Kernels

CPSC 532S: Modern Statistical Learning Theory
7 March 2022
cs.ubc.ca/~dsuth/532S/22/

$f(x) = w^T x$

$\text{sigh}(w^T x) \in \{\pm 1\}$

fiddle at 0

Hard SVM Duality

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called **weak (Lagrange) duality;**

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$$\|w\| = \left(\sum_{i=1}^{n} \alpha_i y_i x_i\right)^2$$

$$= \sum_i \sum_j \alpha_i \alpha_j y_i y_j x_i^\top x_j$$

$$= \max_{\alpha_i \geq 0} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i y_i x_i^\top x_j y_j \alpha_j$$

$$\sum_i \alpha_i y_i x_i^\top \left(\sum_j \alpha_j y_j x_j\right)$$

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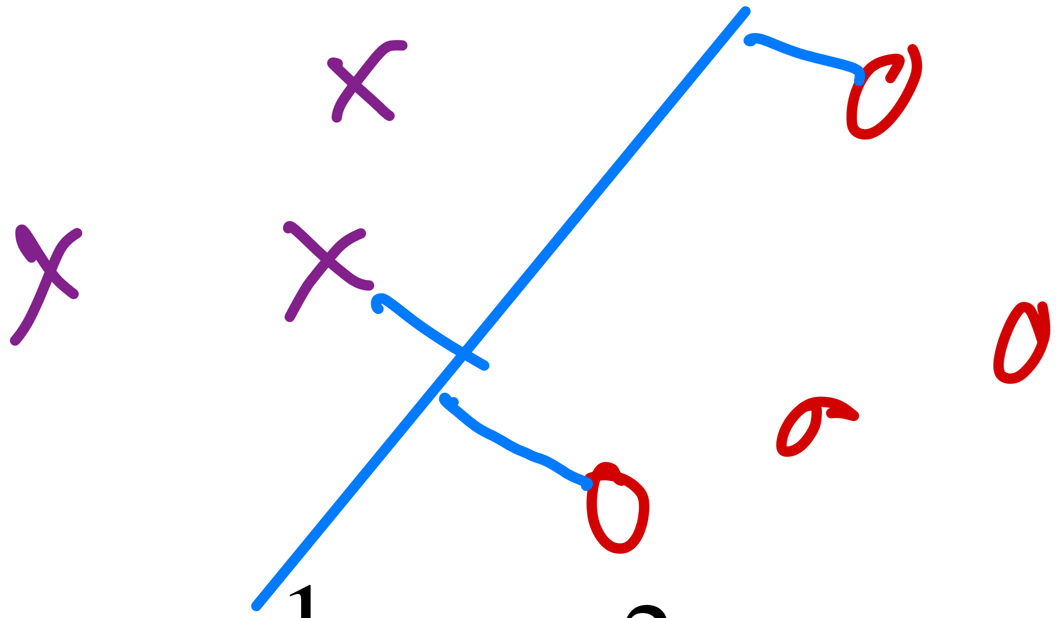
$$w = X^\top \operatorname{diag}(y)\alpha \qquad w^\top x = \alpha^\top \operatorname{diag}(y) \overbrace{X}^{n\times d} \overbrace{x}^{d\times 1}$$



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$$w = X^\top \operatorname{diag}(y) \alpha \qquad w^\top x = \alpha^\top \operatorname{diag}(y) X x$$

α_i is zero if $y_i w^\top x_i > 1$

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$$\min_{w,\xi} \lambda \|w\|^2 + \frac{1}{n} \sum_i \xi_i \quad \text{s.t. } \forall i, \; y_i w^\top x_i \geq 1 - \xi_i, \;\; \xi_i \geq 0$$

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$$2\lambda w - X^\top \operatorname{diag}(y)\alpha = 0$$

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change variables: $2\lambda\tilde{\alpha} = \alpha$

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Only difference from hard SVM is upper bound on $\tilde{\alpha}_i$

