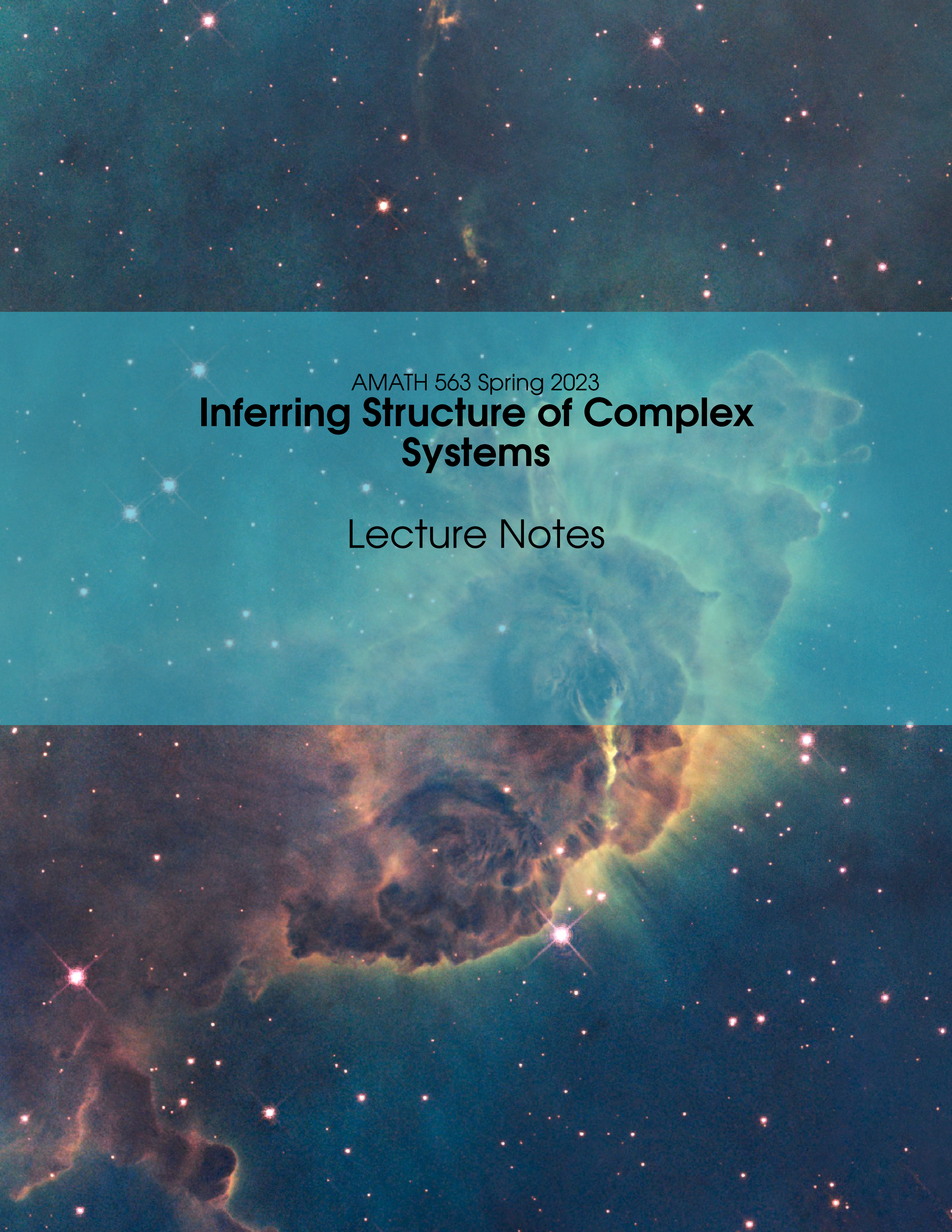


AMATH 563 Spring 2023

# Inferring Structure of Complex Systems

## Lecture Notes

*Release data, TBA*

# Contents

# 1. Convex Sets

## 1.1 Convexity

### 1.1.1 Cone

**Definition 1.1.1 — Cone.** A set $K \in \mathbb{R}^n$, when $x \in K$ implies $\alpha x \in K$.

A non convex cone can be hyper-plane.
For convex cone $x + y \in K, \forall x, y \in K$.
Cone don't need to be "pointed". e.g. [Smi13]
Direct sums of cones $C_1 + C_2 = \{x = x_1 + x_2 | x_1 \in C_1, x_2 \in C_2\}$.

