Probability & Information Theory

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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., $\Pr(x = x_1) = 0.1$, $\Pr(x = x_2) = 0.3$, 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
  - $x \sim P(\theta)$ means "x has distribution P parametrized by θ"

Probability Mass and Density Functions

- If x is discrete, $P(x = x)$ denotes a ***probability mass function*** $P_x(x) = \Pr(x = x)$
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- $p_x(x)$ 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., $P(x, y)$
- The probability distribution over the subset of random variables called the *marginal probability* distribution:

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

  - Also called the sum rule of probability

Conditional Probability

- Conditional density function:

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- Product rule of probability:

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

  - E.g., $P(a, b, c) = P(a \mid b, c) P(b \mid c) P(c)$

Independence and Conditional Independence

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

$$P(x \mid y) = P(x)$$

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

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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]

$$E_{x \sim P}[f(x)] = \sum_x P_x(x)f(x) \text{ or } \int p_x(x)f(x)dx = \mu_{f(x)}$$

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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
- $\mathrm{E}[\mathrm{E}[\mathrm{f}(\mathrm{x})]] = \mathrm{E}[\mathrm{f}(\mathrm{x})]$, 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.,

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

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- $E[f(x)|y = y] = \int p_{x|y}(x|y)f(x)dx$ is called the **conditional expectation**
- $E[f(x)g(y)] = E[f(x)]E[g(y)]$ 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:

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

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- $\mathrm{Var}[f(x)] = \mathrm{E}[f(x)^2] - \mathrm{E}[f(x)]^2$ [Proof]
- $\mathrm{Var}[af(x) + b] = a^2\mathrm{Var}[f(x)]$ for deterministic a and b [Proof]

Covariance I

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

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

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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 $\text{Cov}(x, y) = 0$ [Proof]
  - The converse is *not* true as X and Y may be related in a nonlinear way
  - E.g., $y = \sin(x)$ and $x \sim \text{Uniform}(-\pi, \pi)$

Covariance II

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

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- $\mathrm{Cov}(a\mathrm{x} + b, c\mathrm{y} + d) = ac\mathrm{Cov}(\mathrm{x},\mathrm{y})$ [Proof]
- $\mathrm{Cov}(a\mathrm{x} + b\mathrm{y}, c\mathrm{w} + d\mathrm{v}) =$
  $ac\mathrm{Cov}(\mathrm{x},\mathrm{w}) + ad\mathrm{Cov}(\mathrm{x},\mathrm{v}) + bc\mathrm{Cov}(\mathrm{y},\mathrm{w}) + bd\mathrm{Cov}(\mathrm{y},\mathrm{v})$ [Proof]

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Multivariate Random Variables I

- A multivariate random variable is denoted by $\mathbf{x} = [x_1, \cdots, x_d]^\top$
  - Normally, x_i's (***attributes*** or ***variables*** or ***features***) are dependent with each other
  - $P(\mathbf{x})$ is a joint distribution of $x_1, \cdots, x_d$

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$$\Sigma_{\mathbf{x}} = \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x_1,x_2} & \cdots & \sigma_{x_1,x_d} \\ \sigma_{x_2,x_1} & \sigma_{x_2}^2 & \cdots & \sigma_{x_2,x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{x_d,x_1} & \sigma_{x_d,x_2} & \cdots & \sigma_{x_d}^2 \end{bmatrix}$$

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- $\Sigma_{\mathbf{x}} = \mathrm{Cov}(\mathbf{x}) = E\left[(\mathbf{x} - \mu_{\mathbf{x}})(\mathbf{x} - \mu_{\mathbf{x}})^\top\right] = E(\mathbf{x}\mathbf{x}^\top) - \mu_{\mathbf{x}}\mu_{\mathbf{x}}^\top$

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

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

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

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$$\hat{\Sigma}_{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \hat{\mu}_{\mathbf{x}})(x^{(i)} - \hat{\mu}_{\mathbf{x}})^\top$$

