Lecture 18: Functional Calculus

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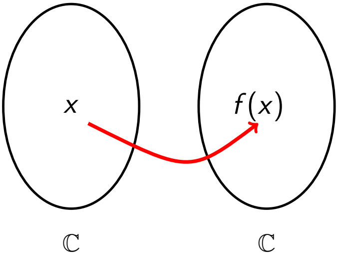
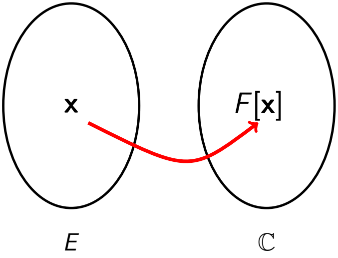
Functionals

- Function: Map complex number x onto complex number $f(x)$
- Domain and range are both $\mathbb{C}$



- Function**al**: Map vector $\mathbf{x}$ onto complex number $F[\mathbf{x}]$
- Domain is vector space E, range is $\mathbb{C}$
- Functionals over a d-dimensional vector space are simply multivariate functions of d variables



Linear Functionals

- A linear functional $L : E \to \mathbb{C}$ satisfies $\forall \mathbf{x}_1, \mathbf{x}_2 \in E, \forall \alpha, \beta \in \mathbb{C}$
  (i) $L[\mathbf{x}_1 + \mathbf{x}_2] = L[\mathbf{x}_1] + L[\mathbf{x}_2]$
  (ii) $L[(\alpha + \beta)\mathbf{x}]] = \alpha L[\mathbf{x}] + \beta L[\mathbf{x}]$
- Riesz: Every linear functional on an inner product space E is representable by an inner product,

$$L_{\boldsymbol{\xi}}[\mathbf{x}] = \langle \boldsymbol{\xi} | \mathbf{x} \rangle \,,$$

  where $\boldsymbol{\xi}$ labels L. The converse also holds, i.e., every inner product is a linear functional.
- "bra" vectors are linear functionals on E. They also form a linear space, E^*, the dual of E.

Functional Derivative

- The (first) functional derivative of $F : E \to \mathbb{C}$ at $\mathbf{x}$ is the "bra" vector

$$\frac{\delta F}{\delta \mathbf{x}} \equiv \mathbf{y}^\dagger \in E^*.$$

- Definition: $\forall \mathbf{u} \in E, \forall \lambda \in \mathbb{R}$,

$$\langle \mathbf{y} | \mathbf{u} \rangle = \left. \frac{d}{d\lambda} F[\mathbf{x} + \lambda \mathbf{u}] \right|_{\lambda=0}$$

- Generalizes the (total) derivative of a multivariate function
- The functional derivative of a linear functional is its defining "bra" vector,

$$\frac{\delta}{\delta \mathbf{x}} \langle \boldsymbol{\xi} | \mathbf{x} \rangle = \langle \boldsymbol{\xi} |$$

Variational Principle

- Linear variational method: The solutions of the stationary Schrödinger equation

$$\hat{H}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$$

are exactly given by the stationary points of the energy functional

$$E[\Psi] = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}.$$

- The stationary points are the energy eigenvalues E_n, and the the corresponding stationarizing states are the eigenstates Ψ_n.
- The ground state energy is the minimum of $E[\Psi]$,

$$E_0 = \min_{\Psi\in H} E[\Psi].$$

- For a normalized "trial" ground state wavefunction Φ_0, the error in E_0 is quadratic in $\|\Psi_0 - \Phi_0\|$.