■ **Example 1.1** $S_1^n\{X|X = X^n, \lambda(x) \geq 0\}$
A matrix with positive eigenvalues. ■

#### Operations preserving convexity

Intersection $C \cap_{i \in \mathbb{I}} C_i$
Linear map Let $A : \mathbb{R}^n \to \mathbb{R}^n$ be a linear map. If $C \in \mathbb{R}^n$ is convex, so is $A(C) = \{Ax \forall x \in C\}$
Inverse image $A^{-1}(D) = \{x \in \mathbb{R} | Ax \in D\}$

#### Operations that induce convexity

Convex hull on $S = \cap\{C|S \in C, Cisconvex\}$

■ **Example 1.2** $Co\{x_1, x_2, \cdots, x_m\} = \{\sum_{i=1}^m \alpha_i x_i | \alpha \in \delta_m\}$ ■

For a convex set $x \in C \Rightarrow x = \sum \alpha_i x_i$.

**Theorem 1.1.1 — Carathéodory's theorem.** If a point $x \in \mathbb{R}^d$ lies in the convex hull of a set $P$, there is a subset $P'$ of $P$ consisting of $d+1$ or fewer points such that $x$ lies in the convex hull of $P'$. Equivalently, x lies in an r-simplex with vertices in P.

## 1.2 Convex Functions

**Definition 1.2.1 — Convex function.** Let $C \in \mathbb{R}^n$ be convex, $f : C \to \mathbb{R}$ is convex on f if $x, y \in C \times C$. $\forall \alpha \in (0,1)$, $f(\alpha x + (1-\alpha)y) \leq f(\alpha x) + f((1-\alpha)y)$

**Definition 1.2.2 — Strictly Convex function.** Let $C \in \mathbb{R}^n$ be convex, $f : C \to \mathbb{R}$ is strictly convex on f if $x, y \in C \times C$. $\forall \alpha \in (0,1)$, $f(\alpha x + (1-\alpha)y) \langle f(\alpha x) + f((1-\alpha)y)$

**Definition 1.2.3 — Strongly convex.** $f : C \to \mathbb{R}$ is strongly convex with modules $u \geq 0$ if $f - \frac{1}{2}u || \cdot ||^2$ is convex.

Interpretation: There is a convex quadratic $\frac{1}{2}u|| \cdot ||^2$ that lower bounds f.

■ **Example 1.3** $\min_{x \in C} f(x) \leftrightarrow \min \bar{f}(x)$ Useful to turn this into an unconstrained problem.

$$\bar{f}(x) = \begin{cases} f(x) & if x \in C \\ \infty & elsewhere \end{cases}$$

■

**Definition 1.2.4** A function $f : \mathbb{R}^n \to \mathbb{R} \cup \infty$ $\bar{\mathbb{R}}$ is convex if $x, y \in \mathbb{R}^n \times \mathbb{R}^n$, $\forall x, y, \bar{f}(\alpha x + (1 - \alpha)y) \leq f(\alpha x) + f((1-\alpha)y)$

Definition 1 is equivalent to definition 2 if $f(x) = \infty$.

■ **Example 1.4** $f(x) = \sup_{j \in J} f_j(x)$ ■

### 1.2.1 Epigraph

**Definition 1.2.5 — Epigraph.** For $f : \mathbb{R}^n \to \bar{R}$, its epigraph $epi(f) \in \mathbb{R}^{n+1} is the set epi(f) \{(x, \alpha) | f(x) \in \alpha\}$

Next: a function is convex i.f.f. its epigraph is convex.

**Definition 1.2.6** A function $f : C \to \mathbb{R}, C \in \mathbb{R}^n$ is convex if $\forall x, y \in C$, $f(ax + (1-a)x) \leq af(x) + (1-a)f(x) \quad \forall a \in (0,1)$.
Strict convex: $x \neq y \Rightarrow f(ax + (1-a)x) \leq af(x) + (1-a)f(x)$

R $f$ is convex $\Rightarrow -f$ is concave.

Level set: $S_\alpha f = \{x | f(x) \leq \alpha\}$.
$S_\alpha f$ is convex $\Leftrightarrow f$ is convex.