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

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- $\hat{\sigma}_{\mathbf{x}_i, \mathbf{x}_j}^2 = \frac{1}{n} \sum_{s=1}^{n} (x_i^{(s)} - \hat{\mu}_{\mathbf{x}_i})(x_j^{(s)} - \hat{\mu}_{\mathbf{x}_j})$
- 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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  - Each $w^{(j)}$ keeps information that cannot be explained by others, so together they preserve the most info
- Why $\|w^{(j)}\| = 1$ for all j?
  - Only directions matter—we don't want to maximize $\mathrm{Var}(z_j)$ by finding a long $w^{(j)}$

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- By Rayleigh's Quotient, the optimal $w^{(1)}$ is given by the eigenvector of $X^\top X$ corresponding to the largest eigenvalue

Solving W II

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

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

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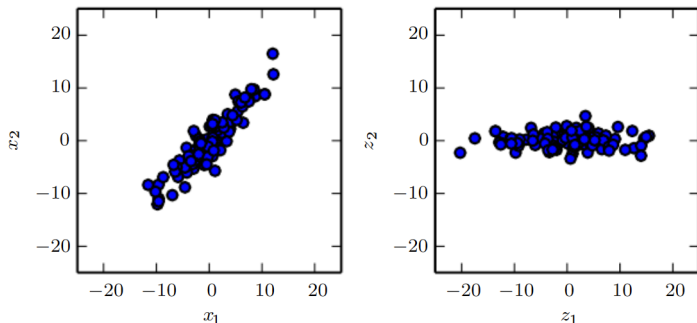
Figure: PCA learns a linear projection that aligns the direction of greatest variance with the axes of the new space. With these new axes, the estimated covariance matrix $\hat{\Sigma}_{\mathbf{z}} = W^\top \hat{\Sigma}_{\mathbf{x}} W \in \mathbb{R}^{K \times K}$ is always diagonal.

Outline

Sure and Almost Sure Events

- Given a continuous random variable x, we have $\Pr(\mathrm{x} = x) = 0$ for any value x
- Will the event $\mathrm{x} = x$ occur?

Sure and Almost Sure Events

- Given a continuous random variable x, we have $\Pr(\mathrm{x} = x) = 0$ for any value x
- 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 $\Pr(x \le a) = \Pr(y \le a)$ for all a.

Definition (Almost Sure Equality)

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

Definition (Equality)

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

Equality of Random Variables II

- What's the difference between the "equality in distribution" and "almost sure equality?"

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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
  $P_x(0) = P_x(1) = P_y(0) = P_y(1) = 0.5$
  - They are equal in distribution
  - But $\Pr(x = y) = 0.5 \neq 1$

Convergence of Random Variables I

Definition (Convergence in Distribution)

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

Definition (Convergence in Probability)

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

Definition (Almost Sure Convergence)

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

Convergence of Random Variables II

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

Distribution of Derived Variables I

- Consider a continuous scalar random variable x
- Suppose $y = f(x)$ and f^{-1} exists, does $P(y = y) = P(x = f^{-1}(y))$ always hold?

Distribution of Derived Variables I

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- Suppose $y = f(x)$ and f^{-1} exists, does $P(y = y) = P(x = f^{-1}(y))$ always hold? *No*, when x and y are continuous
- 1D example: let $x \sim \text{Unifrom}(0, 1)$ and $y = 2x \sim \text{Unifrom}(0, 2)$
- If $p_y(y) = p_x(\frac{1}{2}y)$, then

$$\int_{y=0}^{2} p_y(y)dy = \int_{y=0}^{2} p_x(\frac{1}{2}y)dy = 2 \neq 1$$

- Violates the *unit measure* axiom of probability
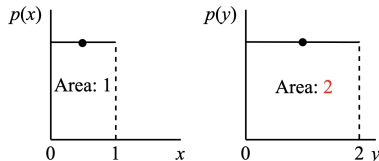
Distribution of Derived Variables II

