Lecture 1. Mathematical Background

Advanced Optimization (Fall 2024)

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Outline

- Calculus
- Linear Algebra
- Probability & Statistics
- Information Theory
- Optimization in Machine Learning

Notational Convention

- $[n] = \{1, \dots, n\}$
- $\mathbf{x}, \mathbf{y}, \mathbf{v}$: vectors
- A, B: matrices
- $\mathcal{X}, \mathcal{Y}, \mathcal{K}$: domain
- d, m, n: dimensions
- I: identity matrix
- X, Y: random variables
- $\boldsymbol{p}, \boldsymbol{q}$: probability distributions

Function

- Function mapping $f : \mathrm{dom}\, f \subseteq \mathcal{X} \subseteq \mathbb{R}^n \to \mathcal{Y} \subseteq \mathbb{R}^m$

Definition 1 (Continuous Function)**.** A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is continuous at $\mathbf{x} \in \mathrm{dom}\ f$ if for all $\epsilon > 0$ there exists a $\delta > 0$ with $\mathbf{y} \in \mathrm{dom}\, f$, such that

$$\|\mathbf{y} - \mathbf{x}\|_2 \leq \delta \Rightarrow \|f(\mathbf{y}) - f(\mathbf{x})\|_2 \leq \epsilon.$$

Part 1. Calculus

- Gradient and Derivatives

- Hessian

- Chain Rule

Gradient and Derivatives (First Order)

- The gradient and derivative of a scalar function ($f : \mathbb{R} \mapsto \mathbb{R}$) is the same.
- The derivative of vector functions ($f : \mathcal{X} \subseteq \mathbb{R}^d \mapsto \mathbb{R}$) is the transpose of its gradient.

we focus on the "gradient" language (i.e., column vector)

Definition 2 (Gradient). Let $f : \mathcal{X} \subseteq \mathbb{R}^d \to \mathbb{R}$ be a differentiable function. Let $\mathbf{x} = [x_1, \cdots, x_d]^\top \in \mathcal{X}$. Then, the gradient of f at $\mathbf{x}$ is a vector in $\mathbb{R}^d$ denoted by $\nabla f(\mathbf{x})$ and defined by

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{bmatrix}.$$

Example

Example 1. The gradient of $f(\mathbf{x}) = \|\mathbf{x}\|_2^2 \triangleq \sum_{i=1}^d x_i^2$ is

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2x_1 \\ \vdots \\ 2x_d \end{bmatrix} = 2\mathbf{x}.$$

Example 2. The gradient of $f(\mathbf{x}) = -\sum_{i=1}^d x_i \ln x_i$ is

$$\nabla f(\mathbf{x}) = \begin{bmatrix} -(\ln x_1 + 1) \\ \vdots \\ -(\ln x_d + 1) \end{bmatrix}.$$

Hessian (Second Order)

Definition 3 (Hessian). Let $f : \mathcal{X} \subseteq \mathbb{R}^d \to \mathbb{R}$ be a twice differentiable function. Let $\mathbf{x} = [x_1, \cdots, x_d]^\top \in \mathcal{X}$. Then, the Hessian of f at $\mathbf{x}$ is the matrix in $\mathbb{R}^{d \times d}$ denoted by $\nabla^2 f(\mathbf{x})$ and defined by

$$\nabla^2 f(\mathbf{x}) = \left[\frac{\partial^2 f}{\partial x_i, x_j}(\mathbf{x})\right]_{1 \leq i,j \leq d}.$$

Example 3. The Hessian of $f(\mathbf{x}) = -\sum_{i=1}^d x_i \ln x_i$ is $\nabla^2 f(\mathbf{x}) = \mathrm{diag}(-\frac{1}{x_1}, \ldots, -\frac{1}{x_d})$.

Example 4. The Hessian of $f(\mathbf{x}) = x_1^3 x_2^2 - 3x_1 x_2^3 + 1$ is $\nabla^2 f(\mathbf{x}) = \begin{bmatrix} 6x_1 x_2^2 & 6x_1^2 x_2 - 6x_2 \\ 6x_1^2 x_2 - 9x_2^2 & 2x_1^3 - 18x_1 x_2 \end{bmatrix}$.

Chain Rule

- Consider scalar functions for simplicity.

> **Chain Rule.** For $h(x) = f(g(x))$,
>
> - the gradient of $h(x)$ is $h'(x) = f'(g(x))g'(x)$.
> - the Hessian of $h(x)$ is $h''(x) = f''(g(x))(g'(x))^2 + f'(g(x))g''(x)$.

Reference: The Matrix Cookbook

The derivatives of **vectors, matrices, norms, determinants, etc** can be found therein.

2.4.1 First Order

$$\frac{\partial \mathbf{x}^T\mathbf{a}}{\partial \mathbf{x}} = \frac{\partial \mathbf{a}^T\mathbf{x}}{\partial \mathbf{x}} = \mathbf{a} \quad (69)$$

$$\frac{\partial \mathbf{a}^T\mathbf{X}\mathbf{b}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{b}^T \quad (70)$$

$$\frac{\partial \mathbf{a}^T\mathbf{X}^T\mathbf{b}}{\partial \mathbf{X}} = \mathbf{b}\mathbf{a}^T \quad (71)$$

$$\frac{\partial \mathbf{a}^T\mathbf{X}\mathbf{a}}{\partial \mathbf{X}} = \frac{\partial \mathbf{a}^T\mathbf{X}^T\mathbf{a}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{a}^T \quad (72)$$

$$\frac{\partial \mathbf{X}}{\partial X_{ij}} = \mathbf{J}^{ij} \quad (73)$$

$$\frac{\partial (\mathbf{X}\mathbf{A})_{ij}}{\partial X_{mn}} = \delta_{im}(\mathbf{A})_{nj} = (\mathbf{J}^{mn}\mathbf{A})_{ij} \quad (74)$$

$$\frac{\partial (\mathbf{X}^T\mathbf{A})_{ij}}{\partial X_{mn}} = \delta_{in}(\mathbf{A})_{mj} = (\mathbf{J}^{nm}\mathbf{A})_{ij} \quad (75)$$

https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

2 Derivatives

This section is covering differentiation of a number of expressions with respect to a matrix $\mathbf{X}$. Note that it is always assumed that $\mathbf{X}$ has *no special structure*, i.e. that the elements of $\mathbf{X}$ are independent (e.g. not symmetric, Toeplitz, positive definite). See section 2.8 for differentiation of structured matrices. The basic assumptions can be written in a formula as

$$\frac{\partial X_{kl}}{\partial X_{ij}} = \delta_{ik}\delta_{lj} \quad (32)$$

that is for e.g. vector forms,

$$\left[\frac{\partial \mathbf{x}}{\partial y}\right]_i = \frac{\partial x_i}{\partial y} \qquad \left[\frac{\partial x}{\partial \mathbf{y}}\right]_i = \frac{\partial x}{\partial y_i} \qquad \left[\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right]_{ij} = \frac{\partial x_i}{\partial y_j}$$