**Definition 1.2.7 — Strongly convex.** $f : C \to \mathbb{R}$ is strongly convex with modules $\mu$ if $\forall x, y \in C$, $\forall \alpha \in (0,1)$, $f(ax + (1-a)x) \leq af(x) + (1-a)f(x) - \frac{1}{2\mu}\alpha(1-\alpha)||x-y||^2$.

R

- $f$ is 2nd-differentiable, $f$ ix convex $\iff \nabla^2 f(x) \rangle 0$.
- $f$ is strongly convex $\iff \nabla^2 f(x) \rangle \mu I \iff x \geq \mu$

**Definition 1.2.8 — 2.** $f : \mathbb{R}^n \to \bar{\mathbb{R}}$ is convexif $x, y \in \mathbb{R}, \alpha \in (0,1), f(ax + (1-a)x) \leq af(x) + (1-a)f(x)$.

The effective domain of $f$ is $domf = \{x | f(x) \langle +\infty\}$

■ **Example 1.5 — Iudcator function.** $\delta_c(x) = \begin{cases} 0 & x \in C \\ +\infty & elsewhere \end{cases}$.

$dom\delta_c(x) = C$ ■

**Definition 1.2.9 — Epigraph.** The epigraph of f is $epif = \{(x, \alpha) | f(x) \leq \alpha\}$

The graph of $epif$ is $\{(x, f(x) | x \in domf\}$.

**Definition 1.2.10 — III.** A function $f : \mathbb{R}^n \to \bar{\mathbb{R}}$ is

**Theorem 1.2.1** $f : \mathbb{R}^n \to \bar{\mathbb{R}}$ is convex $\iff \forall x, y \in \mathbb{R}^n, \alpha \in (0,1), f(ax + (1-a)x) \leq af(x) + (1-a)f(x)$.

*Proof.* $\Rightarrow$ take $x, y \in domf$, $(x, f(x)) \in epif$,$(y, f(y)) \in epif$. ■

■ **Example 1.6 — Distance.** Distance to a convexset $d_c(x) = \inf\{\|z - x\| | z \in C\}$. Take any two sequence $\{y_k\} and \{\bar{y}_k\} \subset C$ s.t. $\|y_k - x\| \to d_c(x)$, $\|\bar{y}_k - \bar{x}\| \to d_c(\bar{x})$. $z_k = \alpha y_k + (1-\alpha)\bar{y}_k$.

$$\begin{aligned} d_c(\alpha x + (1-\alpha)\bar{x}) &\leq \|z_k - \alpha x - (1-\alpha)\bar{x}\| \\ &= \|\alpha(y_k - x) + (1-\alpha)(\bar{y}_k - \bar{x})\| \\ &\leq \alpha\|y_k - x\| + (1-\alpha)\|\bar{y}_k - \bar{x}\| \end{aligned}$$

Take $k \to \infty$, $d_c(\alpha x + (1-\alpha)\bar{x}) \leq \alpha d(x) + (1-\alpha)d(\bar{x})$ ■

■ **Example 1.7 — Eigenvalues.** Let $X \in S^n := \{n \times nsymmetricmatrix\}$. $\lambda_1(x) \geq \lambda_2(X) \geq \ldots \geq \lambda_n(x)$.
$f_k(x) = \sum_1^n \lambda_i(x)$.
Equivalent characterization

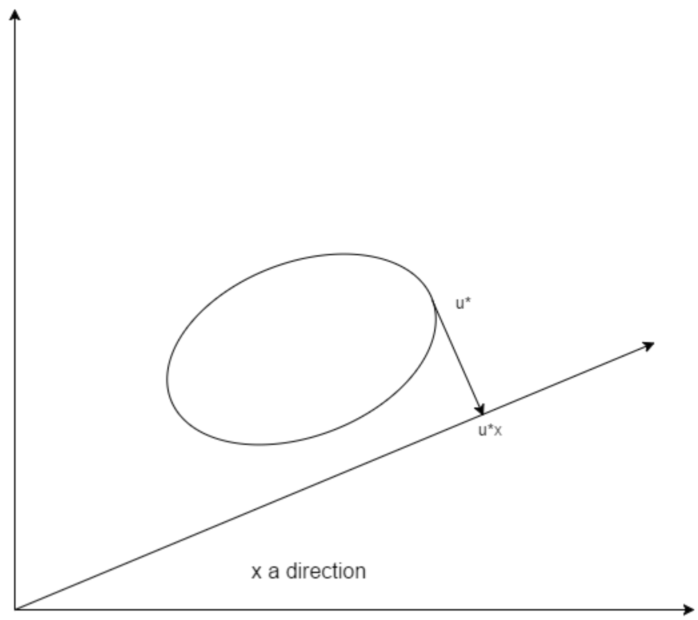
$$\begin{aligned} f_k(x) &= \max\{\sum_i v_i^T X v_i | v_i \perp v_j, i \neq j\} \\ &= \max\{tr(V^T XV | V^T V = I_k\} \end{aligned}$$