- Recall that $\Pr(y = y) = p_y(y)dy$ and $\Pr(x = x) = p_x(x)dx$
- To preserve unit measure, we need to ensure that

$$p_y(f(x))dy = p_x(x)dx, \forall x$$
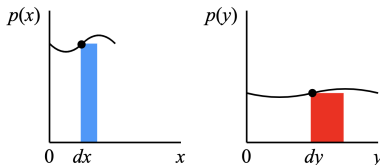
- We have

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

- Absolute values deal with the case where $y = -cx$
- In 1D example: $p_y(y) = \frac{1}{2} p_x(\frac{1}{2} y)$ for all y

Distribution of Derived Variables III

- In multivariate case where $\mathbf{y} = \boldsymbol{f}(\mathbf{x})$, we need to ensure that

$$p_{\mathbf{y}}(\boldsymbol{f}(\boldsymbol{x}))|\det(\Delta)| = p_{\mathbf{x}}(\boldsymbol{x})dx_1 dx_2 \cdots, \forall \boldsymbol{x}$$

- $dx_1 dx_2 \cdots$: volume of $d\boldsymbol{x}$
- $|\det(\Delta)|$: volume of $d\boldsymbol{y}$, where Δ captures the linear relationship between $d\boldsymbol{y}$ and $d\boldsymbol{x}$
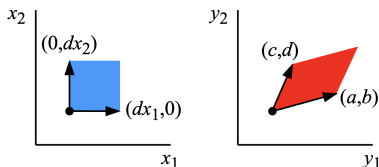
- We have $p_{\mathbf{x}}(\boldsymbol{x}) = p_{\mathbf{y}}(\boldsymbol{f}(\boldsymbol{x})) \left| \frac{1}{dx_1 dx_2 \cdots} \det(\Delta) \right| = p_{\mathbf{y}}(\boldsymbol{f}(\boldsymbol{x})) \left| \det(\boldsymbol{J}(\boldsymbol{f})(\boldsymbol{x})) \right|$
  - $\boldsymbol{J}(\boldsymbol{f})(\boldsymbol{x})$ is the Jacobian matrix of $\boldsymbol{f}$ at input $\boldsymbol{x}$
  - Or equivalently, $p_{\mathbf{y}}(\boldsymbol{y}) = p_{\mathbf{x}}(\boldsymbol{f}^{-1}(\boldsymbol{y})) \left| \det(\boldsymbol{J}(\boldsymbol{f}^{-1})(\boldsymbol{y})) \right|$

Distribution of Derived Variables IV

- Why $\frac{1}{dx_1 dx_2 \cdots} \det(\Delta) = \det(\boldsymbol{J}(\boldsymbol{f})(\boldsymbol{x}))$?
- 2D example:

$$\frac{1}{dx_1 dx_2} \det\left(\begin{bmatrix} a & c \\ b & d \end{bmatrix}\right) = \frac{1}{dx_1 dx_2} \det\left(\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right)$$

$$= \det\left(\begin{bmatrix} \frac{a}{dx_1} & \frac{b}{dx_1} \\ \frac{c}{dx_2} & \frac{d}{dx_2} \end{bmatrix}\right) = \det\left(\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} \end{bmatrix}\right)$$

$$== \det\left(\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{bmatrix}\right) = \det(\boldsymbol{J}(\boldsymbol{f})(\boldsymbol{x}))$$
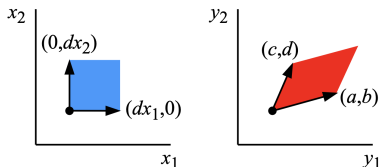
Outline

Random Experiments

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

Bernoulli Distribution (Discrete)

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

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

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

Categorical Distribution (Discrete)

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

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

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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:

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

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

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
- $\mu_x = \mu$ and $\sigma_x^2 = \sigma^2$
- To avoid inverting σ^2, we can parametrize the distribution using the **precision** β:

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

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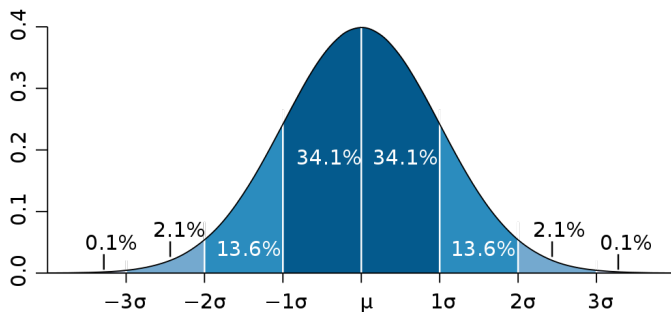
Figure: Graph of $\mathcal{N}(\mu, \sigma^2)$.