The following rules are general and very useful when deriving the differential of an expression ([19]):

$$\begin{aligned}
\partial \mathbf{A} &= 0 \qquad (\mathbf{A} \text{ is a constant}) && (33)\\
\partial(\alpha\mathbf{X}) &= \alpha\partial\mathbf{X} && (34)\\
\partial(\mathbf{X}+\mathbf{Y}) &= \partial\mathbf{X}+\partial\mathbf{Y} && (35)\\
\partial(\mathrm{Tr}(\mathbf{X})) &= \mathrm{Tr}(\partial\mathbf{X}) && (36)\\
\partial(\mathbf{X}\mathbf{Y}) &= (\partial\mathbf{X})\mathbf{Y}+\mathbf{X}(\partial\mathbf{Y}) && (37)\\
\partial(\mathbf{X}\circ\mathbf{Y}) &= (\partial\mathbf{X})\circ\mathbf{Y}+\mathbf{X}\circ(\partial\mathbf{Y}) && (38)\\
\partial(\mathbf{X}\otimes\mathbf{Y}) &= (\partial\mathbf{X})\otimes\mathbf{Y}+\mathbf{X}\otimes(\partial\mathbf{Y}) && (39)\\
\partial(\mathbf{X}^{-1}) &= -\mathbf{X}^{-1}(\partial\mathbf{X})\mathbf{X}^{-1} && (40)\\
\partial(\det(\mathbf{X})) &= \mathrm{Tr}(\mathrm{adj}(\mathbf{X})\partial\mathbf{X}) && (41)\\
\partial(\det(\mathbf{X})) &= \det(\mathbf{X})\mathrm{Tr}(\mathbf{X}^{-1}\partial\mathbf{X}) && (42)\\
\partial(\ln(\det(\mathbf{X}))) &= \mathrm{Tr}(\mathbf{X}^{-1}\partial\mathbf{X}) && (43)\\
\partial\mathbf{X}^T &= (\partial\mathbf{X})^T && (44)\\
\partial\mathbf{X}^H &= (\partial\mathbf{X})^H && (45)
\end{aligned}$$

Part 2. Linear Algebra

- Positive (Semi-)Definite Matrix

- Rank

- Inner Product, Norm, Matrix Norm

- Matrix Decomposition

Positive (Semi-)Definite Matrix

Definition 4 (Positive Definite, PD)**.** A matrix $A \in \mathbb{R}^{d\times d}$ is positive definite, if for all $\mathbf{x} \neq \mathbf{0}, \mathbf{x}^\top A\mathbf{x} > 0$, usually denoted as $A \succ 0$.

Definition 5 (Positive Semi-Definite, PSD)**.** A matrix $A \in \mathbb{R}^{d\times d}$ is positive semi-definite, if for all $\mathbf{x} \in \mathbb{R}^d, \mathbf{x}^\top A\mathbf{x} \geq 0$, usually denoted as $A \succeq 0$.

Rank

- **Rank**: the dimension of the vector space spanned by its columns, or the maximal number of linearly independent columns.

Example 5.

$$A = \begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix} \xrightarrow{2R_1+R_2\to R_2} \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 3 \\ 3 & 5 & 0 \end{bmatrix} \xrightarrow{-3R_1+R_3\to R_3} \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 3 \\ 0 & -1 & -3 \end{bmatrix}$$

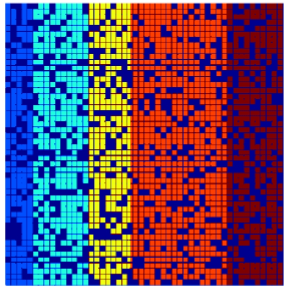
$$\xrightarrow{R_2+R_3\to R_3} \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix} \xrightarrow{-2R_2+R_1\to R_1} \begin{bmatrix} 1 & 0 & -5 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}.$$

The rank of matrix A is 2.

Low rank: Robust PCA

- Robust PCA formulation

$$\min_{\hat{X}} \|X - \hat{X}\|_1 + \|\hat{X}\|_*$$



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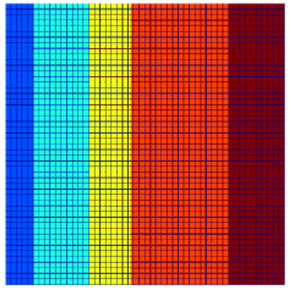

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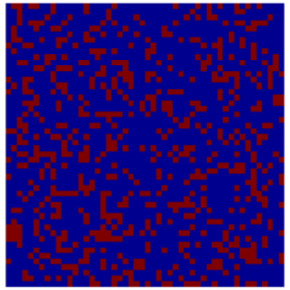
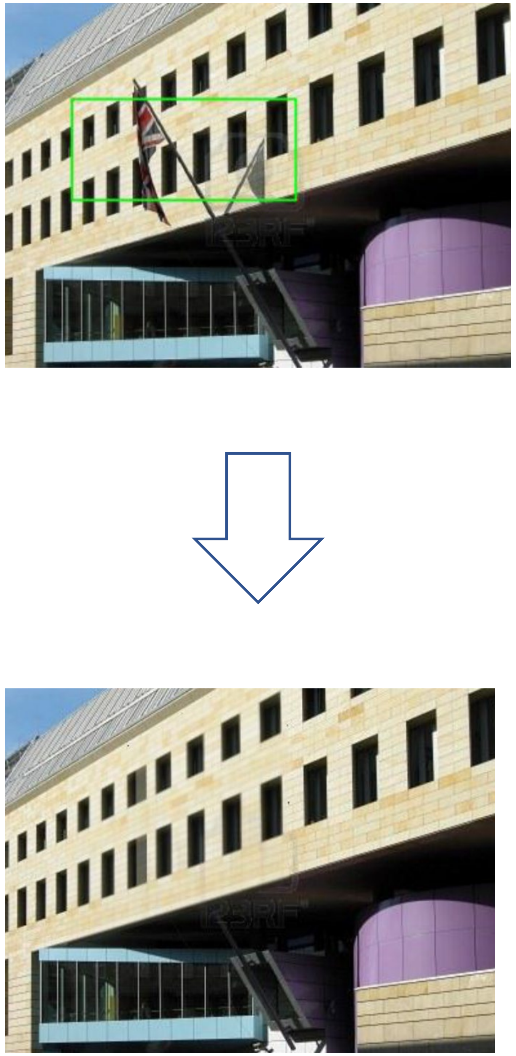


input X | *low rank* $\|\hat{X}\|_*$ | *sparse* $\|X - \hat{X}\|_1$



Inner Product

- Vector Space: consider $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, then

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\top \mathbf{y} = \sum_{i=1}^{d} x_i y_i$$

- Matrix Space: consider $A, B \in \mathbb{R}^{m \times n}$, then

$$\langle A, B \rangle = \mathrm{Tr}\left(A^\top B\right) = \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} B_{ij}$$

Norm

- Typically used vector norms.