$\max\{tr(VV^T X)\}$by circularity

Note $\langle A, B\rangle = tr(A, B)$ is true for symmetric matrix.
$\langle A, A\rangle = |A|_F^2 = \sum_i A_{ii}^2$ ■

## 1.3 Support Function

Take a set $C \in \mathbb{R}^n$, not necessarily convex.The support function is $\sigma_C = \mathbb{R}^n \to \bar{\mathbb{R}}$. $\sigma_C(x) =$




$\sum\{\langle x,u\rangle | u \in C\}$.

**Fact 1.3.1** The support function binds the supporting hyper-plane.

Supporting functions are

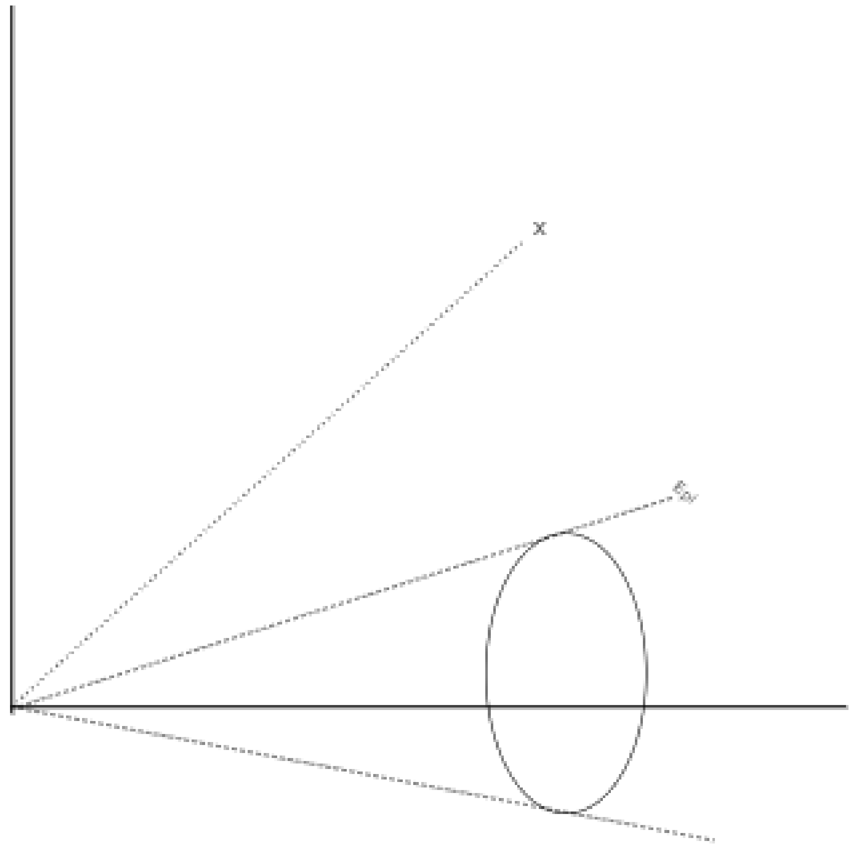
- Positively homogeneous
  $\sigma_C(\alpha x) = \alpha\sigma_C(x)\forall\alpha\rangle 0$
  $\sigma_C(\alpha x) = \sup_{u\in C}\langle \alpha x, u\rangle = \alpha \sup_{u\in C}\langle x,u\rangle = \alpha\sigma_C(x)$
- Sub-linear( a special case of convex, linear combination holds $\forall\alpha$.
  $\sigma_C(\alpha x + (1-\alpha)y) = \sup_{u\in C}\langle \alpha x + (1-\alpha)y, u\rangle \leq \alpha \sup_{u\in C}\langle x,u\rangle + (1-\alpha)\sup_{u\in C}\langle y,u\rangle$

