Sigma_{\mathbf{x}}$ is always positive semidefinite [Homework]
- $\Sigma_{\mathbf{x}}$ is nonsingular iff it is positive definite
- $\Sigma_{\mathbf{x}}$ is singular implies that $\mathbf{x}$ has either:
  - Deterministic/independent/non-linearly dependent attributes causing zero rows, or
  - Redundant attributes causing linear dependency between rows

Derived Random Variables

- Let $\mathrm{y} = \mathrm{f}(\mathbf{x}; \boldsymbol{w}) = \boldsymbol{w}^\top \mathbf{x}$ be a random variable transformed from $\mathbf{x}$
- $\mu_{\mathrm{y}} = \mathrm{E}(\boldsymbol{w}^\top \mathbf{x}) = \boldsymbol{w}^\top \mathrm{E}(\mathbf{x}) = \boldsymbol{w}^\top \mu_{\mathbf{x}}$
- $\sigma_{\mathrm{y}}^2 = \boldsymbol{w}^\top \Sigma_{\mathbf{x}} \boldsymbol{w}$ [Homework]

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1. ***Bayesian probability***: it's a degree of belief or qualitative levels of certainty
2. ***Frequentist probability***: if we can draw samples of x, then the proportion of frequency of samples having the value x is equal to $\Pr(\mathrm{x} = x)$

Bayes' Rule

$$P(y|x) = \frac{P(x|y)P(y)}{P(x)} = \frac{P(x|y)P(y)}{\Sigma_y P(x|y=y)P(y=y)}$$

- Bayes' Rule is so important in statistics (and ML as well) such that each term has a name:

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- Why is it so important?
- E.g., a doctor diagnoses you as having a disease by letting x be "symptom" and y be "disease"
  - $\mathrm{P}(\mathrm{x}\,|\,\mathrm{y})$ and $\mathrm{P}(\mathrm{y})$ may be estimated from sample frequencies more easily

Point Estimation

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- Let $\{x^{(1)}, \cdots, x^{(n)}\}$ be a set of n independent and identically distributed (***i.i.d.***) samples of a random variable x, a ***point estimator*** or ***statistic*** is a function of the data:

$$\hat{\theta}_n = g(x^{(1)}, \cdots, x^{(n)})$$

  - $\hat{\theta}_n$ is called the ***estimate*** of θ

Sample Mean and Covariance

- Given $\boldsymbol{X} = [\boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(n)}]^\top \in \mathbb{R}^{n \times d}$ the i.i.d samples, what are the estimates of the mean and covariance of $\mathbf{x}$?

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  - $\hat{\sigma}^2_{\mathrm{x}_i, \mathrm{x}_j} = \frac{1}{n} \sum_{s=1}^{n} (x_i^{(s)} - \hat{\mu}_{\mathrm{x}_i})(x_j^{(s)} - \hat{\mu}_{\mathrm{x}_j})$

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  - If each $\boldsymbol{x}^{(i)}$ is centered (by subtracting $\hat{\mu}_{\mathbf{x}}$ first), then $\hat{\Sigma}_{\mathbf{x}} = \frac{1}{n} \boldsymbol{X}^\top \boldsymbol{X}$

Outline

Principal Components Analysis (PCA) I

- Give a collection of data points $\mathbb{X} = \{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$, where $\boldsymbol{x}^{(i)} \in \mathbb{R}^D$
- Suppose we want to lossily compress $\mathbb{X}$, i.e., to find a function f such that $f(\boldsymbol{x}^{(i)}) = \boldsymbol{z}^{(i)} \in \mathbb{R}^K$, where $K < D$
- How to keep the maximum info in $\mathbb{X}$?

Principal Components Analysis (PCA) II

- Let $\boldsymbol{x}^{(i)}$'s be i.i.d. samples of a random variable $\mathbf{x}$
- Let f be linear, i.e., $f(\mathbf{x}) = \boldsymbol{W}^\top \mathbf{x}$ for some $\boldsymbol{W} \in \mathbb{R}^{D \times K}$

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- ***Principal Component Analysis (PCA)*** finds K orthonormal vectors $\boldsymbol{W} = \left[\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}\right]$ such that the transformed variable $\mathbf{z} = \boldsymbol{W}^\top \mathbf{x}$ has the most "spread out" attributes, i.e., each attribute $\mathrm{z}_j = \boldsymbol{w}^{(j)\top} \mathbf{x}$ has the maximum variance $\mathrm{Var}(\mathrm{z}_j)$
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  - $\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}$ are called the ***principle components***
- Why $\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}$ need to be orthogonal with each other?
  - Each $\boldsymbol{w}^{(j)}$ keeps information that cannot be explained by others, so together they preserve the most info

Principal Components Analysis (PCA) II

- Let $\boldsymbol{x}^{(i)}$'s be i.i.d. samples of a random variable $\mathbf{x}$
- Let f be linear, i.e., $f(\mathbf{x}) = \boldsymbol{W}^\top \mathbf{x}$ for some $\boldsymbol{W} \in \mathbb{R}^{D \times K}$
- ***Principal Component Analysis (PCA)*** finds K orthonormal vectors $\boldsymbol{W} = \left[\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}\right]$ such that the transformed variable $\mathbf{z} = \boldsymbol{W}^\top \mathbf{x}$ has the most "spread out" attributes, i.e., each attribute $\mathrm{z}_j = \boldsymbol{w}^{(j)\top} \mathbf{x}$ has the maximum variance $\mathrm{Var}(\mathrm{z}_j)$
  - $\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}$ are called the ***principle components***
- Why $\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}$ need to be orthogonal with each other?
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- Why $\|\boldsymbol{w}^{(j)}\| = 1$ for all j?
  - Only directions matter—we don't want to maximize $\mathrm{Var}(\mathrm{z}_j)$ by finding a long $\boldsymbol{w}^{(j)}$

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- For simplicity, let's consider $K = 1$ first
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- $\boldsymbol{X}^\top\boldsymbol{X}$ is symmetric thus can be eigendecomposed
- By Rayleigh's Quotient, the optimal $\boldsymbol{w}^{(1)}$ is given by the eigenvector of $\boldsymbol{X}^\top\boldsymbol{X}$ corresponding to the largest eigenvalue

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- Optimization problem for $\boldsymbol{w}^{(2)}$:

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- By Rayleigh's Quotient again, $\boldsymbol{w}^{(2)}$ is the eigenvector corresponding to the 2-nd largest eigenvalue
- For general case where $K > 1$, the $\boldsymbol{w}^{(1)}, \cdots, \boldsymbol{w}^{(K)}$ are eigenvectors of $\boldsymbol{X}^\top\boldsymbol{X}$ corresponding to the largest K eigenvalues
  - Proof by induction [Proof]

Visualization

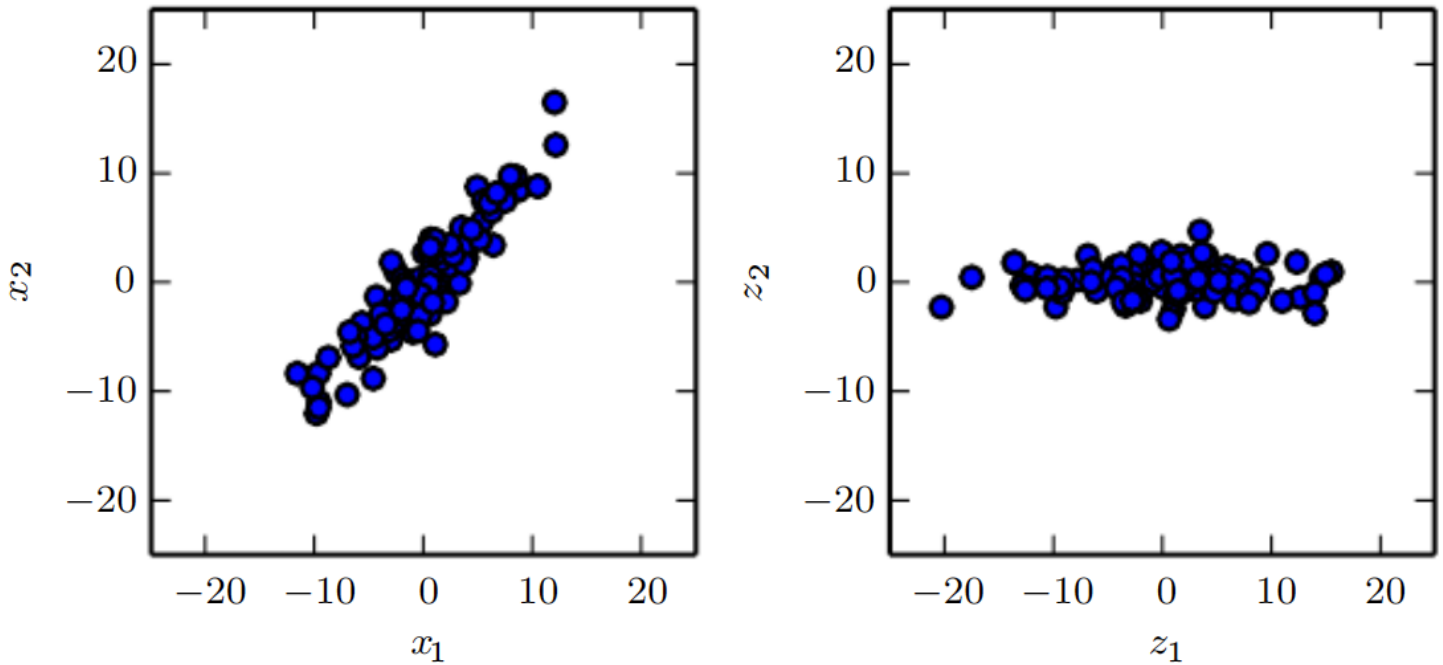

Figure: PCA learns a linear projection that aligns the direction of greatest variance with the axes of the new space. With these new axes, the estimated covariance matrix $\hat{\boldsymbol{\Sigma}}_{\mathbf{z}} = \boldsymbol{W}^\top \hat{\boldsymbol{\Sigma}}_{\mathbf{x}} \boldsymbol{W} \in \mathbb{R}^{K \times K}$ is always diagonal.