  - ℓ_1-norm:

$$\|\mathbf{x}\|_1 = |x_1| + \cdots + |x_d|$$

  - ℓ_2-norm:

$$\|\mathbf{x}\|_2 = \left(\mathbf{x}^\top \mathbf{x}\right)^{1/2} = \sqrt{x_1^2 + \cdots + x_d^2}$$

or called *Euclidean norm*

  - ℓ_∞-norm:

$$\|\mathbf{x}\|_\infty = \max\left\{|x_1|, \ldots, |x_d|\right\}$$

Norm

- Typically used vector norms.

  - General ℓ_p-norm:

$$\|\mathbf{x}\|_p = \left(|x_1|^p + \cdots + |x_d|^p\right)^{1/p}$$

  - Quadratic norm:

$$\|\mathbf{x}\|_A = \sqrt{\mathbf{x}^\top A \mathbf{x}}, \text{ where } A \text{ is positive semi-definite.}$$

Dual Norm

Let $\|\cdot\|$ be a vector norm on $\mathbb{R}^d$. The associated dual norm $\|\cdot\|_*$ is defined as

$$\|\mathbf{y}\|_* = \sup\left\{\mathbf{y}^\top \mathbf{x} \mid \|\mathbf{x}\| \le 1\right\}.$$

Proposition 1. The dual of ℓ_p-norm is the ℓ_q-norm with $\frac{1}{p} + \frac{1}{q} = 1$.

e.g., the dual of ℓ_2-norm is still ℓ_2-norm, the dual of ℓ_1-norm is ℓ_∞-norm

Proposition 2. Hölder's inequality: $\langle \mathbf{x}, \mathbf{y} \rangle \le \|\mathbf{x}\| \cdot \|\mathbf{y}\|_*$.

Norm Relationship

Qualitative:

Lemma 1 (Mathematical Equivalence of Norms). *Suppose that* $\|\cdot\|_a$ *and* $\|\cdot\|_b$ *are norms on* $\mathbb{R}^d$*, there exist positive "constants"* α *and* β*, for all* $\mathbf{x} \in \mathbb{R}^d$*, such that*

$$\alpha\|\mathbf{x}\|_a \leq \|\mathbf{x}\|_b \leq \beta\|\mathbf{x}\|_a.$$

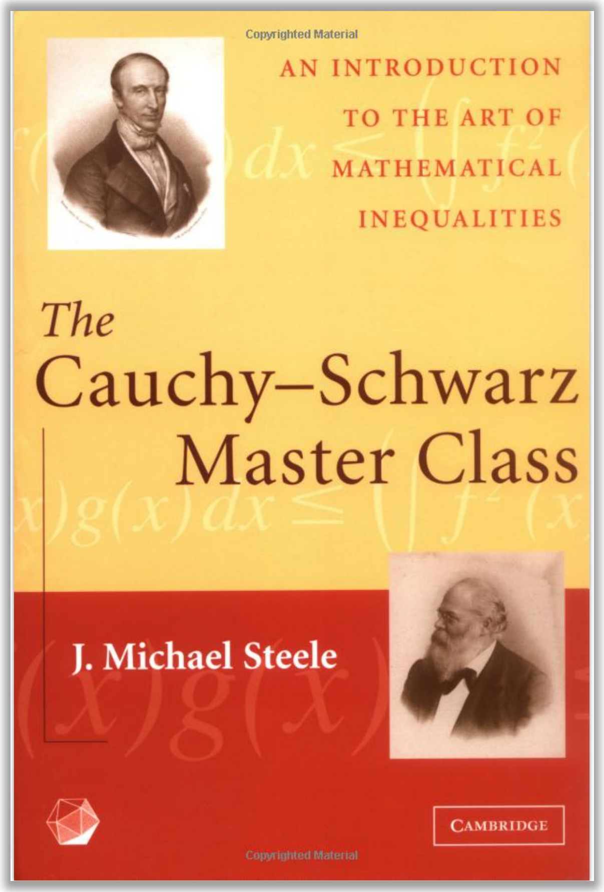
Notice: constants may depend on dimension!

For example: for any $\mathbf{x} \in \mathbb{R}^d$, the following inequalities hold:

- $\frac{1}{d}\|\mathbf{x}\|_1 \leq \|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_1$
- $\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_2 \leq \sqrt{d}\|\mathbf{x}\|_\infty$

Cauchy-Schwarz Inequality

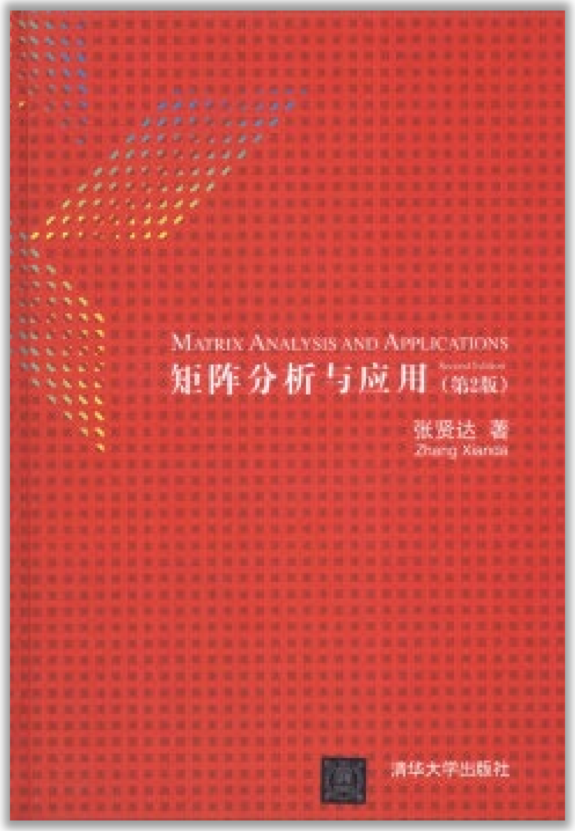
- $\langle \mathbf{x}, \mathbf{y} \rangle \leq \|\mathbf{x}\| \cdot \|\mathbf{y}\|_*$
- $\left(\sum_{i=1}^{n} a_i b_i \right)^2 \leq \left(\sum_{i=1}^{n} a_i^2 \right) \cdot \left(\sum_{i=1}^{n} b_i^2 \right)$
- $\left(\int_a^b f(x) g(x) \mathrm{d}x \right)^2 \leq \left(\int_a^b f^2(x) \mathrm{d}x \right) \cdot \left(\int_a^b g^2(x) \mathrm{d}x \right)$



Matrix Norm

Three different versions:

- operator norm
- entrywise norm
- Schatten norm



矩阵分析与应用. 张贤达

related pages can be found in readings of the course web

Matrix Operator Norm

- Consider a matrix $A \in \mathbb{R}^{m \times n}$.