■ **Example 1.8 — L2-norm.** $\|x\| = \sup_{u\in C}\{\langle x,u\rangle, u \in \mathbb{R}^n\}$.
$\|x\|_p = \sup\{\langle x,u\rangle, u \in B_q\}$ where $\frac{1}{p}+\frac{1}{q} = 1$. $B_q = \{\|x\|_q \leq 1\}$.
The norm is

- Positive homogeneous
- sub-linear
- If $0 \in C$, $\sigma_C$ is non-negative.
- If $C$ is central-symmetric, $\sigma_C(0) = 0$ and $\sigma_C(x) = \sigma_C(-x)$

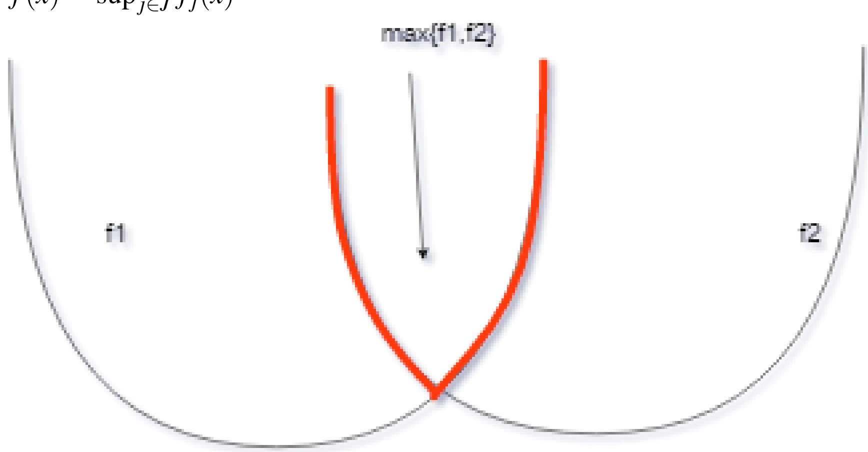
■

**Fact 1.3.2 — Epigraph of a support function.** $epi\sigma_C = \{(x,t)|\sigma_C(x) \leq t\}$. Suppose $(x,t) \in epi\sigma_C$.
Take any $\alpha > 0$. $\alpha(x,t) = (\alpha x, \alpha t)$.
$\alpha\sigma_C(x) = \alpha\sigma_C(x) \leq \alpha t$. $\alpha(x,c) \in epi\sigma_C$