Outline

Sure and Almost Sure Events

- Given a continuous random variable x, we have $\Pr(\mathrm{x} = x) = 0$ for any value x
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- Will the event $\mathrm{x} = x$ occur? ***Yes!***
- An event $\mathbb{A}$ happens ***surely*** if always occurs
- An event $\mathbb{A}$ happens ***almost surely*** if $\Pr(\mathbb{A}) = 1$ (e.g., $\Pr(\mathrm{x} \neq x) = 1$)

Equality of Random Variables I

Definition (Equality in Distribution)

Two random variables x and y are ***equal in distribution*** iff $\Pr(\mathrm{x} \leq a) = \Pr(\mathrm{y} \leq a)$ for all a.

Definition (Almost Sure Equality)

Two random variables x and y are ***equal almost surely*** iff $\Pr(\mathrm{x} = \mathrm{y}) = 1$.

Definition (Equality)

Two random variables x and y are ***equal*** iff they maps the same events to same values.

Equality of Random Variables II

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- Almost sure equality implies equality in distribution, but converse not true
- E.g., let x and y be binary random variables and $P_{\mathrm{x}}(0) = P_{\mathrm{x}}(1) = P_{\mathrm{y}}(0) = P_{\mathrm{y}}(1) = 0.5$
  - They are equal in distribution
  - But $\Pr(\mathrm{x} = \mathrm{y}) = 0.5 \neq 1$

Convergence of Random Variables I

Definition (Convergence in Distribution)

A sequence of random variables $\{\mathrm{x}^{(1)}, \mathrm{x}^{(2)}, \cdots\}$ *converges in distribution* to x iff $\lim_{n\to\infty} \mathrm{P}\left(\mathrm{x}^{(n)} = x\right) = \mathrm{P}(\mathrm{x} = x)$

Definition (Convergence in Probability)

A sequence of random variables $\{\mathrm{x}^{(1)}, \mathrm{x}^{(2)}, \cdots\}$ *converges in probability* to x iff for any $\varepsilon > 0$, $\lim_{n\to\infty} \Pr\left(|\mathrm{x}^{(n)} - \mathrm{x}| < \varepsilon\right) = 1$.

Definition (Almost Sure Convergence)

A sequence of random variables $\{\mathrm{x}^{(1)}, \mathrm{x}^{(2)}, \cdots\}$ *converges almost surely* to x iff $\Pr\left(\lim_{n\to\infty} \mathrm{x}^{(n)} = \mathrm{x}\right) = 1$.

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- Almost sure convergence implies convergence in probability, but converse not true
- $\lim_{n\to\infty} \Pr\left(|\mathrm{x}^{(n)} - \mathrm{x}| < \varepsilon\right) = 1$ leaves open the possibility that $|\mathrm{x}^{(n)} - \mathrm{x}| > \varepsilon$ happens an infinite number of times
- $\Pr\left(\lim_{n\to\infty} \mathrm{x}^{(n)} = \mathrm{x}\right) = 1$ guarantees that $|\mathrm{x}^{(n)} - \mathrm{x}| > \varepsilon$ almost surely will not occur

Distribution of Derived Variables I

- Suppose $\mathrm{y} = f(\mathrm{x})$ and f^{-1} exists, does $\mathrm{P}(\mathrm{y} = y) = \mathrm{P}(\mathrm{x} = f^{-1}(y))$ always hold?

Distribution of Derived Variables I

- Suppose $\mathrm{y} = f(\mathrm{x})$ and f^{-1} exists, does $\mathrm{P}(\mathrm{y} = y) = \mathrm{P}(\mathrm{x} = f^{-1}(y))$ always hold? ***No***, when x and y are continuous
- Suppose $\mathrm{x} \sim \mathrm{Uniform}(0, 1)$ is continuous and $p(x) = c$ for $x \in (0, 1)$
- Let $\mathrm{y} = \mathrm{x}/2 \sim \mathrm{Uniform}(0, 1/2)$
- If $p_{\mathrm{y}}(y) = p_{\mathrm{x}}(2y)$, then

$$\int_{y=0}^{1/2} p_{\mathrm{y}}(y)dy = \int_{y=0}^{1/2} c \cdot dy = \frac{1}{2} \neq 1$$

  - Violates the axiom of probability

Distribution of Derived Variables II

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$$|p_{\mathrm{y}}(f(x))dy| = |p_{\mathrm{x}}(x)dx|$$

- We have

$$p_{\mathrm{y}}(y) = p_{\mathrm{x}}(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right| \quad (\text{or } \; p_{\mathrm{x}}(x) = p_{\mathrm{y}}(f(x)) \left| \frac{\partial f(x)}{\partial x} \right|)$$

  - In previous example: $p_{\mathrm{y}}(y) = \mathbf{2} \cdot p_{\mathrm{x}}(2y)$

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  - In previous example: $p_{\mathrm{y}}(y) = \mathbf{2} \cdot p_{\mathrm{x}}(2y)$
- In multivariate case, we have

$$p_{\mathbf{y}}(\boldsymbol{y}) = p_{\mathbf{x}}(\boldsymbol{f}^{-1}(\boldsymbol{y})) \left| \det \left(\boldsymbol{J}(\boldsymbol{f}^{-1})(\boldsymbol{y}) \right) \right|,$$

  where $\boldsymbol{J}(\boldsymbol{f}^{-1})(\boldsymbol{y})$ is the Jacobian matrix of $\boldsymbol{f}^{-1}$ at input $\boldsymbol{y}$
  - $J(\boldsymbol{f}^{-1})(\boldsymbol{y})_{i,j} = \partial f_i^{-1}(\boldsymbol{y}) / \partial y_j$

Outline

Random Experiments

- The value of a random variable x can be think of as the outcome of an random experiment
- Helps us define $\mathrm{P}(\mathrm{x})$

Bernoulli Distribution (Discrete)

- Let $\mathrm{x} \in \{0, 1\}$ be the outcome of tossing a coin, we have:

$$\text{Bernoulli}(\mathrm{x} = x; \rho) = \begin{cases} \rho, & \text{if } x = 1 \\ 1 - \rho, & \text{otherwise} \end{cases} \quad \text{or } \rho^x (1 - \rho)^{1-x}$$

- Properties: [Proof]
  - $\mathrm{E}(\mathrm{x}) = \rho$
  - $\mathrm{Var}(\mathrm{x}) = \rho(1 - \rho)$

Categorical Distribution (Discrete)

- Let $\mathrm{x} \in \{1, \cdots, k\}$ be the outcome of rolling a k-sided dice, we have:

$$\text{Categorical}(\mathrm{x} = x; \rho) = \prod_{i=1}^{k} \rho_i^{1(x; x=i)}, \text{ where } \mathbf{1}^\top \rho = 1$$

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- An extension of the Bernoulli distribution for k states

Multinomial Distribution (Discrete)

- Let $\mathbf{x} \in \mathbb{R}^k$ be a random vector where x_i the number of the outcome i after rolling a k-sided dice n times:

$$\text{Multinomial}(\mathbf{x} = \boldsymbol{x}; n, \rho) = \frac{n!}{x_1! \cdots x_k!} \prod_{i=1}^{k} \rho_i^{x_i}, \text{ where } \mathbf{1}^\top \rho = 1 \text{ and } \mathbf{1}^\top \boldsymbol{x} = n$$

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- Properties: [Proof]
  - $\mathrm{E}(\mathbf{x}) = n\rho$
  - $\mathrm{Var}(\mathbf{x}) = n\left(\mathrm{diag}(\rho) - \rho\rho^\top\right)$
    (i.e., $\mathrm{Var}(\mathrm{x}_i) = n\rho_i(1-\rho_i)$ and $\mathrm{Var}(\mathrm{x}_i, \mathrm{x}_j) = -n\rho_i\rho_j$)

Normal/Gaussian Distribution (Continuous)

Theorem (Central Limit Theorem)

The sum x *of many independent random variables is approximately normally/Gaussian distributed:*

$$\mathcal{N}(\mathrm{x} = x; \mu, \sigma^2) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right).$$

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- Holds regardless of the original distributions of individual variables
- $\mu_{\mathrm{x}} = \mu$ and $\sigma_{\mathrm{x}}^2 = \sigma^2$
- To avoid inverting σ^2, we can parametrize the distribution using the ***precision*** β:

$$\mathcal{N}(\mathrm{x} = x; \mu, \beta^{-1}) = \sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{\beta}{2}(x-\mu)^2\right)$$