We define its ***operator norm*** based on the aforementioned ***vector norm***.

Definition 6 (Matrix Operator Norm)**.** The operator norm (or called induced norm) of a matrix $A \in \mathbb{R}^{m \times n}$ is defined by

$$\|A\|_{\mathrm{op},p} \triangleq \max \left\{ \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p} \;\middle|\; \mathbf{x} \in \mathbb{R}^d, \mathbf{x} \neq \mathbf{0} \right\}.$$

the norm in the right-hand side is defined over the *vector space*.

Matrix Operator Norm

- Consider a matrix $A \in \mathbb{R}^{m \times n}$
  - ℓ_1-norm (max-column-sum norm):

$$\|A\|_{\text{op},1} = \max_{j \in [n]} \sum_{i=1}^{m} |A_{ij}|$$

  - ℓ_∞-norm (max-row-sum norm):

$$\|A\|_{\text{op},\infty} = \max_{i \in [m]} \sum_{j=1}^{n} |A_{ij}|$$

Matrix Operator Norm

- Consider a matrix $A \in \mathbb{R}^{m \times n}$
  - ℓ_2-norm (spectral norm):

$$\|A\|_{\mathrm{op},2} = \max_{i \in [r]} |\sigma_i|$$

where $A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$, namely, σ_i is the i-th singular value.

Matrix Entrywise Norm

- Consider a matrix $A \in \mathbb{R}^{m \times n}$

The entrywise norm is defined by ***treating matrices as vectors***.

Definition 7 (Matrix Entrywise Norm). The entrywise norm of a matrix $A \in \mathbb{R}^{m \times n}$ is defined by

$$\|A\|_{\mathrm{en},p} \triangleq \left(\sum_{i=1}^{m} \sum_{j=1}^{n} |A_{ij}|^p \right)^{1/p}.$$

Matrix Entrywise Norm

- Consider a matrix $A \in \mathbb{R}^{m \times n}$
  - ℓ_1-norm (sum norm):

$$\|A\|_{\text{en},1} = \sum_{i=1}^{m} \sum_{j=1}^{n} |A_{ij}|$$

  - Frobenius-norm:

$$\|A\|_{\text{F}} = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij}^2}$$

  - ℓ_∞-norm (max norm):

$$\|A\|_{\text{en},\infty} = \max_{i \in [m]} \max_{j \in [n]} |A_{ij}|$$

Eigen Value Decomposition

Let A be an $d \times d$ PSD matrix, then it can be factored as

$$A = Q\Lambda Q^\top,$$

where (a) $Q = (\mathbf{v}_1, \ldots, \mathbf{v}_d) \in \mathbb{R}^{d\times d}$ is orthogonal, i.e., $Q^\top Q = I$ and $\mathbf{v}_1, \ldots, \mathbf{v}_d$ are eigenvectors; and (b) $\Lambda = \mathrm{diag}(\lambda_1, \cdots, \lambda_d)$ and $\lambda_1, \cdots, \lambda_d$ are eigenvalues.

Some concerned terms can be expressed by eigenvalues:

- $A = \sum_{i=1}^d \lambda_i \mathbf{v}_i \mathbf{v}_i^\top$
- $\det(A) = \prod_{i=1}^d \lambda_i$
- $\mathrm{Tr}(A) = \sum_{i=1}^d \lambda_i$
- $\|A\|_{\mathrm{op},2} = \max_{i\in[d]} |\lambda_i|$
- $\|A\|_{\mathrm{F}} = \sqrt{\sum_{i=1}^d \lambda_i^2}$

Singular Value Decomposition

Suppose $A \in \mathbb{R}^{m \times n}$ has rank r, then it can be factored as

$$A = U \Sigma V^\top,$$

where (a) $U = (\mathbf{u}_1, \ldots, \mathbf{u}_r) \in \mathbb{R}^{m \times r}$ satisfies $U^\top U = I, V = (\mathbf{v}_1, \ldots, \mathbf{v}_r) \in \mathbb{R}^{n \times r}$ satisfies $V^\top V = I$; and (b) $\Sigma = \operatorname{diag}(\sigma_1, \cdots, \sigma_r)$ and $\sigma_1, \cdots, \sigma_r$ are sigular values.

Some concerned terms can be expressed by sigular values:

- $A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$
- $\|A\|_{\text{op},2} = \max_{i \in [r]} |\sigma_i|$
- $\|A\|_{\text{F}} = \sqrt{\sum_{i=1}^{r} \sigma_i^2}$

Schatten Norm

- Consider a matrix $A \in \mathbb{R}^{m \times n}$

The Schatten norm is defined via the ***sigular values***.

Definition 8 (Matrix Schatten Norm). The Schatten norm of a matrix $A \in \mathbb{R}^{m \times n}$ with rank r is defined by

$$\|A\|_{\mathrm{Sc},p} \triangleq \begin{cases} \left(\sum_{i=1}^{r} \sigma_i^p\right)^{1/p}, & \text{for } 1 \leq p < \infty \\ \max_{i \in [r]} |\sigma_i|, & \text{for} \quad p = \infty \end{cases}$$

where $\sigma_1, \cdots, \sigma_r$ are the singular values of A.

Part 3. Probability and Statistics

- Expectation and Variance

- Conditional Expectation

- Concentration Inequalities

Expectation and Variance

Expectation

$$\mathbb{E}[X] = \sum_{x \in \mathcal{X}} x \Pr[X = x]$$

Linearity of expecation: $\mathbb{E}[aX + bY] = a\mathbb{E}[X] + b\mathbb{E}[Y]$.