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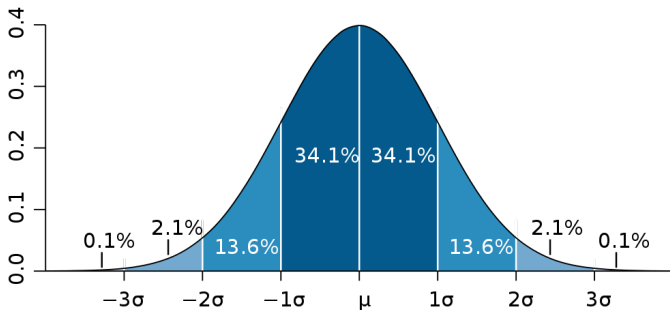
Figure: Graph of $\mathcal{N}(\mu, \sigma^2)$.

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

Multivariate Gaussian Distribution

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

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

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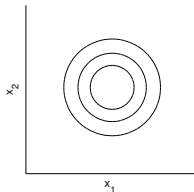$$\mathcal{N}(\mathbf{x} = \boldsymbol{x}; \mu, \Sigma) = \sqrt{\frac{1}{(2\pi)^d \det(\Sigma)}} \exp\left[-\frac{1}{2}(\boldsymbol{x} - \mu)^\top \Sigma^{-1}(\boldsymbol{x} - \mu)\right]$$

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

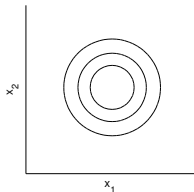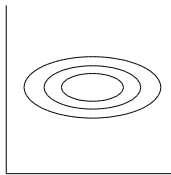# Bivariate Example I

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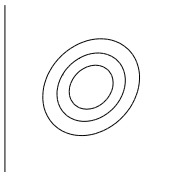
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Cov(x_1,x_2)=0, Var(x_1)=Var(x_2)

Cov(x_1,x_2)=0, Var(x_1)>Var(x_2)
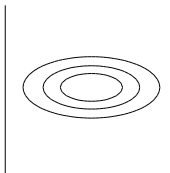
- The level sets closer to the center $\boldsymbol{\mu_x}$ are lower

Cov(x_1,x_2)>0
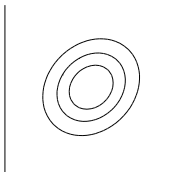
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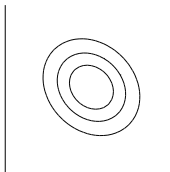
Bivariate Example I

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

Cov(x_1,x_2)=0, Var(x_1)=Var(x_2)
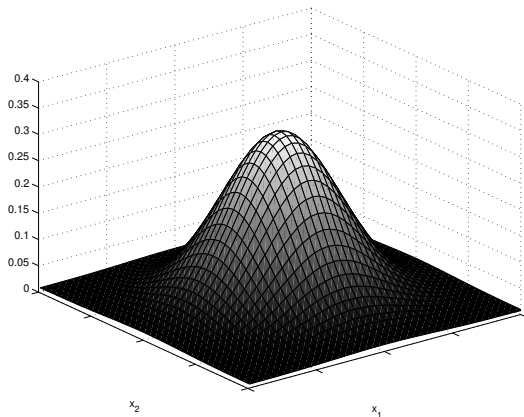
Cov(x_1,x_2)=0, Var(x_1)>Var(x_2)