Confidence Intervals

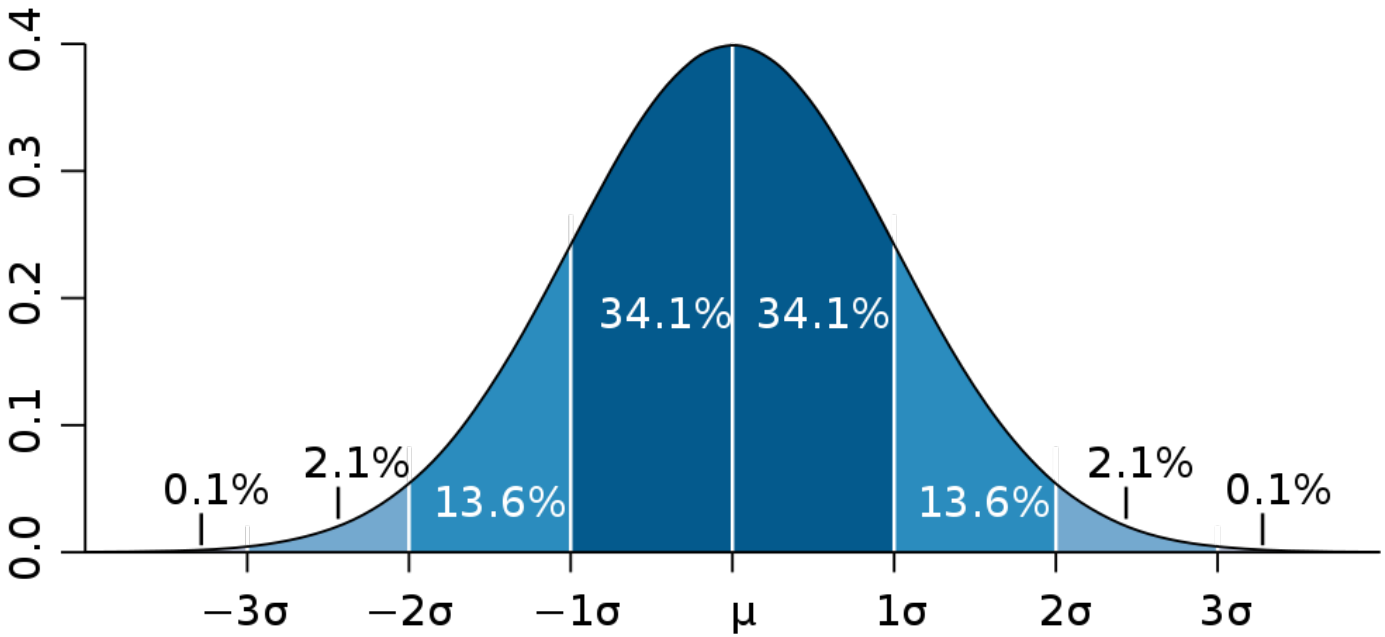

Figure: Graph of $\mathcal{N}(\mu, \sigma^2)$.

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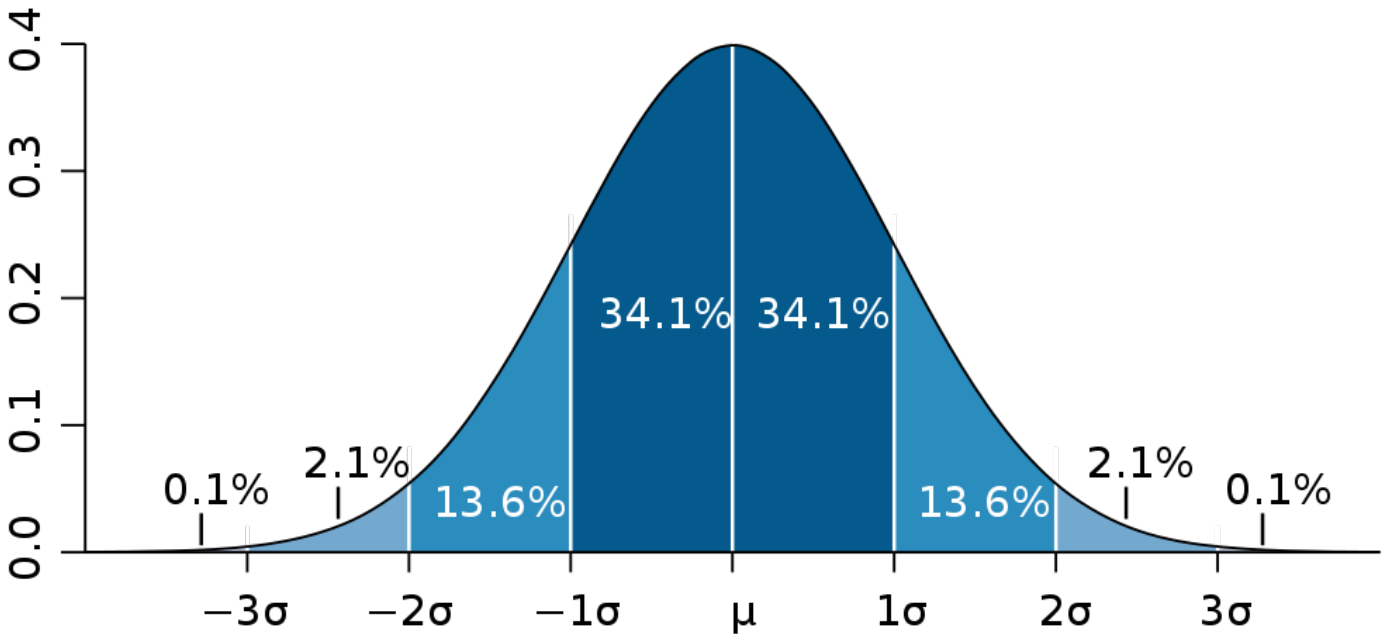

Figure: Graph of $\mathcal{N}(\mu, \sigma^2)$.

- We say the interval $[\mu - 2\sigma, \mu + 2\sigma]$ has about the 95% confidence

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3. Convenient for many analytical manipulations
   - Closed under affine transformation, summation, marginalization, conditioning, etc.
   - Many of the integrals involving Gaussian distributions that arise in practice have simple closed form solutions

Properties

- Closed under affine transformation: if $\mathrm{x} \sim \mathcal{N}(\mu, \sigma^2)$, then $a\mathrm{x}+b \sim \mathcal{N}(a\mu+b, a^2\sigma^2)$ for any deterministic $a, b \in \mathbb{R}$, $a \neq 0$ [Proof]
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  - ***Not*** true if $\mathrm{x}^{(1)}$ and $\mathrm{x}^{(2)}$ are dependent

Multivariate Gaussian Distribution

- When $\mathbf{x}$ is sum of many random vectors:

$$\mathcal{N}(\mathbf{x}=\boldsymbol{x};\mu,\Sigma)=\sqrt{\frac{1}{(2\pi)^d\det(\Sigma)}}\exp\left[-\frac{1}{2}(\boldsymbol{x}-\mu)^\top\Sigma^{-1}(\boldsymbol{x}-\mu)\right]$$

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- What does the graph of $\mathcal{N}(\mu,\Sigma)$ look like?

Bivariate Example I

- Consider the ***Mahalanobis distance*** first

$$\mathcal{N}(\mu,\Sigma) = \sqrt{\frac{1}{(2\pi)^d \det(\Sigma)}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\mu)^\top \Sigma^{-1}(\boldsymbol{x}-\mu)\right]$$

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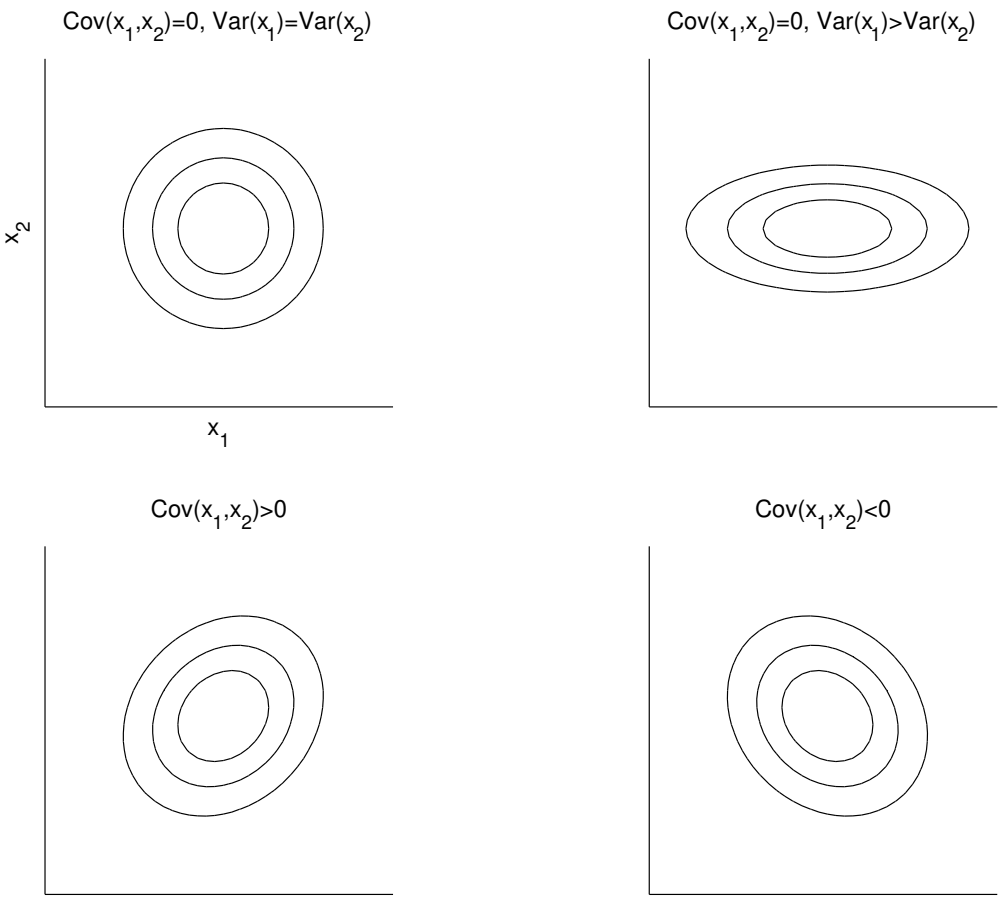