Variance

$$\mathrm{Var}[X] = \mathbb{E}\left[(X - \mathbb{E}[X])^2\right]$$

- $\mathrm{Var}[X] = \mathbb{E}\left[X^2\right] - \mathbb{E}[X]^2$
- $\mathrm{Var}[aX] = a^2\,\mathrm{Var}[X]$
- $\mathrm{Var}[X + Y] = \mathrm{Var}[X] + \mathrm{Var}[Y]$

Cauchy-Schwarz Inequality in Probability

- $\langle \mathbf{x}, \mathbf{y} \rangle \leq \|\mathbf{x}\| \cdot \|\mathbf{y}\|_*$
- $\left(\sum_{i=1}^n a_i b_i \right)^2 \leq \left(\sum_{i=1}^n a_i^2 \right) \cdot \left(\sum_{i=1}^n b_i^2 \right)$
- $\left(\int_a^b f(x) g(x) \mathrm{d}x \right)^2 \leq \left(\int_a^b f^2(x) \mathrm{d}x \right) \cdot \left(\int_a^b g^2(x) \mathrm{d}x \right)$
- $(\mathbb{E}[XY])^2 \leq \mathbb{E}[X^2] \cdot \mathbb{E}[Y^2]$

Conditional Expectation

Conditional Expectation

$$\mathbb{E}[X|Y=y] = \sum_{x \in \mathcal{X}} x \Pr[X=x|Y=y]$$

Theorem 1 (Double Expectation Theorem). *Let X, Y be arbitrary random variables. Suppose $\mathbb{E}[X], \mathbb{E}[Y], \mathbb{E}[X|Y], \mathbb{E}[Y|X]$ all exist, then it holds that*

$$\mathbb{E}[X] = \mathbb{E}_Y[\mathbb{E}_X[X|Y]], \ \mathbb{E}[Y] = \mathbb{E}_X[\mathbb{E}_Y[Y|X]].$$

$\mathbb{E}[X] = \mathbb{E}_Y[\mathbb{E}_X[X|Y]]$ means that to measure the expectation of X, we can first measure the expectation of X ***given the information of Y***, then measure the expectation of Y.

Concentration Inequalities

Theorem 2 (Markov's Inequality). *Let X be a non-negative random variable with $\mathbb{E}[X] < \infty$, then for all $t > 0$,*

$$\Pr[X \geq t\mathbb{E}[X]] \leq \frac{1}{t}.$$

Proof.

$$\begin{aligned}
\Pr[X \geq t\mathbb{E}[X]] &= \sum_{x \geq t\mathbb{E}[X]} \Pr[X = x] \\
&\leq \sum_{x \geq t\mathbb{E}[X]} \Pr[X = x] \cdot \frac{x}{t\mathbb{E}[X]} && \text{(using } \tfrac{x}{t\mathbb{E}[X])} \geq 1\text{)} \\
&\leq \sum_{x} \Pr[X = x] \cdot \frac{x}{t\mathbb{E}[X]} && \text{(extending non-negative sum)} \\
&= \mathbb{E}\left[\frac{X}{t\mathbb{E}[X]}\right] = \frac{1}{t} && \text{(linearity of expectation)}
\end{aligned}$$

Concentration Inequalities

Theorem 3 (Chebyshev's Inequality). *Let X be a non-negative random variable with $\mathbb{E}[X], \mathrm{Var}[X] < \infty$, then for all $\epsilon > 0$,*

$$\Pr\left[|X - \mathbb{E}[X]| \geq \epsilon\right] \leq \frac{\mathrm{Var}[X]}{\epsilon^2}.$$

Chebyshev's inequality can be immediately obtained from Markov's inequality.

Theorem 4 (Hoeffding's Inequality). *Let $X_1, \ldots, X_m$ be* ***independent*** *random variables with X_i taking values in $[a_i, b_i]$ for all $i \in [m]$. Then, for any $\epsilon > 0$, the following inequalities hold for $S_m = \sum_{i=1}^m X_i$,*

$$\Pr\left[S_m - \mathbb{E}\left[S_m\right] \geq \epsilon\right] \leq e^{-2\epsilon^2 / \sum_{i=1}^m (b_i - a_i)^2},$$

$$\Pr\left[S_m - \mathbb{E}\left[S_m\right] \leq -\epsilon\right] \leq e^{-2\epsilon^2 / \sum_{i=1}^m (b_i - a_i)^2}.$$

Part 4. Information Theory

- Entropy
- Conditional Entropy
- KL divergence
- Bregman Divergence

Entropy

- Entropy measures the uncertainty, which is the most basic concept in the information theory.

Definition 9 (Entropy)**.** The entropy of a discrete random variable X with probability mass function $\boldsymbol{p}(x) = \Pr[X = x]$ is denoted by $H(X)$:

$$H(X) = -\sum_{x \in X} \boldsymbol{p}(x) \log(\boldsymbol{p}(x)).$$

An explanation of entropy: $\log_2(1/\boldsymbol{p}(x))$ is the code length needed to encode the info., then entropy $H(X)$ measures the ***expected code length*** to encode a distribution $\boldsymbol{p}$.

⇨ The entropy is a lower bound on ***lossless data compression*** and is therefore a critical quantity to consider in information theory.

Conditional Entropy & Mutual Information

Definition 10 (Conditional Entropy).

$$H(Y|X) = -\sum_{x\in\mathcal{X},y\in\mathcal{Y}} \boldsymbol{p}(x,y)\log\frac{\boldsymbol{p}(x,y)}{\boldsymbol{p}(x)}$$

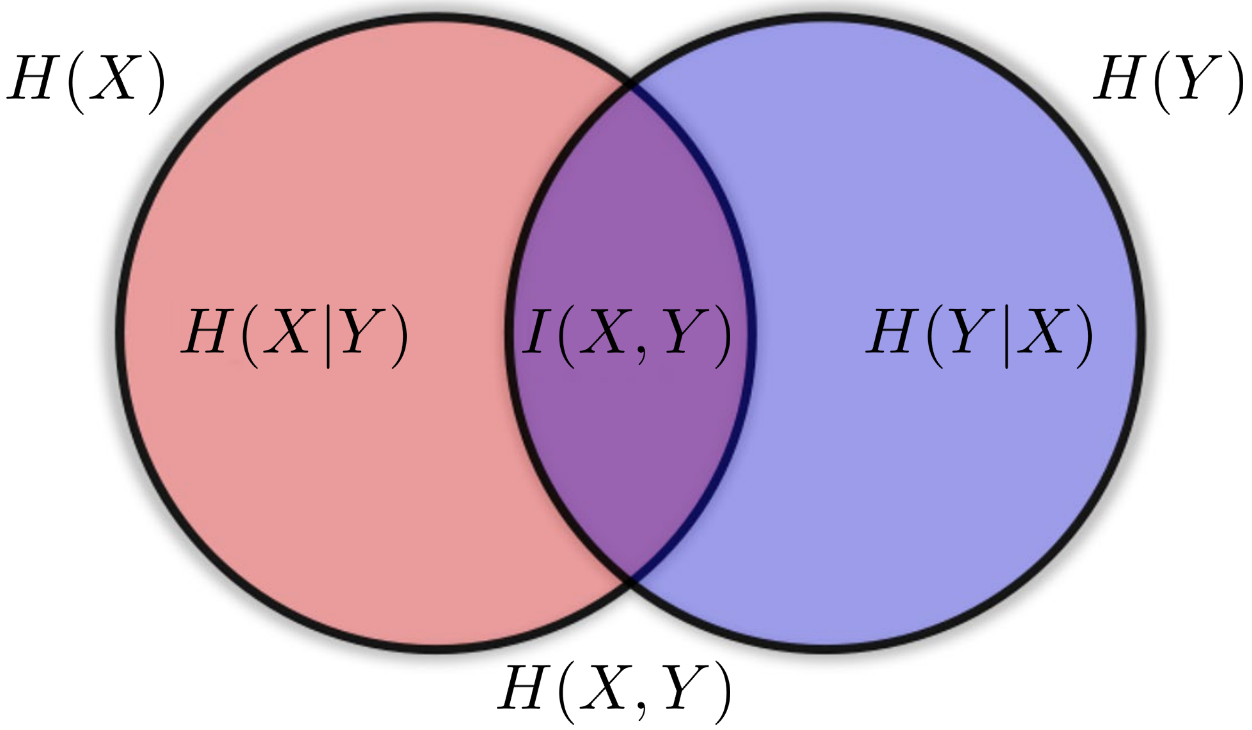
Conditional entropy $H(Y|X)$ measures the uncertainty of Y ***given the uncertainty of*** X.