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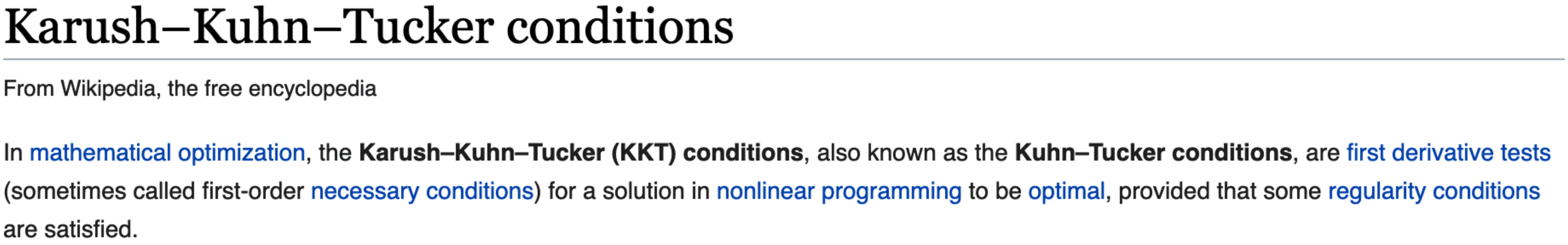
Can do with b also:
add $\alpha^\top y = 0$ constraint,
set $b = w^\top x_i - y_i$ for any SV

FYI



Karush–Kuhn–Tucker conditions

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In mathematical optimization, the **Karush–Kuhn–Tucker (KKT) conditions**, also known as the **Kuhn–Tucker conditions**, are first derivative tests (sometimes called first-order necessary conditions) for a solution in nonlinear programming to be optimal, provided that some regularity conditions are satisfied.

- Summarize the process of going through Lagrange duality for you
    - Like Lagrange multipliers, but allow inequality constraints
- Make things a lot faster once you're familiar with them
- Related conditions for when strong duality holds
    - Especially important: "Slater's condition"

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- Machine learning! ...but how do we actually do it?
- Linear models! $f(x) = w_0 + wx$, $\hat{y}(x) = \textbf{sign}(f(x))$

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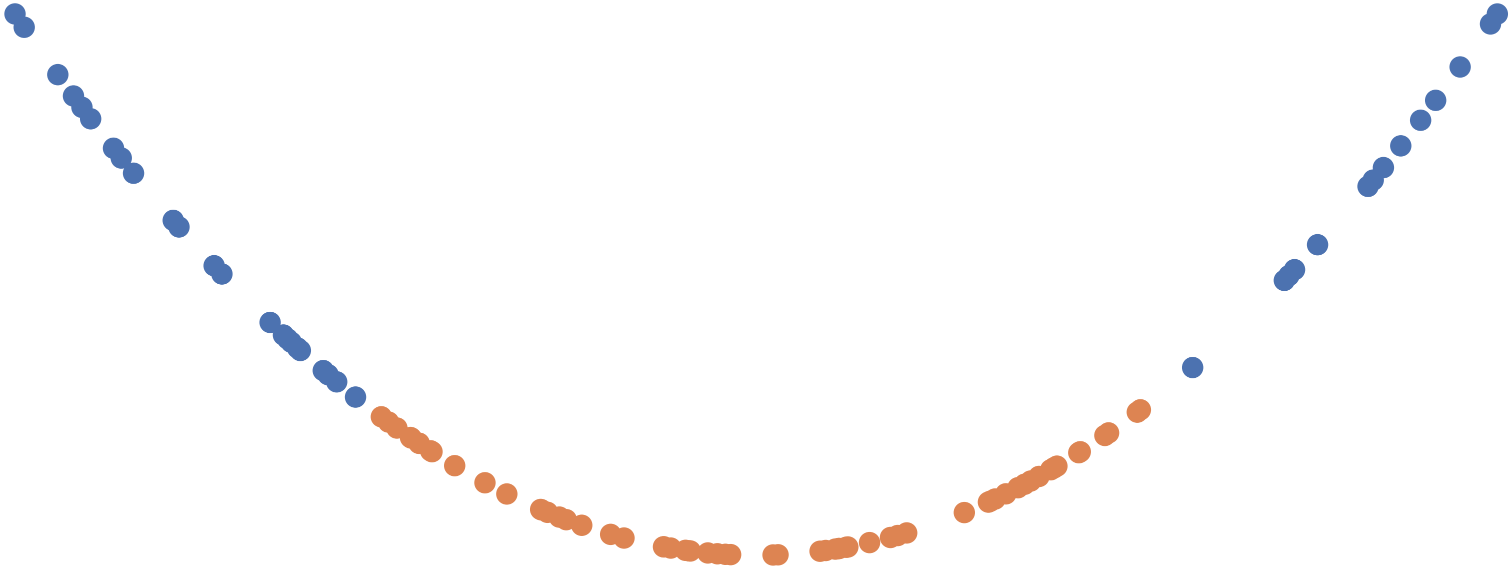