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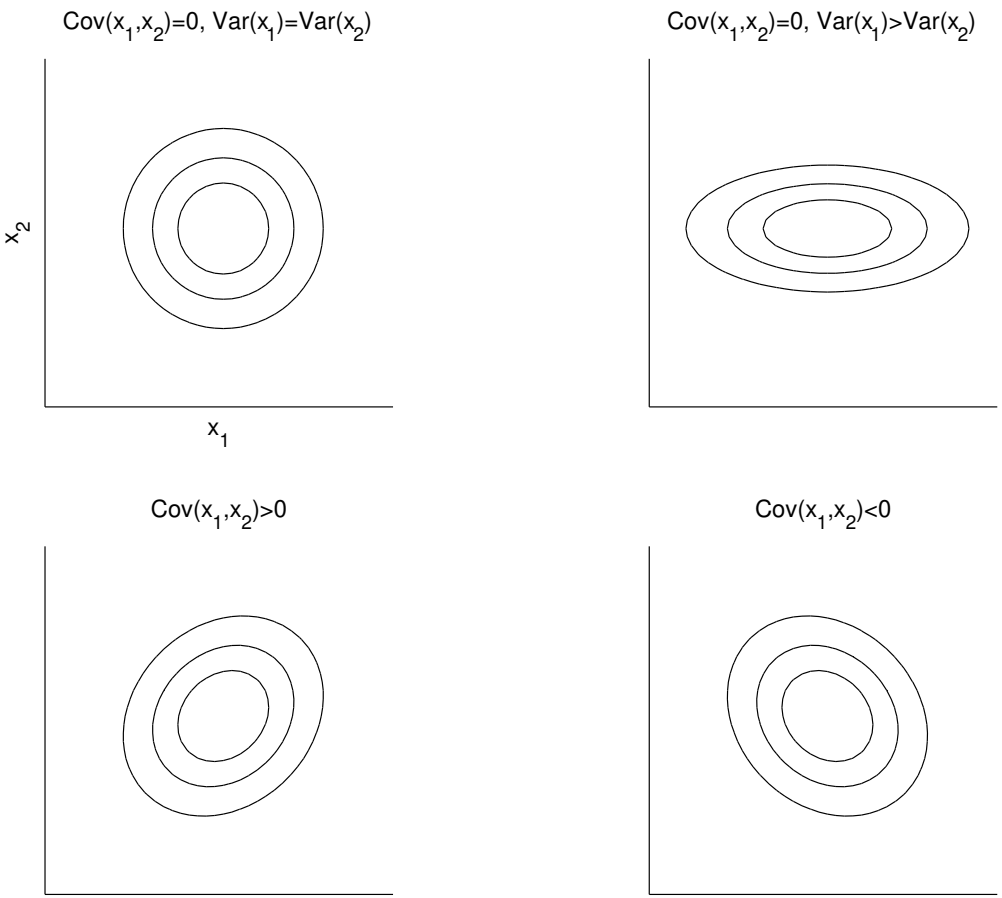
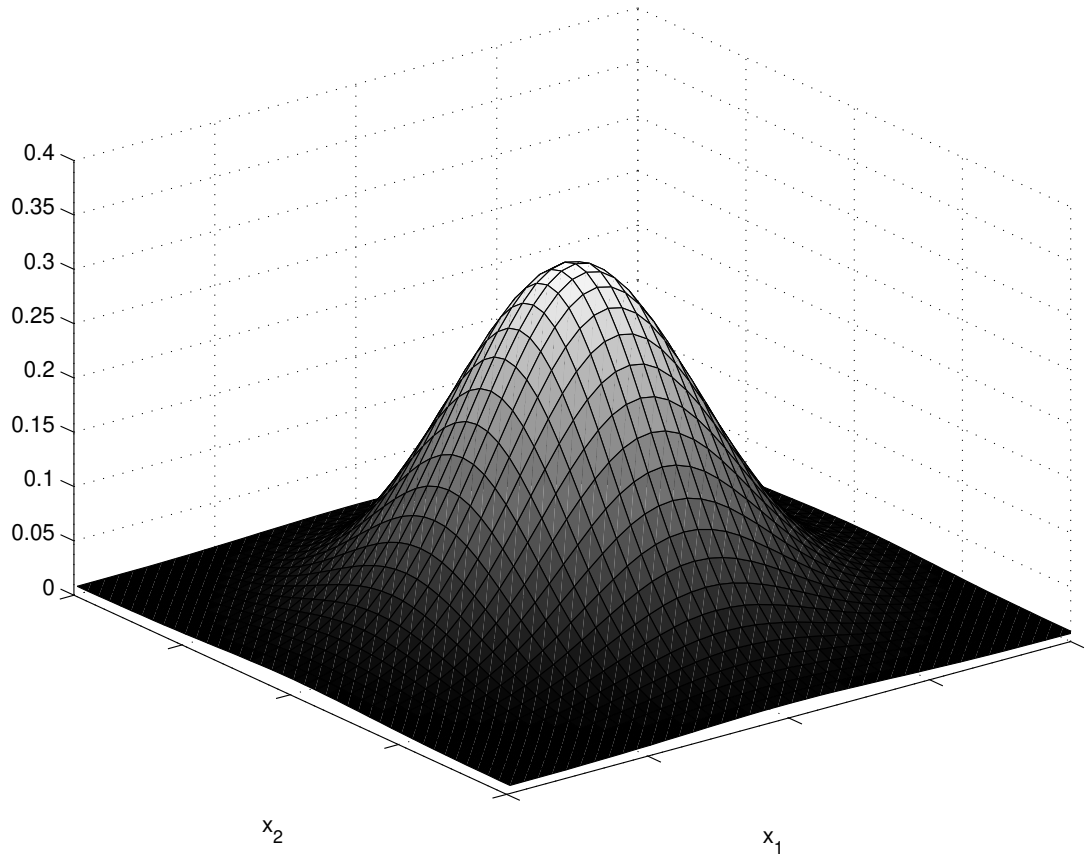


- The level sets closer to the center $\mu_{\mathbf{x}}$ are lower
- Increasing $\mathrm{Cov}[\mathrm{x}_1,\mathrm{x}_2]$ stretches the level sets along the 45° axis
- Decreasing $\mathrm{Cov}[\mathrm{x}_1,\mathrm{x}_2]$ stretches the level sets along the -45° axis

Bivariate Example II

- The hight of $\mathcal{N}(\mu,\Sigma) = \sqrt{\frac{1}{(2\pi)^d \det(\Sigma)}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\mu)^\top \Sigma^{-1}(\boldsymbol{x}-\mu)\right]$ in its graph is inversely proportional to the Mahalanobis distance



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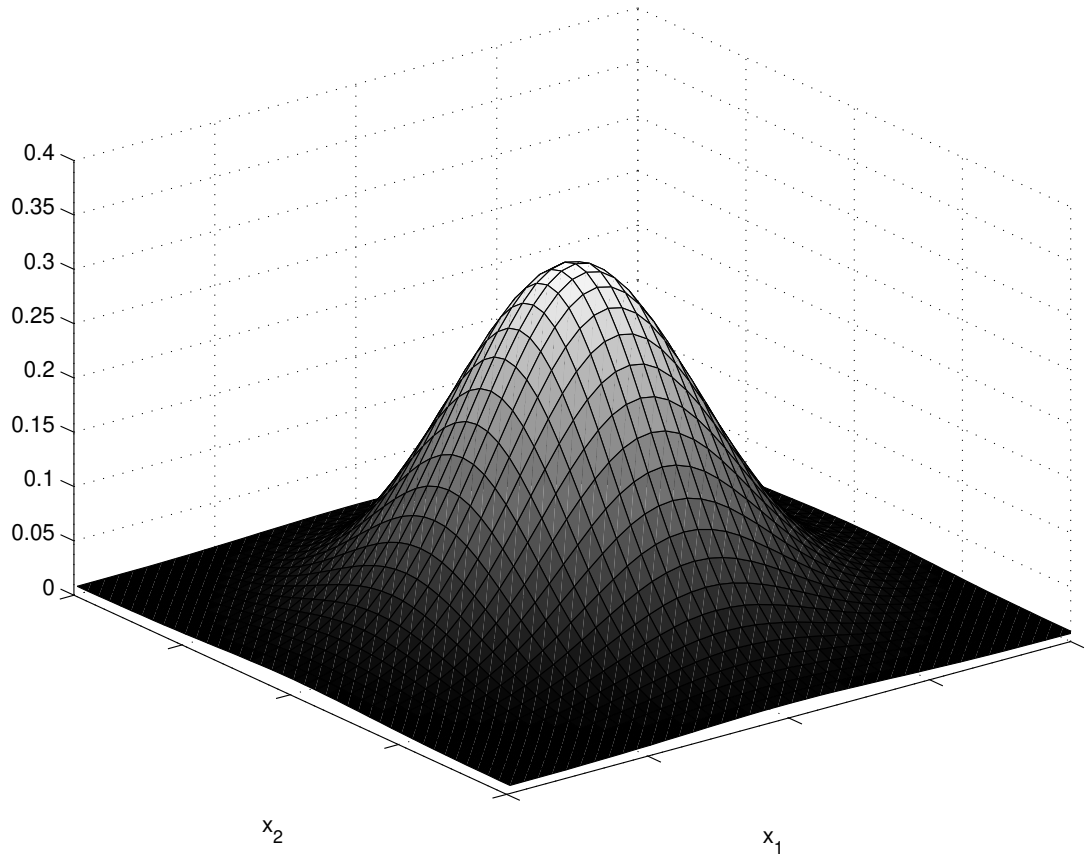