Cov(x_1,x_2)>0

Cov(x_1,x_2)<0

- The level sets closer to the center μ_x are lower
- Increasing $\mathrm{Cov}[x_1, x_2]$ stretches the level sets along the $45°$ axis
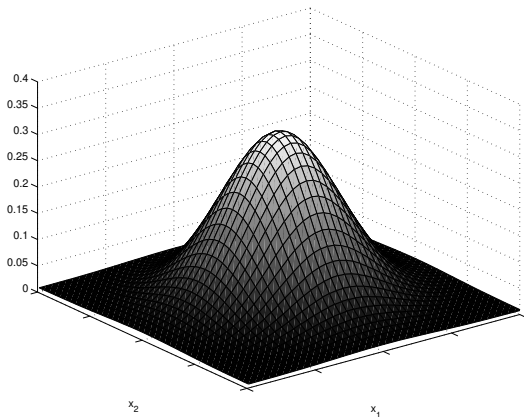- Decreasing $\mathrm{Cov}[x_1, x_2]$ stretches the level sets along the $-45°$ axis

Bivariate Example II

- The hight of $\mathcal{N}(\boldsymbol{\mu}, \Sigma) = \sqrt{\frac{1}{(2\pi)^d \det(\Sigma)}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right]$ 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 $\mathbf{x} \sim \mathscr{N}(\mu, \Sigma)$, then $\mathbf{w}^\top \mathbf{x} \sim \mathscr{N}(\mathbf{w}^\top \mu, \mathbf{w}^\top \Sigma \mathbf{w})$ for any deterministic $\mathbf{w} \in \mathbb{R}^d$
  - More generally, given $\mathbf{W} \in \mathbb{R}^{d \times k}$, $k < d$, we have $\mathbf{W}^\top \mathbf{x} \sim \mathscr{N}(\mathbf{W}^\top \mu, \mathbf{W}^\top \Sigma \mathbf{W})$ that is k-variate normal
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- Consider $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \sim \mathcal{N}(\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \Sigma = \begin{bmatrix} \Sigma_{1,1} & \Sigma_{1,2} \\ \Sigma_{2,1} & \Sigma_{2,2} \end{bmatrix})$:

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- Closed under marginalization: $\mathbf{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_{1,1})$ [Proof: $P(\mathbf{x}_1) = \int_{\boldsymbol{x}_2} P(\mathbf{x}_1, \boldsymbol{x}_2\,; \mu, \Sigma) d\boldsymbol{x}_2)]$

- 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]
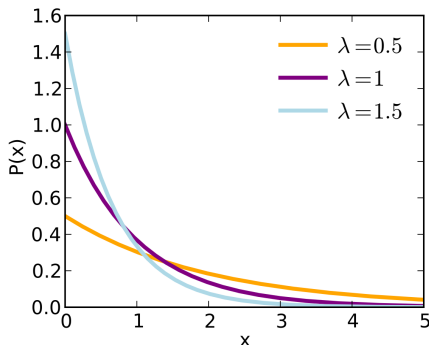
Exponential Distribution (Continuous)

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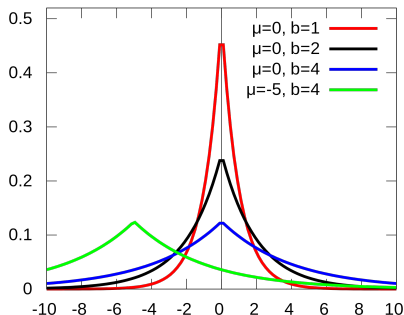- To accomplish this, we can use the *exponential distribution*:

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

Laplace Distribution (Continuous)

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

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

Dirac Distribution (Continuous)

- In some cases, we wish to specify that all of the mass in a probability distribution clusters around a single data point μ

Dirac Distribution (Continuous)

- In some cases, we wish to specify that all of the mass in a probability distribution clusters around a single data point μ
- This can be accomplished by using the *Dirac distribution*:

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

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 $\mathbf{x}$
- What is the distribution $P(\theta)$ that maximizes the likelihood $P(\theta|\mathbb{X})$ of $\mathbb{X}$?