Definition 11 (Mutual Information).

$$I(X,Y) = \mathrm{KL}(\boldsymbol{p}(x,y)\|\boldsymbol{p}(x)\boldsymbol{p}(y)) = \sum_{x\in X,y\in y} \boldsymbol{p}(x,y)\log\left[\frac{\boldsymbol{p}(x,y)}{\boldsymbol{p}(x)\boldsymbol{p}(y)}\right],$$

with the conventions $0\log 0 = 0, 0\log\frac{0}{0} = 0$, and $a\log\frac{a}{0} = +\infty$ for $a > 0$.

Relationship



$$I(X,Y) = H(X) - H(X|Y)$$

$$I(X,Y) = H(Y) - H(Y|X)$$

KL Divergence (Relative Entropy)

Definition 12 (KL Divergence)**.** The Kullback-Leibler (KL) divergence (relative entropy) of two distributions $\boldsymbol{p}$ and $\boldsymbol{q}$ is defined by $\mathrm{KL}(\boldsymbol{p}\|\boldsymbol{q})$:

$$\mathrm{KL}(\boldsymbol{p}\|\boldsymbol{q}) = \sum_{x \in \mathcal{X}} \boldsymbol{p}(x) \log \left[\frac{\boldsymbol{p}(x)}{\boldsymbol{q}(x)}\right]$$

with the conventions $0 \log 0 = 0, 0 \log \frac{0}{0} = 0$, and $a \log \frac{a}{0} = +\infty$ for $a > 0$.

Proposition 1.

- *KL divergence is always non-negative;*
- *Pinsker's inequality:* $KL(\boldsymbol{p}\|\boldsymbol{q}) \geq \frac{1}{2} \|\boldsymbol{p} - \boldsymbol{q}\|_1^2$.

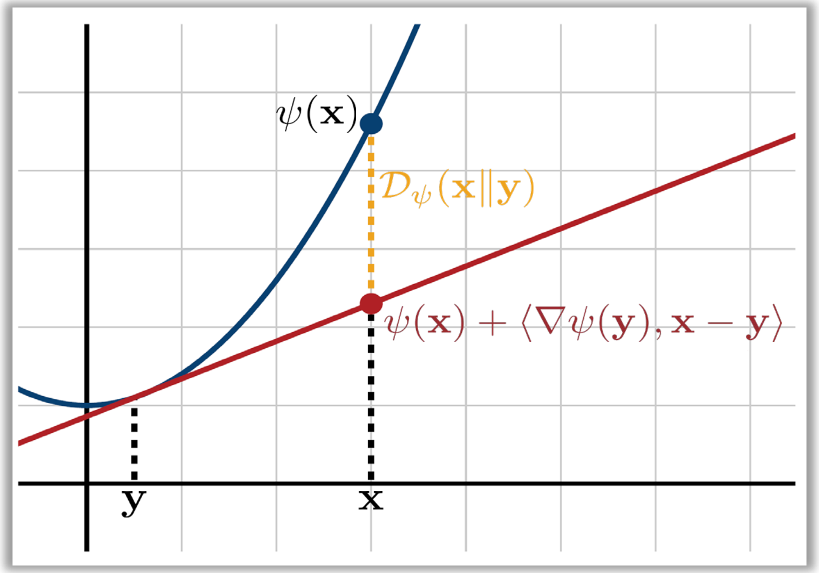
Bregman Divergence

Definition 13 (Bregman Divergence)**.** Let ψ be a convex and differentiable function over a convex set $\mathcal{K}$, then for any $\mathbf{x}, \mathbf{y} \in \mathcal{K}$, the bregman divergence $\mathcal{D}_\psi$ associated to ψ is defined as

$$\mathcal{D}_\psi(\mathbf{x} \| \mathbf{y}) = \psi(\mathbf{x}) - \psi(\mathbf{y}) - \langle \nabla \psi(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle.$$

Table 1: Choice of $\psi(\cdot)$ and the Bregman divergence.

	$\psi(\mathbf{x})$	$\mathcal{D}_\psi(\mathbf{x} \| \mathbf{y})$
Squared L_2-distance	$\|\mathbf{x}\|_2^2$	$\|\mathbf{x} - \mathbf{y}\|_2^2$
Mahalanobis distance	$\|\mathbf{x}\|_Q^2$	$\|\mathbf{x} - \mathbf{y}\|_Q^2$
negative entropy	$\sum_i x_i \log x_i$	$\mathrm{KL}(\mathbf{x} \| \mathbf{y})$



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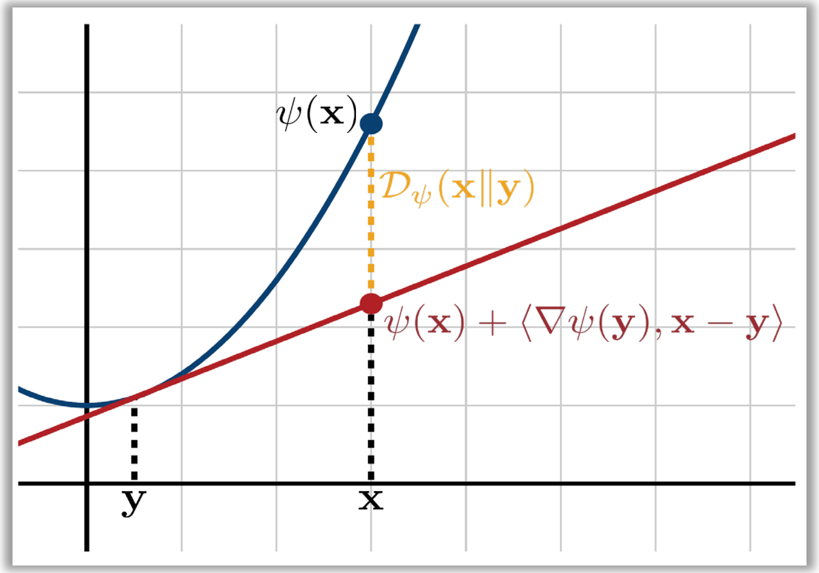
Q: *Is its importance due to generality?*