- A multivariate Gaussian distribution is ***isotropic*** iff $\Sigma = \sigma \boldsymbol{I}$

Properties

- Closed under affine transformation: if $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$, then $\boldsymbol{w}^\top \mathbf{x} \sim \mathcal{N}(\boldsymbol{w}^\top \mu, \boldsymbol{w}^\top \Sigma \boldsymbol{w})$ for any deterministic $\boldsymbol{w} \in \mathbb{R}^d$
  - More generally, given $\boldsymbol{W} \in \mathbb{R}^{d \times k}$, $k < d$, we have $\boldsymbol{W}^\top \mathbf{x} \sim \mathcal{N}(\boldsymbol{W}^\top \mu, \boldsymbol{W}^\top \Sigma \boldsymbol{W})$ that is k-variate normal
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- Closed under marginalization: $\mathbf{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_{1,1})$ [Proof: $\mathrm{P}(\mathbf{x}_1) = \int_{\boldsymbol{x}_2} \mathrm{P}(\mathbf{x}_1, \boldsymbol{x}_2; \mu, \Sigma) d\boldsymbol{x}_2$)]
- Closed under conditioning: $(\mathbf{x}_1 | \boldsymbol{x}_2) \sim \mathcal{N}(\mu_1 + \Sigma_{1,2}\Sigma_{2,2}^{-1}(\boldsymbol{x}_2 - \mu_2), \Sigma_{1,1} - \Sigma_{1,2}\Sigma_{2,2}^{-1}\Sigma_{2,1})$ [Proof]

Exponential Distribution (Continuous)

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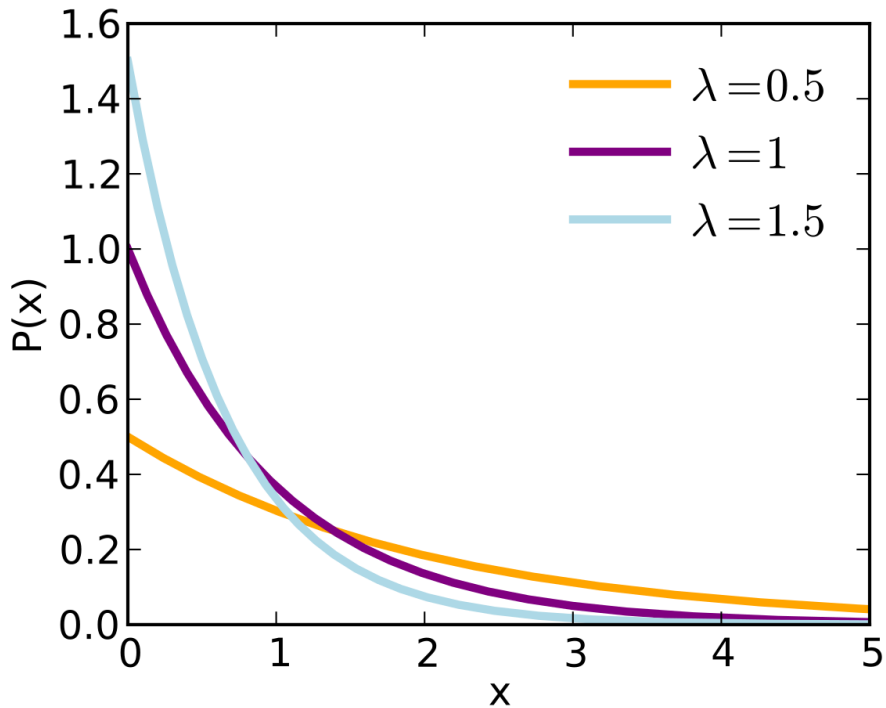
- To accomplish this, we can use the ***exponential distribution***:

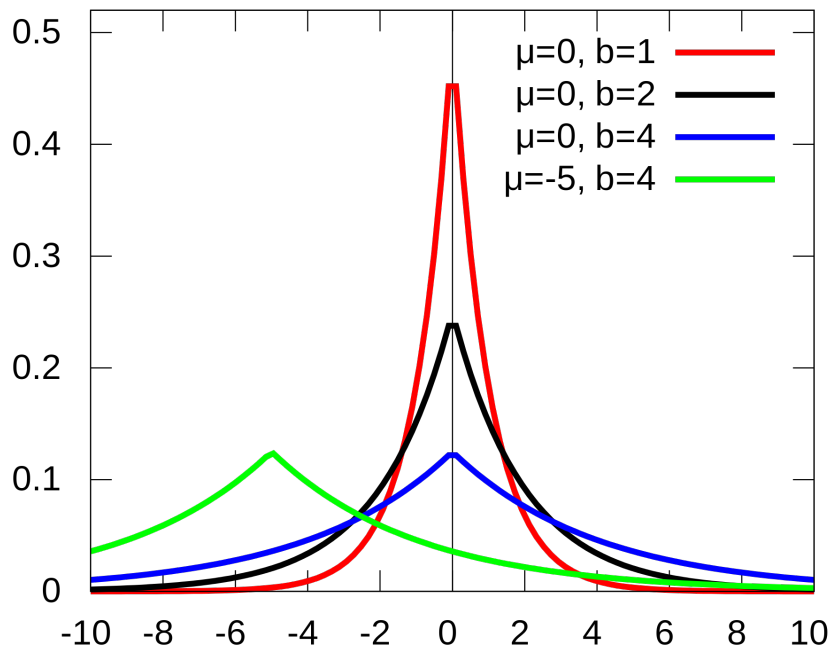
$$\text{Exponential}(\mathrm{x} = x; \lambda) = \lambda 1(x; x \geq 0) \exp(-\lambda x)$$



Laplace Distribution (Continuous)

- ***Laplace distribution*** can be think of as a "two-sided" exponential distribution centered at μ:

$$\text{Laplace}(\text{x} = x; \mu, b) = \frac{1}{2b} \exp\left(-\frac{|x-\mu|}{b}\right)$$



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- This can be accomplished by using the ***Dirac distribution***:

$$\text{Dirac}(\mathbf{x} = \boldsymbol{x}; \mu) = \delta(\boldsymbol{x} - \mu),$$

where $\delta(\cdot)$ is the Dirac delta function that

1. Is zero-valued everywhere except at input $\mathbf{0}$
2. Integrals to 1

Empirical Distribution (Continuous)

- Given a dataset $\mathbb{X} = \{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$ where $\boldsymbol{x}^{(i)}$'s are i.i.d. samples of $\mathbf{x}$
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- If $\mathbf{x}$ is continuous, we have the ***empirical distribution***:

$$\text{Empirical}(\mathbf{x} = \boldsymbol{x}; \mathbb{X}) = \frac{1}{N} \sum_{i=1}^{N} \delta(\boldsymbol{x} - \boldsymbol{x}^{(i)})$$

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- We may define a probability distribution by combining other simpler probability distributions $\{\mathrm{P}^{(i)}(\boldsymbol{\theta}^{(i)})\}_i$

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- The component identity variable c is a ***latent variable***
  - Whose values are not observed

Gaussian Mixture Model

- A mixture model is called the ***Gaussian mixture model*** iff $\mathrm{P}^{(i)}(\mathbf{x} = \boldsymbol{x} | \mathrm{c} = i; \boldsymbol{\theta}^{(i)}) = \mathcal{N}^{(i)}(\mathbf{x} = \boldsymbol{x} | \mathrm{c} = i; \boldsymbol{\mu}^{(i)}, \Sigma^{(i)}), \forall i$

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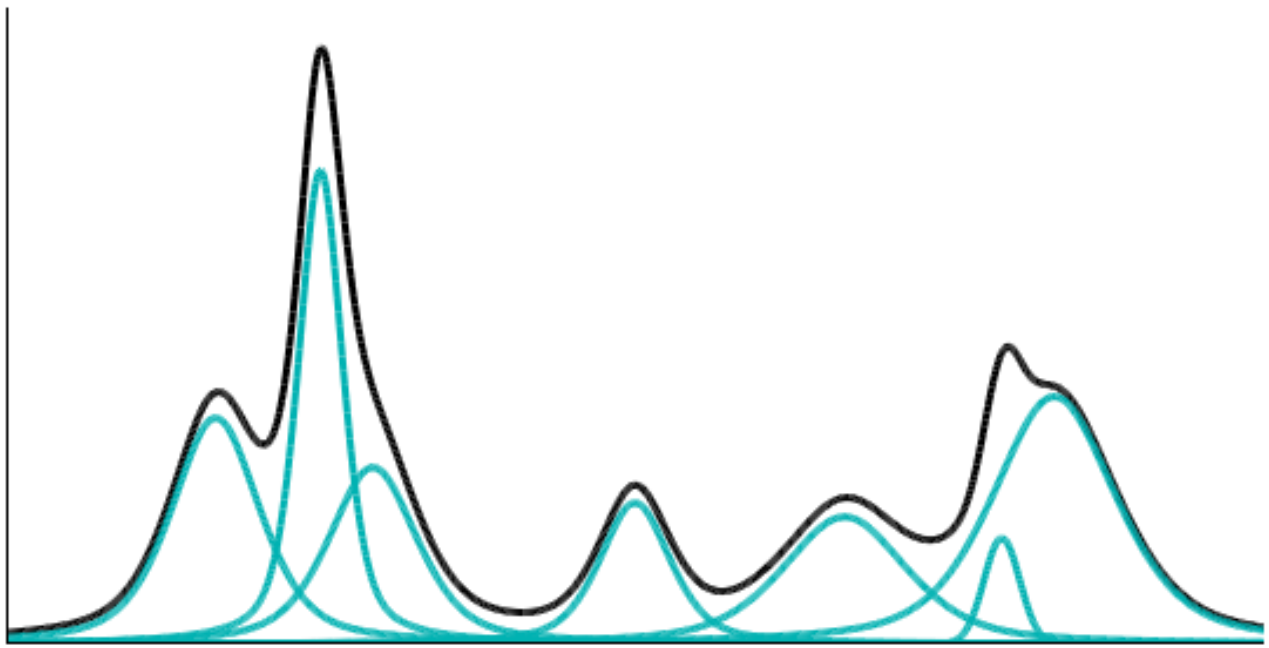
- Any smooth density can be approximated by a Gaussian mixture model with enough components