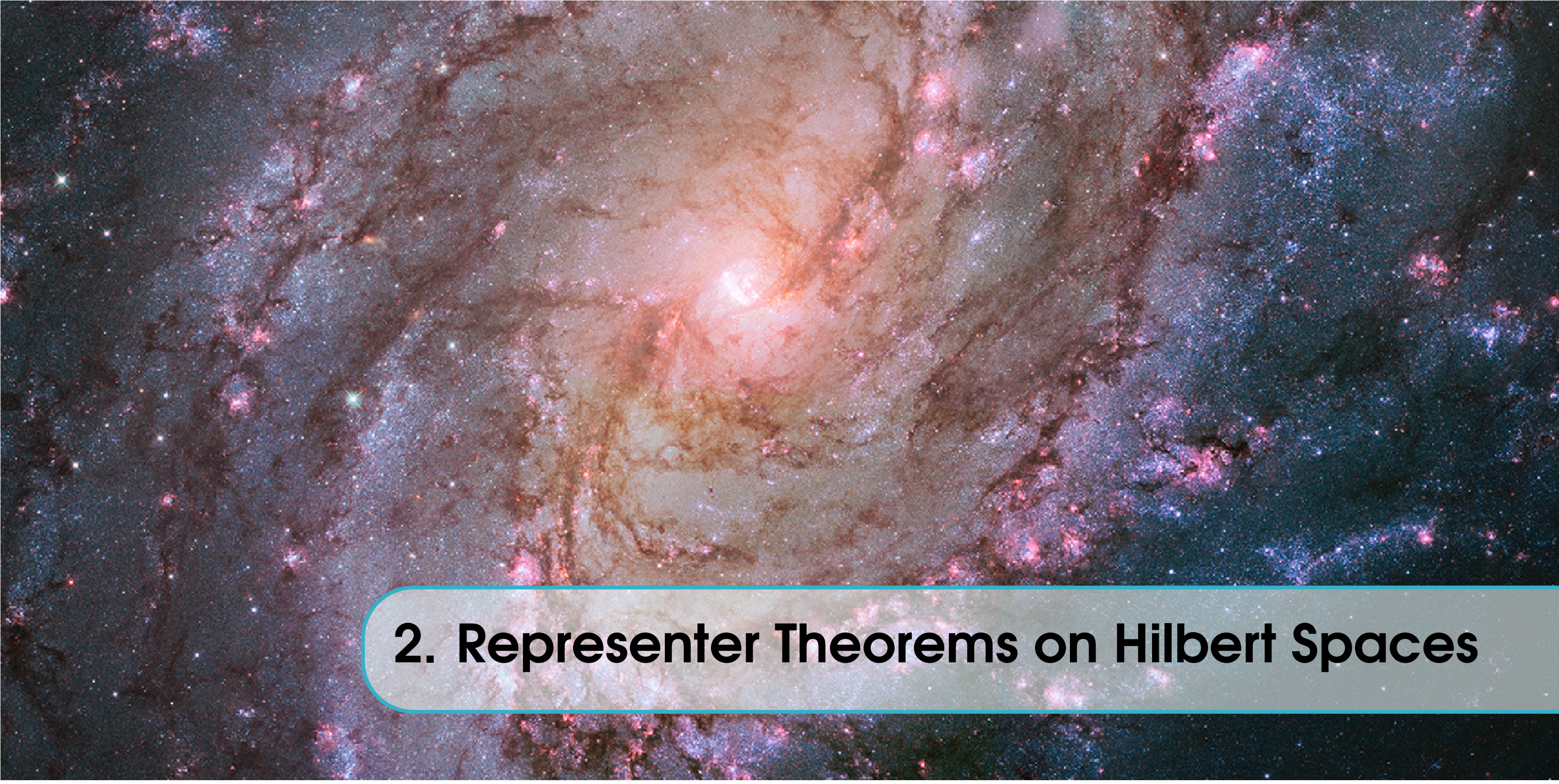

## 1.4 Operations Preserve Convexity of Functions

- Positive affine transformation
  $f_1, f_2, \ldots, f_k \in cvx\mathbb{R}^n$.
  $f = \alpha_1 f_1 + \alpha_2 f_2 + \ldots + \alpha_k f_k$
- Supremum of functions. Let $\{f_i\}_{i\in I}$ be arbitrary family of functions. If $\exists x \sup_{j\in J} f_j(x) < \infty \Leftrightarrow$ $f(x) = \sup_{j\in J} f_j(x)$




- Composition with linear map.
  $f \in cvx\mathbb{R}^n, A : \mathbb{R}^n \to \mathbb{R}^m$ is a linear map. $f \circ A(x) = f(Ax) \in cvx\mathbb{R}^n$

$$
\begin{aligned}
f \circ A(x) &= f(A(\alpha x + (1-\alpha)y)) \\
&= f(A\alpha x + (1-\alpha)Ay) \\
&\leq \alpha f(Ax) + (a-\alpha)f(Ay)
\end{aligned}
$$



# 2. Representer Theorems on Hilbert Spaces

■ **Example 2.1** Optimal recovery in $L^2([-\pi,\pi])$
Let $h_0 = \frac{1}{\sqrt{2\pi}}, h_j(x) = \frac{1}{\sqrt{\pi}}\cos(j\pi x)$ for $j = 1,\cdots,n$. Consider the optimization problem
$\min_{L^2} J(h) = \sum_{j=0}^{n} |\int_{-\pi}^{\pi} h(t)h_j(t)dt - y_j| + \|h\|^2_{L^2([-\pi,\pi])}$.
Apply representer theorem to get, $\tilde{h} = \sum_{j=1}^{n} \alpha_j h_j$. In fact, here the $h_j$ are an orthonormal set and so, we have the $n$-dimensional problem, $\min J(\alpha) = \sum_{j=0}^{n} |\alpha_j - y_j| + \|\alpha\|_2^2$.
■

While the representer theorem is quite powerful, it may seem limited at first since we require the "measurements" to be of the form $\langle h, h_j\rangle$. However, the result can be generated to all bounded linear functionals on $H$ thanks to Riesz representation theorem. (This is a different representation theorem.)