Not exactly, consider more general one like

$$\mathcal{D}_\psi^{\alpha,\beta,\gamma}(\mathbf{x}\|\mathbf{y}) = \psi(\mathbf{x})^\alpha - \psi(\mathbf{y})^\beta - \langle \nabla\psi(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle^\gamma.$$

⇨ Bregman divergence measures the difference of a function and its *linear approximation*



Part 5. Asymptotic Notations

- Definition

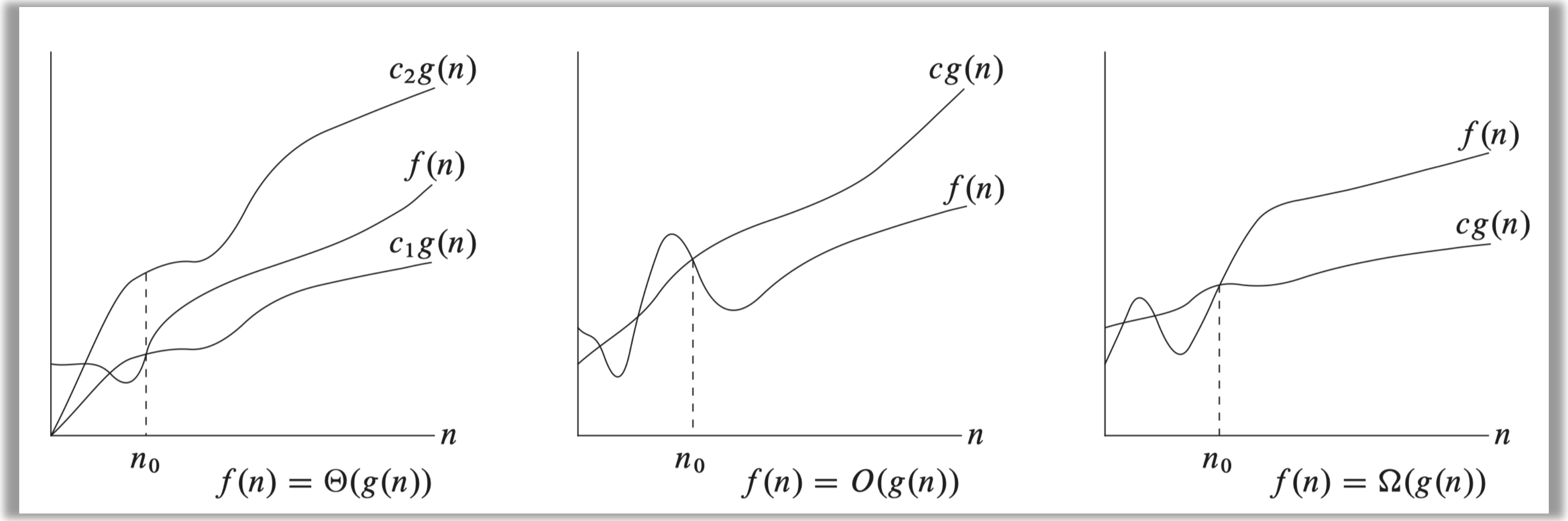
- Illustration

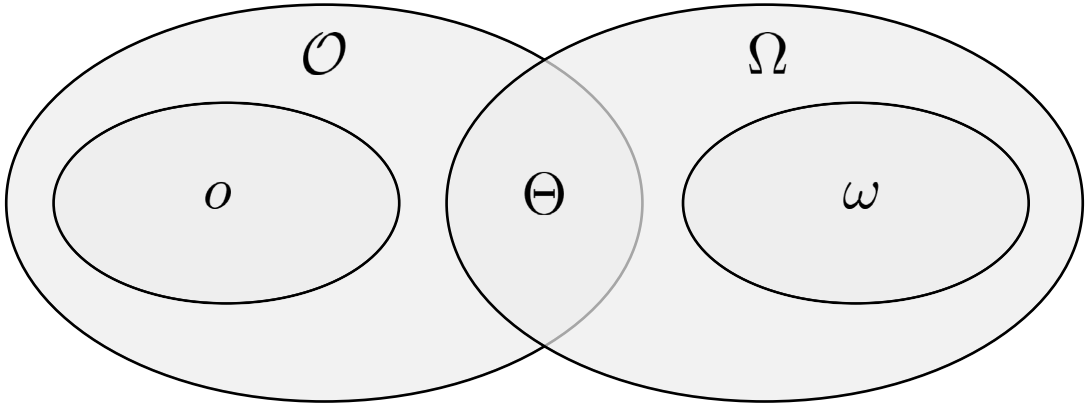
- Example

Definition

- $\Theta(g(n)) = \{f(n) \mid$ there exist positive constants c_1, c_2, and n_0 such that $0 \leq c_1 g(n) \leq f(n) \leq c_2 g(n)$ for all $n \geq n_0\}$.
- $\mathcal{O}(g(n)) = \{f(n) \mid$ there exist positive constants c and n_0 such that $0 \leq f(n) \leq cg(n)$ for all $n \geq n_0\}$.
- $\Omega(g(n)) = \{f(n) \mid$ there exist positive constants c and n_0 such that $0 \leq cg(n) \leq f(n)$ for all $n \geq n_0\}$.
- $o(g(n)) = \{f(n) \mid$ for any positive constant $c > 0$, there exists a constant $n_0 > 0$ such that $0 \leq f(n) < cg(n)$ for all $n \geq n_0\}$.
- $\omega(g(n)) = \{f(n) \mid$ for any positive constant $c > 0$, there exists a constant $n_0 > 0$ such that $0 \leq cg(n) < f(n)$ for all $n \geq n_0\}$.