Outline

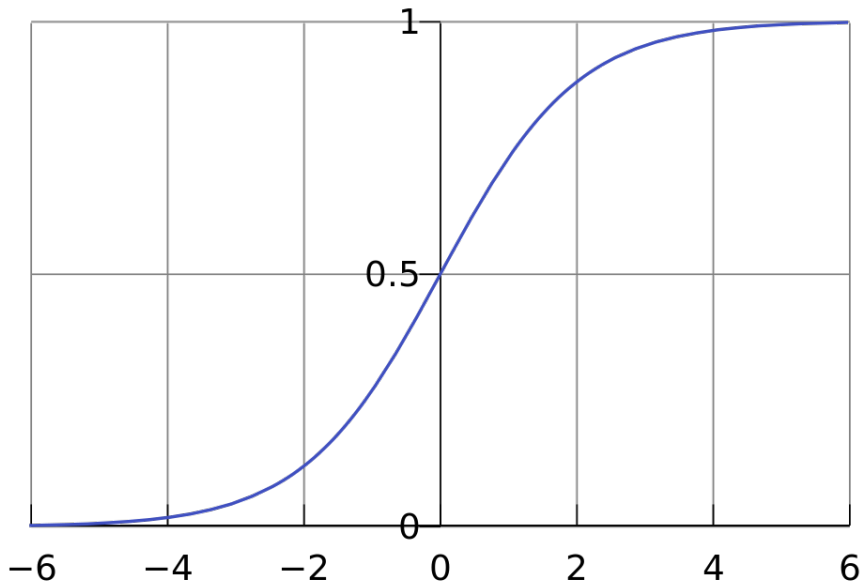
Parametrizing Functions

- A probability distribution $\mathrm{P}(\theta)$ is parametrized by θ
- In ML, θ may be the output value of a deterministic function
  - Called ***parametrizing function***

Logistic Function

- The ***logistic function*** (a special case of ***sigmoid functions***) is defined as:

$$\sigma(x) = \frac{\exp(x)}{\exp(x)+1} = \frac{1}{1+\exp(-x)}$$



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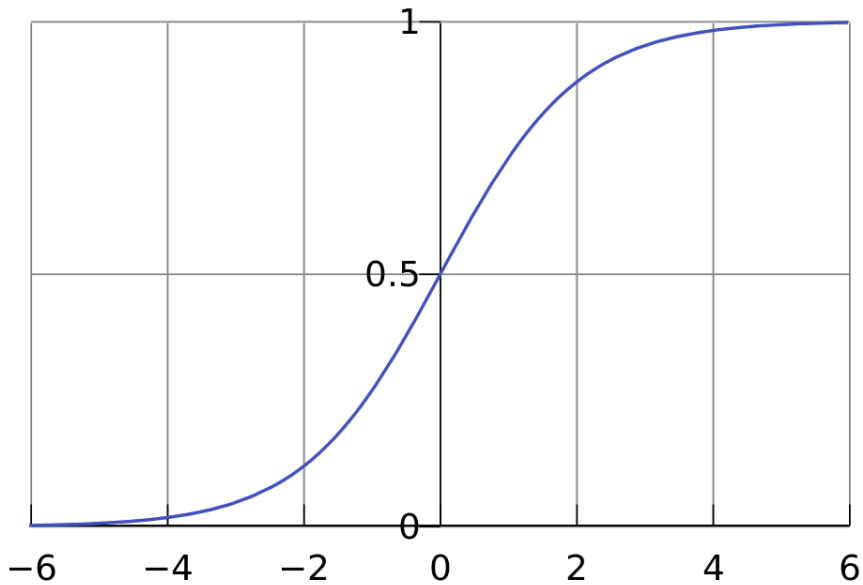

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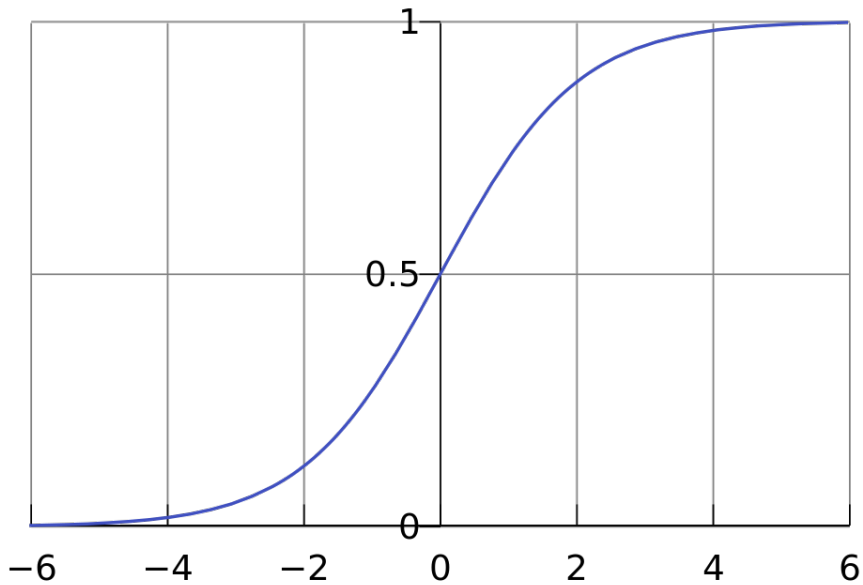

- Always takes on values between $(0,1)$
- Commonly used to produce the ρ parameter of Bernoulli distribution

Softplus Function

- The ***softplus function*** :

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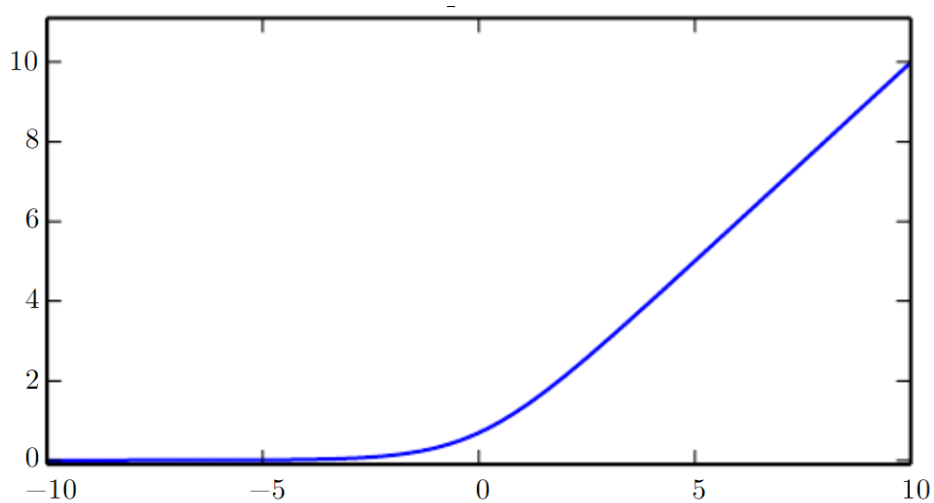

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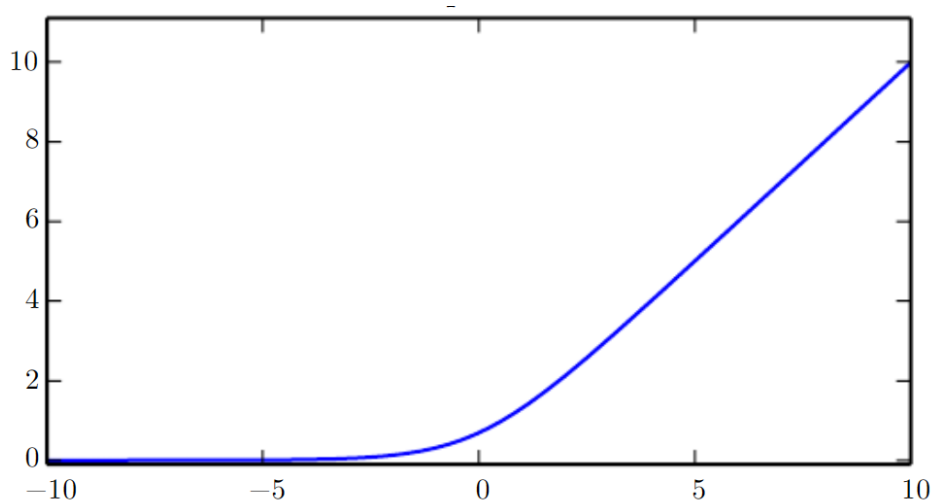