**Theorem 2.0.1 — Riesz representation theorem.** Every bounded linear functional $\phi$ on a Hilbert space $H$ (ie $\phi \in H^*$) can be represented in terms of the $H$-inner product $\phi(h) = \langle \hat{\phi}, h\rangle$ where $\hat{\phi} \in H$ depends on $\phi$, it is uniquely determined by $\phi$ and satisfies $\|\hat{\phi}\|^2 = \|\phi\|_*$

Since the Riesz representation theorem allows us to identify bounded linear functionals with inner product with elements of the Hilbert space, we can now generalize our representation theorem to the following form:

**Theorem 2.0.2** Let $H(\cdot, \|\cdot\|, \langle\cdot,\cdot\rangle)$ be a Hilbert space and consider the optimization problem, $\min_{h\in H} J(h) = L(\phi_1(h),\ldots,\phi_n(h)) + R(\|h\|)$ where $\phi_j \in H^*$ are fixed and $R : \mathbb{R} \mapsto \mathbb{R}$ is non-decreasing. Then if $J$ admits minimizers, then it has at least one minimizer $\tilde{h}$ of the form

$\tilde{h} = \sum_{j=1}^{n} \alpha_j \hat{\phi}_j$, where the $\hat{\phi}_j$ are the Riesz representers of $\phi_j$.

*Proof.* Apply Riesz's representation theorem to write $\phi_j(h) = \langle h, \hat{\phi} \rangle$ and apply the original representation theorem. ■

This form of the representation theorem is very useful in our study of reproducing kernel Hilbert spaces (RKHS's) where the $\hat{\phi}$ often here are simple and convenient forms in terms of a Kernel function.

# 3. Lecture 8: Representer Theorems in RKHSs

## 3.1 Representer Theorem and Formula in RKHSs

**Theorem 3.1.1 — Representer Theorem.** Suppose $(H, \langle\cdot,\cdot\rangle, \|\cdot\|)$ is a Hilbert space and $R : \mathbb{R} \to \mathbb{R}$ is non-decreasing. Then if

$$J(h) = L(\langle h_1, h\rangle, \ldots, \langle h_n, h\rangle + R(\|h\|)$$

has a minimizer, there exists at least one minimizer $h^* \in \operatorname{span}\{h_1, \ldots, h_n\}$.

Since RKHSs satisfy the reproducing property–$f \in \mathscr{H}$, $f(x) = \langle f, K(x,\cdot)\rangle$– we can immediately obtain a very useful version of the representer theorem.

**Theorem 3.1.2** Let $H$ be an RKHS with kernel $K : \mathscr{X} \times \mathscr{X} \to \mathbb{R}$. Let $X = \{x_1, \ldots, x_n\} \subset \mathscr{X}$ and consider $J : H \to \mathbb{R}$,

$$J(h) = L(\langle h_1, h\rangle, \ldots, \langle h_n, h\rangle + R(\|h\|),$$

where $R : \mathbb{R} \to \mathbb{R}$ is non-decreasing. If $J$ has a minimizer, there exists at least one minimizer $h^*$ such that

$$h^* = \sum_{i=1}^{n} \alpha_i^* K(x_i, \cdot)$$

Since we now have an ansatz for $h^*$ we can now compute $h^*$ in two ways! First observe that

$$\|h^*\|^2 = \langle h^*, h^*\rangle = \langle \sum_i \alpha_i^* K(x_i,\cdot), \sum_j \alpha_j^* K(x_j,\cdot)\rangle = \sum_{ij} \alpha_i^* \alpha_j^* K(x_i, x_j) = (\alpha^*)^T K(X,X)\alpha^*.$$