Illustration





Example

- $3n^3 + 2n^2 + n + \log n = \Theta(n^3)$
- ~~$\mathcal{O}(1) < \mathcal{O}(\log n) < \mathcal{O}(n) < \mathcal{O}(n \log n) < \mathcal{O}\left(n^2\right) < \mathcal{O}\left(2^n\right) < \mathcal{O}(n!)$~~
- $\Theta(1) < \Theta(\log n) < \Theta(n) < \Theta(n \log n) < \Theta\left(n^2\right) < \Theta\left(2^n\right) < \Theta(n!)$

Part 6. Optimization in Machine Learning

- Supervised Learning
- Empirical Risk Minimization
- Structural Risk Minimization
- Example

Learning by Optimization

The fundamental goal of (supervised) learning: ***Risk Minimization (RM)***,

$$\min_{h \in \mathcal{H}} \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}[f(h(\mathbf{x}), y)],$$

where

- h denotes the hypothesis (model) from the hypothesis space $\mathcal{H}$.
- $(\mathbf{x}, y)$ is an instance chosen from a unknown distribution $\mathcal{D}$.
- $f(h(\mathbf{x}), y)$ denotes the loss of using hypothesis h on the instance $(\mathbf{x}, y)$.

Empirical Risk Minimization

Since the distribution of the data, i.e., $\mathcal{D}$, is unavailable to the learner, the risk is not computable.

In practice, the learner instead tries to optimize the following empirical risk, which is called ***empirical risk minimization (ERM)***:

$$\min_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} f\left(h(\mathbf{x}_i), y_i\right).$$

ERM approximates RM: All instances are i.i.d. sampled from the same distribution.

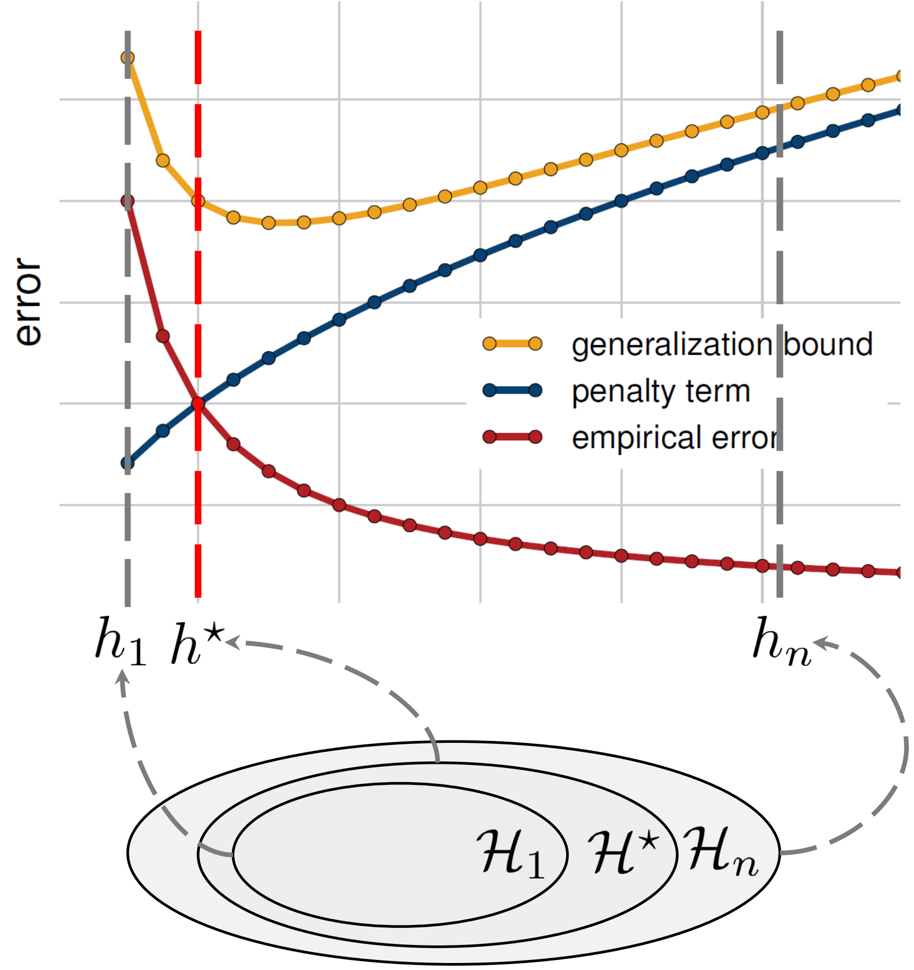
IID assumption: *Independent and Identically Distributed random variables*

Structural ERM

In practice, we often explicitly control the complexity of the learner by adding a regularization term in the optimization objective, i.e.,

$$\min_{h \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} f(h(\mathbf{x}_i), y_i) + \lambda \mathcal{R}(h).$$

This is called ***Structural ERM***.



Example

- Consider the following binary classification task with (i) linear hypothesis $h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$; and (ii) $\mathbf{x}_i \in \mathbb{R}^d$, $y_i \in \{-1, +1\}$ for all $i \in [m]$.

Example 6. Taking $f(h(\mathbf{x}_i), y_i) = \max\{0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i\}$ (hinge loss) and $\mathcal{R}(h) = \|\mathbf{w}\|_2^2$ forms the optimization objective in ***Support Vector Machine (SVM)***:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \sum_{i=1}^{n} \max\{0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i\} + \lambda \|\mathbf{w}\|_2^2 .$$

Example

- Consider the following binary classification task with (i) linear hypothesis $h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$; and (ii) $\mathbf{x}_i \in \mathbb{R}^d$, $y_i \in \{-1, +1\}$ for all $i \in [m]$.

Example 7. Taking $f(h(\mathbf{x}_i), y_i) = \log(1 + \exp(-y_i \mathbf{w}^\top \mathbf{x}_i))$ and $\mathcal{R}(h) = \|\mathbf{w}\|_2^2$ forms the optimization objective in ***Logistic Regression (LR)***:

$$\min_{\mathbf{w} \in \mathbb{R}^d} \sum_{i=1}^{n} \log(1 + \exp(-y_i \mathbf{w}^\top \mathbf{x}_i)) + \lambda \|\mathbf{w}\|_2^2 .$$

Summary

- **CALCULUS**
  - Gradient and Deritives
  - Hessian
  - Chain Rule
  - The Matrix Cookbook
- **LINEAR ALGEBRA**
  - Positive (Semi-)Definite Matrix
  - Rank
  - Inner Product
  - Norm
    - Norm
    - Matrix Norm
    - Norm Relationship
  - Cauchy-Schwarz Inequality
  - Decomposition
    - Eigen Value Decomposition
    - Singular Value Decomposition
- **PROBABILITY & STATISTICS**
  - Expectation and Variance
  - Cauchy-Schwarz Inequality in Probability
  - Conditional Expectation
  - Concentration Inequalities
- **INFORMATION THEORY**
  - Entropy
  - Conditional Entropy
  - Mutual Information
  - KL Divergence (Relative Entropy)
  - Bregman Divergence
- **OPTIMIZATION IN MACHINE LEARNING**
  - Risk Minimization
  - Empirical Risk Minimization (ERM)
  - Structural ERM

Q & A

Thanks!