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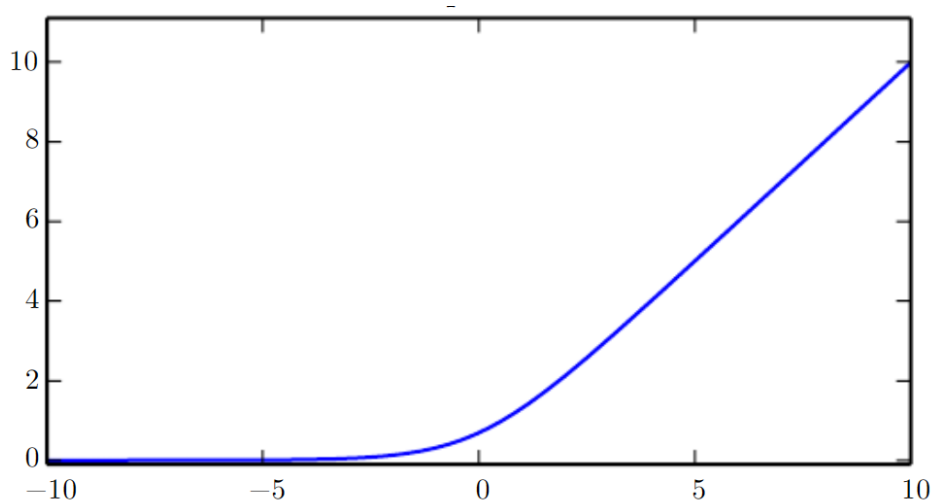

- A "softened" version of $x^+ = \max(0, x)$
- Range: $(0, \infty)$
- Useful for producing the β or σ parameter of Gaussian distribution

Properties [Homework]

- $1-\sigma(x)=\sigma(-x)$
- $\log\sigma(x)=-\zeta(-x)$
- $\frac{d}{dx}\sigma(x)=\sigma(x)(1-\sigma(x))$
- $\frac{d}{dx}\zeta(x)=\sigma(x)$
- $\forall x\in(0,1),\sigma^{-1}(x)=\log\left(\frac{x}{1-x}\right)$
- $\forall x>0,\zeta^{-1}(x)=\log(\exp(x)-1)$
- $\zeta(x)=\int_{-\infty}^{x}\sigma(y)dy$
- $\zeta(x)-\zeta(-x)=x$
  - $\zeta(-x)$ is the softened $x^-=\max(0,-x)$
  - $x=x^+-x^-$

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  - Called ***bit*** if base-2 logarithm is used
  - Called ***nat*** if base-e

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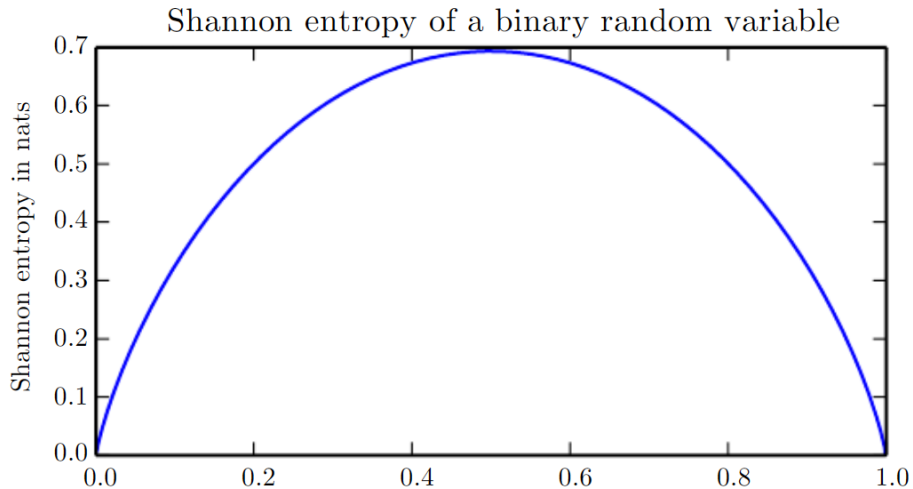

Figure: Shannon entropy $\mathrm{H}(\mathrm{x})$ over Bernoulli distributions with different ρ.

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- If the probabilities of the 8 states are $(\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64})$ instead
  - $\mathrm{H}(\mathrm{x}) = 2$
  - The encoding $0, 10, 110, 1110, 111100, 111101, 111110, 111111$ gives the average code length 2

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$$\mathrm{D_{KL}(P\|Q)} = \mathrm{E_{x\sim P}}\left[\log \frac{\mathrm{P(x)}}{\mathrm{Q(x)}}\right] = -\mathrm{E_{x\sim P}}\left[\log \mathrm{Q(x)}\right] - \mathrm{H(x\sim P)}$$

  - The term $-\mathrm{E_{x\sim P}}\left[\log \mathrm{Q(x)}\right]$ is called the ***cross entropy***

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  - The term $-\mathrm{E}_{\mathrm{x}\sim\mathrm{P}}\left[\log\mathrm{Q}(\mathrm{x})\right]$ is called the ***cross entropy***
- If P and Q are independent, we can solve

$$\arg\min_{Q}\mathrm{D_{KL}}(\mathrm{P}\|\mathrm{Q})$$

by

$$\arg\min_{Q} -\mathrm{E}_{\mathrm{x}\sim\mathrm{P}}\left[\log\mathrm{Q}(\mathrm{x})\right]$$

Properties

- $\mathrm{D_{KL}(P\|Q)} \geq 0$, $\forall \mathrm{P, Q}$
- $\mathrm{D_{KL}(P\|Q)} = 0$ iff P and Q are equal almost surely
- KL divergence is asymmetric, i.e., $\mathrm{D_{KL}(P\|Q)} \neq \mathrm{D_{KL}(Q\|P)}$

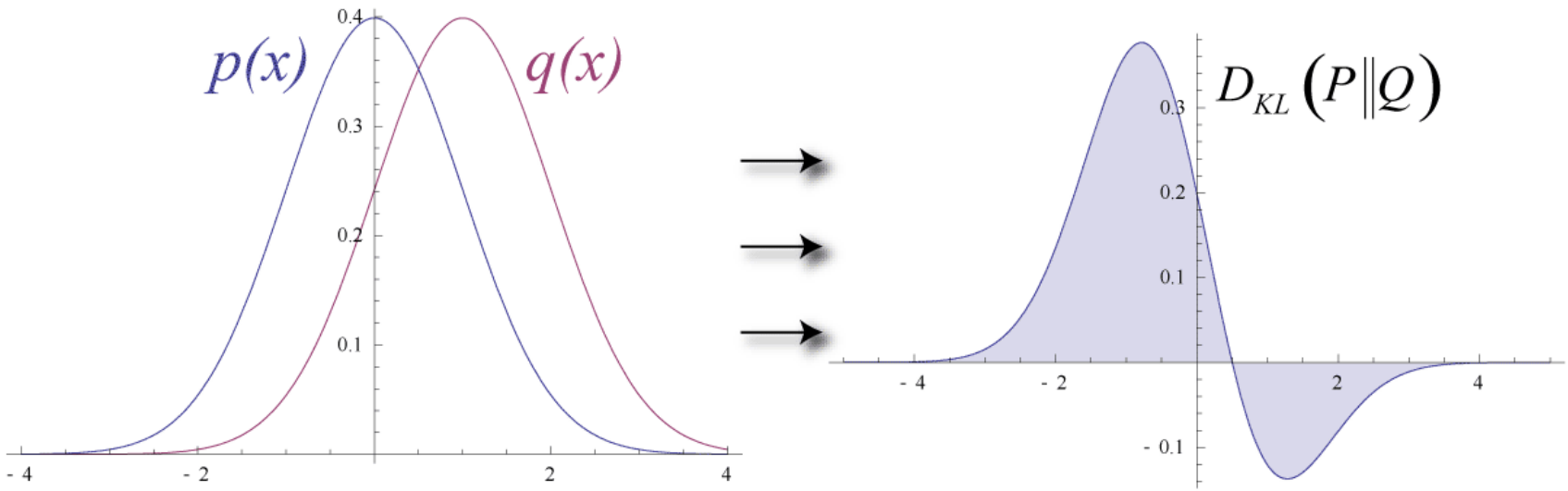

Figure: KL divergence for two normal distributions.

Minimizer of KL Divergence

- Given P, we want to find Q^* that minimizes the KL divergence
- $\mathrm{Q}^{*(\text{from})} = \arg\min_{\mathrm{Q}} \mathrm{D}_{\mathrm{KL}}(\mathrm{P}\|\mathrm{Q})$ or $\mathrm{Q}^{*(\text{to})} = \arg\min_{\mathrm{Q}} \mathrm{D}_{\mathrm{KL}}(\mathrm{Q}\|\mathrm{P})$?