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- If $\mathbf{x}$ is discrete, the distribution simply reflects the empirical frequency of values:

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- If $\mathbf{x}$ is continuous, we have the *empirical distribution*:

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

Mixtures of Distributions

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$$\text{Mixture}(\mathbf{x} = \boldsymbol{x}; \boldsymbol{\rho}, \{\boldsymbol{\theta}^{(i)}\}_i) = \sum_i P^{(i)}(\mathbf{x} = \boldsymbol{x} | \mathbf{c} = i; \boldsymbol{\theta}^{(i)}) \text{Categorical}(\mathbf{c} = i; \boldsymbol{\rho})$$

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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
$P^{(i)}(\mathbf{x} = \boldsymbol{x}|c = i; \boldsymbol{\theta}^{(i)}) = \mathcal{N}^{(i)}(\mathbf{x} = \boldsymbol{x}|c = i; \boldsymbol{\mu}^{(i)}, \Sigma^{(i)}), \ \forall i$

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  - Variants: $\Sigma^{(i)} = \Sigma$ or $\Sigma^{(i)} = \mathrm{diag}(\boldsymbol{\sigma})$ or $\Sigma^{(i)} = \boldsymbol{\sigma} \boldsymbol{I}$

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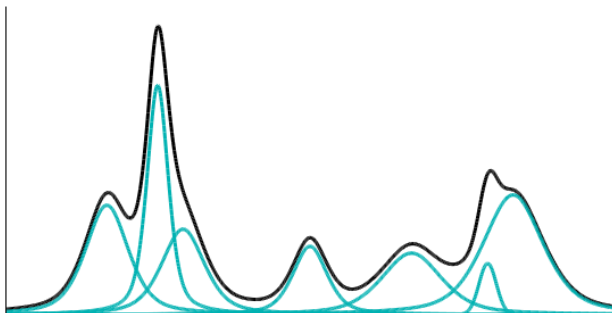
Outline

Parametrizing Functions

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

Logistic Function

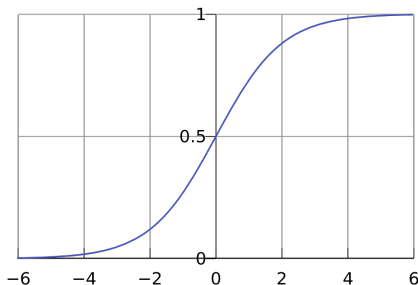- The *logistic function* (a special case of *sigmoid functions*) is defined as:
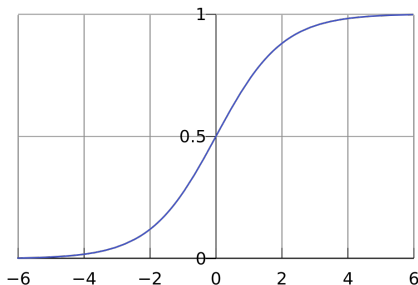
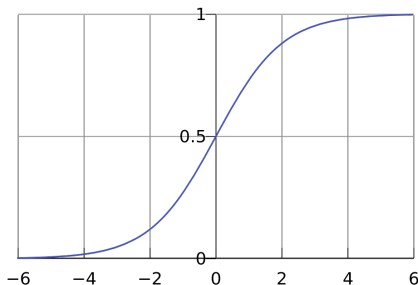$$\sigma(x) = \frac{\exp(x)}{\exp(x) + 1} = \frac{1}{1 + \exp(-x)}$$

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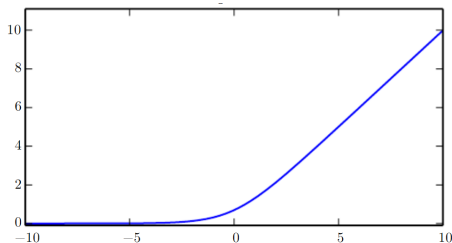

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- Commonly used to produce the ρ parameter of Bernoulli distribution