Furthermore,

$$h^* = \sum_{i=1}^{n} \alpha_i^* K(x_i, \cdot) = K(x, X)\alpha^*$$

where we introduced the vector field

$$K(x,X) = (K(x_1,x),\dots,K(x_n,x)) \in H^{\otimes n}.$$

We obtain the following corollary. Every vector $\alpha^* \in \mathbb{R}^n$ that is a minimizer of

$$J(\alpha) = L(K(x_1,X)\alpha,\dots,K(x_n,X)\alpha) + R(\alpha^T K(X,X)\alpha) \tag{3.1}$$

is associated with the minimizer $h^*$ of $J(h)$ of the form $h^* = K(x,X)\alpha^*$. Observe that 3.1 can be easily implemented numerically and often solved using "off the shelf" optimization algorithms. In the setting where $K(X,X)$ is invertible we can characterize $h^*$ in yet another way which proves to be quite useful in practice. Define

$$x_i \in \mathscr{X}, \quad z_i^* \equiv h^*(x_i) = K(x_i,X)\alpha.$$

Then we have for $\mathbf{z}^* \equiv (z_1,\dots,z_n)^T$,

$$\mathbf{z}^* = K(X,X)\alpha^* \to \alpha^* = K(X,X)^{-1}\mathbf{z}^*.$$

This implies immediately that

$$\|h^*\|^2 = (\alpha^*)^T K(X,X)\alpha^* = (\mathbf{z}^*)^T K(X,X)^{-1}\mathbf{z}^*.$$

So, by substitution in 3.1, we obtain the corollary:

**Corollary 3.1.3 — Representer formula.** Every vector $\mathbf{z}^* \in \mathbb{R}^n$ that is a minimizer of

$$J(\mathbf{z}) = L(\mathbf{z}) + R(\mathbf{z}^T K(X,X)\mathbf{z})$$

is associated with a minimizer $h^*$ of $J(h)$ given by the formula

$$h^*(x) = K(x,X)K(X,X)^{-1}\mathbf{z}^* \tag{3.2}$$

The above corollary is what is often referred to as "the representer theorem" in ML literature on kernel methods, and 3.2 is often called the representer formula.

## 3.2 Application to supervised learning

Consider input and output spaces $X$ and $Y$, respectively. The goal of supervised learning is to approximate/learn a function $f^t : X \to Y$ given a "training data set" of the form $\{(x_i,y_i)\}_{i=1}^n$. For simplicity, let us assume $Y \equiv \mathbb{R}$ so that the $\mathbf{y} = (y_1,\dots,y_n) \in \mathbb{R}^n$ and suppose $X$ is a Banach space. We will derive our approximatin to $f^t$ within an RKHS.

- (**Step 1**) Pick a kernel $K : X \times X \to \mathbb{R}$. A simple choice is the RBF kernel

$$K(x,x') = \exp(-\gamma||x-x'||_X^2)$$

- (**Step 2**) Pick a regularization term

$$R(||f||) = \frac{\lambda}{2}||f||^2, \qquad \lambda > 0$$

  where $||\cdot||$ is the RKHS norm.

- (**Step 3**) Pick a loss function, such as mean squared error.

$$L(f) = \frac{1}{2N}\sum_{j=1}^{N}|f(x_i) - y_i|^2$$

- (**Step 4**) Formulate the optimization problem

$$\min_{f\in\mathscr{H}_k} J(f) := L(f) + \frac{\lambda}{2}||f||^2$$

- (**Step 5**) Apply the representer theorem. We have

$$h^* = K(\cdot,X)K(X,X)^{-1}\mathbf{z}^*$$

  where

$$\mathbf{z}^* = \arg\min_{\mathbf{z}\in\mathbb{R}^n} \frac{1}{2N}||\mathbf{z}-\mathbf{y}||^2 + \frac{\lambda}{2}\mathbf{z}^T K(X,X)^{-1}\mathbf{z}$$

  Since the functional is quadratic, we can solve using the first order optimization condition

$$\mathbf{z}^* - \mathbf{y} + N\lambda K(X,X)^{-1}\mathbf{z}^* = 0 \qquad \Rightarrow \qquad \mathbf{z}^* = (K(X,X)+N\lambda I)^{-1}K(X,X)\mathbf{y}$$

  Substituting this back into the representer formula gives us

$$h^*(x) = K(x,X)K(X,X)^{-1}(K(X,X)+N\lambda I)^{-1}K(X,X)\mathbf{y}$$

In practice, $K(X,X)$ can become very ill-posed. So, we regularize it using a **nugget term**:

$$K(X,X)^{-1} \to \left(K(X,X)+\sigma^2 I\right)^{-1}$$

where $\sigma^2 > 0$ is a small parameter.

# Bibliography


[Smi13] James Smith. "Article title". In: 14.6 (2013), pages 1–8.