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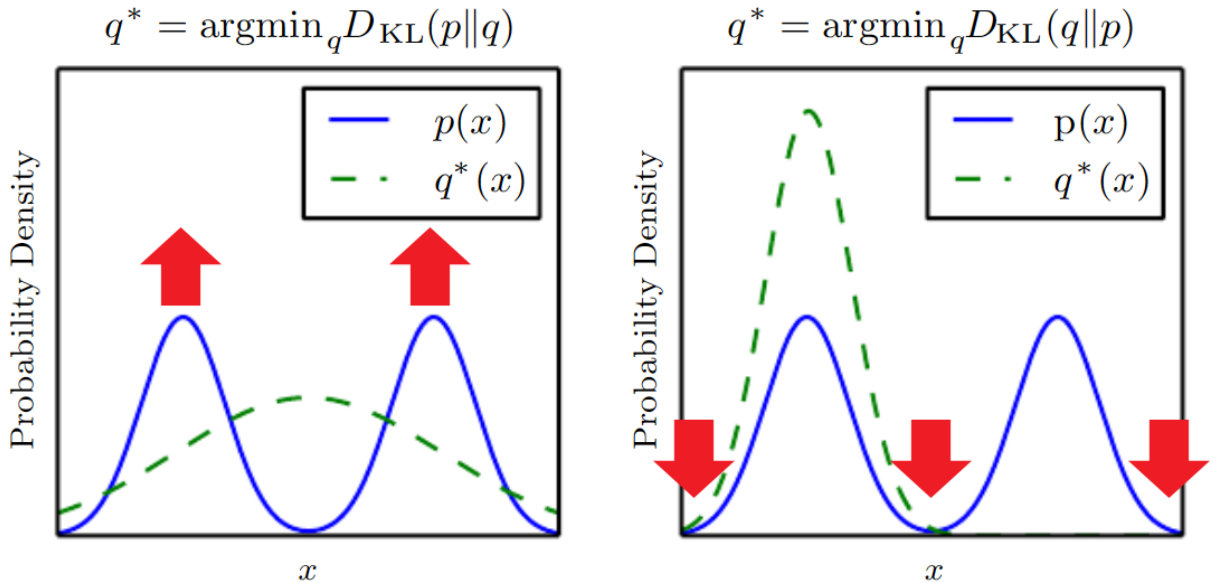
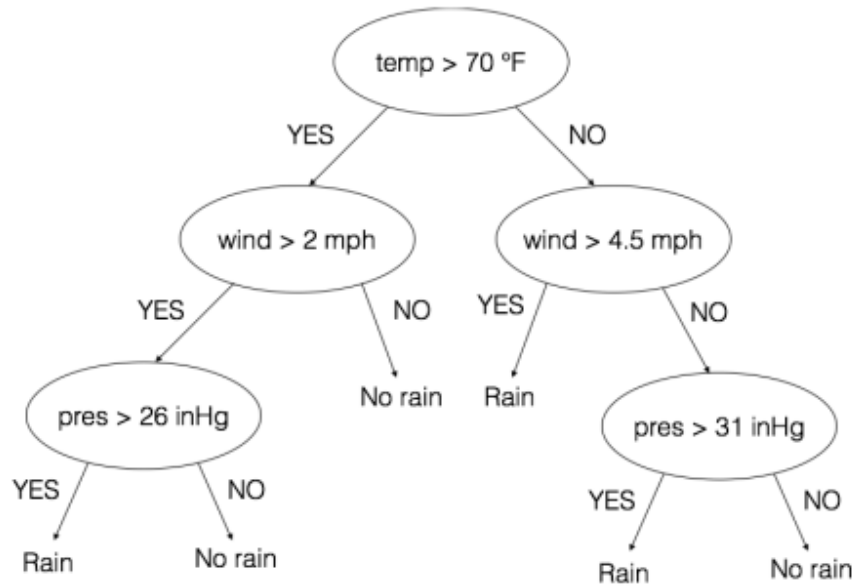


Figure: Approximating a mixture P of two Gaussians using a single Gaussian Q.

Outline

Decision Trees

- Given a supervised dataset $\mathbb{X} = \{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$
- Can we find out a tree-like function f (i.e, a set of rules) such that $f(\boldsymbol{x}^{(i)}) = y^{(i)}$?



Training a Decision Tree

- Start from root which corresponds to all data points $\{(\boldsymbol{x}^{(i)}, y^{(i)}) : \text{Rules} = \emptyset)\}$
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$$\mathbb{X}^{\text{left}} = \{(\boldsymbol{x}^{(i)}, y^{(i)}) : \text{Rules} \cup \{x_j^{(i)} < v\}\}, \text{ and}$$

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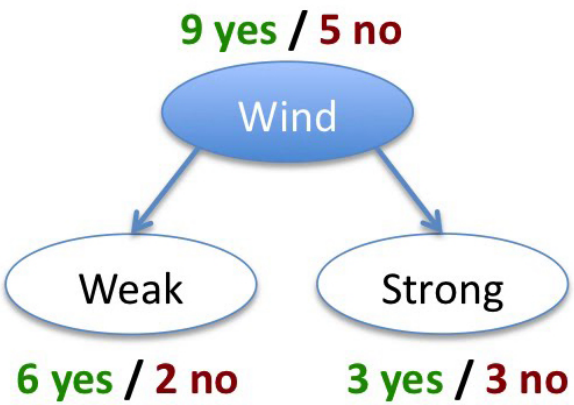
the "impurity" of labels drops the most



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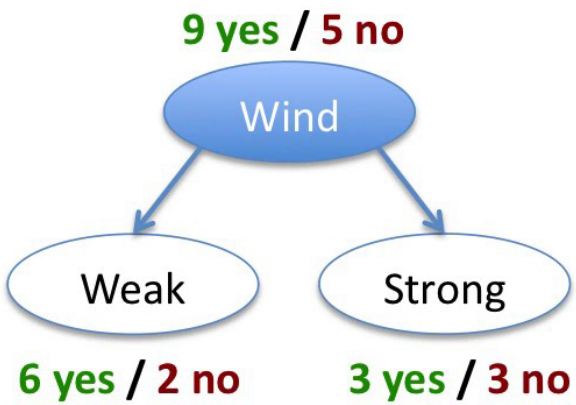

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the "impurity" of labels drops the most, i.e., solve

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- In this case, $\text{Impurity}(\mathbb{X}^{\text{parent}}) - \text{Impurity}(\mathbb{X}^{\text{left}}, \mathbb{X}^{\text{right}})$ is called the ***information gain***

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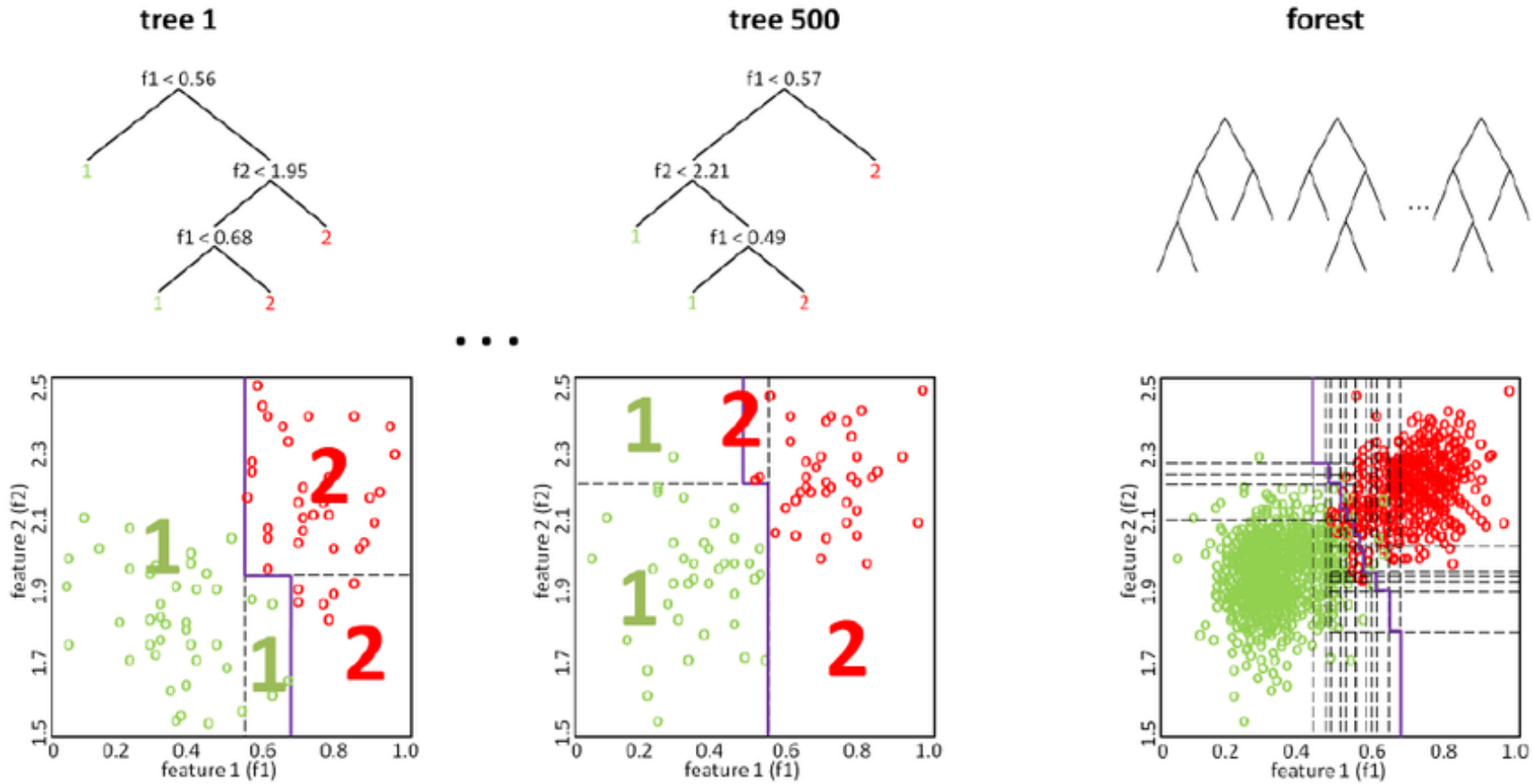
- Each tree is trained slightly differently because of Step 1 and 2(a)
- Provides different "perspectives" when voting

Decision Boundaries



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Decision Trees vs. Random Forests

- Cons of random forests:
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- Pros:
  - Less sensitive to the depth of trees
    - The majority voting can "absorb" the noise from individual trees
  - Can be parallelized
    - Each tree can grow independently