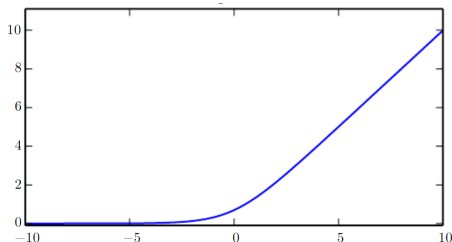# Softplus Function

- The *softplus function* :

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Softplus Function

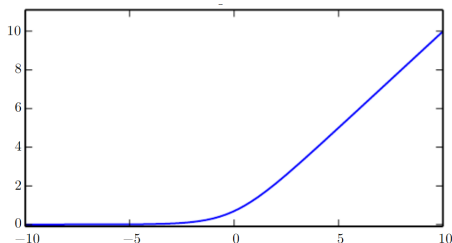- The **softplus function** :

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Softplus Function

- The **_softplus function_** :

$$\zeta(x) = \log(1 + \exp(x))$$

- 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 $x^- = \max(0, -x)$
  - $x = x^+ - x^-$

Outline

What's Information Theory

- Probability theory allows us to make uncertain statements and reason in the presence of uncertainty

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- Information theory allows us to ***quantify*** the amount of uncertainty

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

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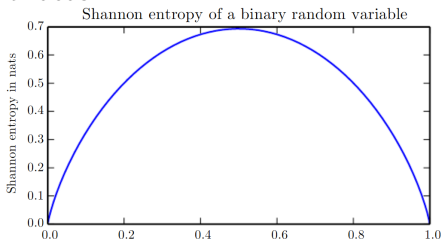- Called *Shannon entropy* when x is discrete; *differential entropy* when x is continuous

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

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  - To send a value x to receiver, we would encode it into 3 bits
  - Shannon entropy: $H(x \sim \text{Uniform}) = -8 \times \frac{1}{8} \log_2 \frac{1}{8} = 3$

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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
  - $H(x) = 2$
  - The encoding $0, 10, 110, 1110, 111100, 111101, 111110, 111111$ gives the average code length 2

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

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

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- If P and Q are independent, we can solve

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

by

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

Properties

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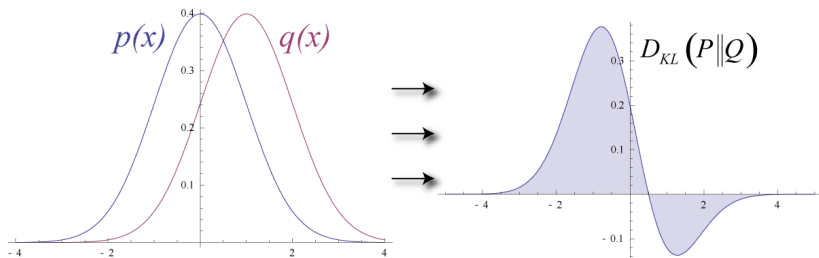- KL divergence is asymmetric, i.e., $D_{KL}(P\|Q) \neq D_{KL}(Q\|P)$

Figure: KL divergence for two normal distributions.

Minimizer of KL Divergence

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

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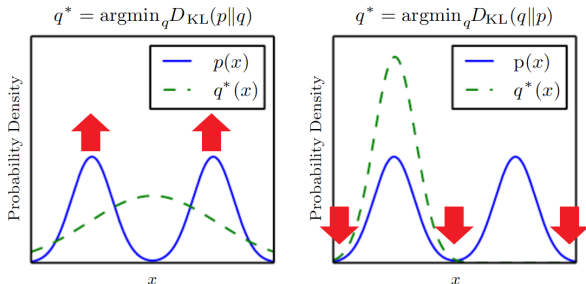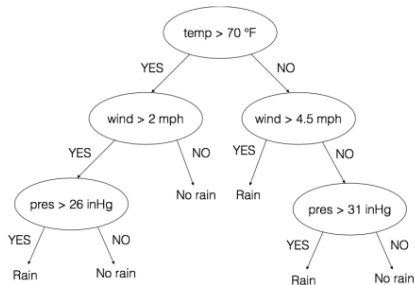- $Q^{*(\text{to})}$ places low probability where P has low probability

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
  $\{(\boldsymbol{x}^{(i)}, y^{(i)}) : \text{Rules} = \emptyset)\}$
- Recursively split leaf nodes until data corresponding to children are "pure" in labels

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- How to split? Find a cutting point (j, v) among all unseen attributes such that after partitioning the corresponding data points
  $\mathbb{X}^{\text{parent}} = \{(\boldsymbol{x}^{(i)}, y^{(i)} : \text{Rules})\}$ into two groups

$$\mathbb{X}^{\text{left}} = \{(\boldsymbol{x}^{(i)}, y^{(i)}) : \text{Rules} \cup \{x_j^{(i)} < v\}\}, \text{ and}$$

$$\mathbb{X}^{\text{right}} = \{(\boldsymbol{x}^{(i)}, y^{(i)}) : \text{Rules} \cup \{x_j^{(i)} \geq v\}\},$$

the "impurity" of labels drops the most

9 yes / 5 no
Wind
Weak   Strong
6 yes / 2 no   3 yes / 3 no

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

$$\arg\max_{j,v} \left(\text{Impurity}(\mathbb{X}^{\text{parent}}) - \text{Impurity}(\mathbb{X}^{\text{left}}, \mathbb{X}^{\text{right}}) \right)$$

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Impurity Measure

$$\arg\max_{j,v} \Big(\text{Impurity}(\mathbb{X}^{\text{parent}}) - \text{Impurity}(\mathbb{X}^{\text{left}}, \mathbb{X}^{\text{right}}) \Big)$$

- What's Impurity$(\cdot)$?

Impurity Measure

$$\arg\max_{j,v} \left(\text{Impurity}(\mathbb{X}^{\text{parent}}) - \text{Impurity}(\mathbb{X}^{\text{left}}, \mathbb{X}^{\text{right}}) \right)$$

- What's Impurity$(\cdot)$?
- Entropy is a common choice:

$$\text{Impurity}(\mathbb{X}^{\text{parent}}) = \text{H}[y \sim \text{Empirical}(\mathbb{X}^{\text{parent}})]$$

$$\text{Impurity}(\mathbb{X}^{\text{left}}, \mathbb{X}^{\text{right}}) = \sum_{i=\text{left,right}} \frac{|\mathbb{X}^{(i)}|}{|\mathbb{X}^{\text{parent}}|} \text{H}[y \sim \text{Empirical}(\mathbb{X}^{(i)})]$$

Impurity Measure

$$\arg\max_{j,v} \left(\text{Impurity}(\mathbb{X}^{\text{parent}}) - \text{Impurity}(\mathbb{X}^{\text{left}}, \mathbb{X}^{\text{right}}) \right)$$

- What's Impurity$(\cdot)$?
- Entropy is a common choice:

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

Decision Boundaries
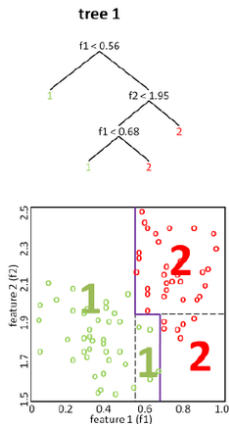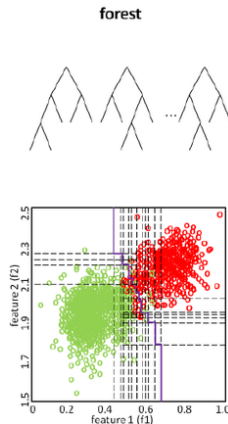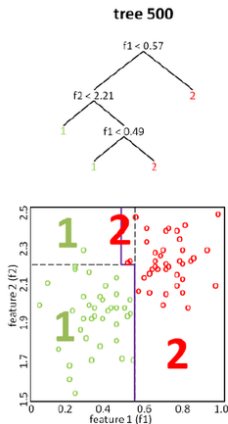
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Decision Trees vs. Random Forests

- Cons of random forests:
  - Less interpretable model
- 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