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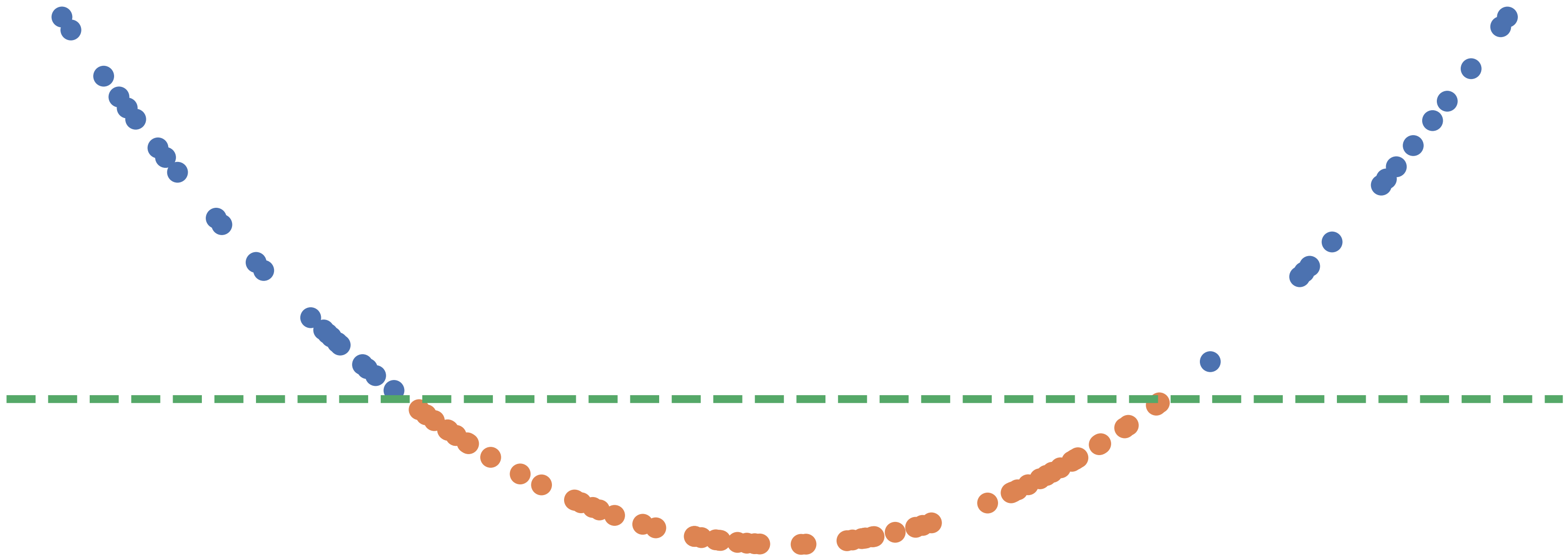

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- ϕ will live in a *reproducing kernel Hilbert space*

Hilbert spaces

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  - $\langle \alpha_1 f_1 + \alpha_2 f_2, g \rangle_{\mathcal{H}} = \alpha_1 \langle f_1, g \rangle_{\mathcal{H}} + \alpha_2 \langle f_2, g \rangle_{\mathcal{H}}$
  - $\langle f, g \rangle_{\mathcal{H}} = \langle g, f \rangle_{\mathcal{H}}$
  - $\langle f, f \rangle_{\mathcal{H}} > 0$ for $f \neq 0$, $\langle 0, 0 \rangle_{\mathcal{H}} = 0$

$\mathbb{R}^d \quad \langle a, b \rangle_{\mathbb{R}^d} = a^T b$

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  Induces a **norm**: $\|f\|_{\mathcal{H}} = \sqrt{\langle f, f \rangle_{\mathcal{H}}}$
- Complete: "well-behaved" (Cauchy sequences have limits in $\mathcal{H}$)

$x_1, x_2, x_3, x_4, \cdots$

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- $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel on $\mathcal{X}$ if there exists a Hilbert space $\mathcal{H}$ and a *feature map* $\phi : \mathcal{X} \to \mathcal{H}$ so that

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- *Linear kernel* on $\mathbb{R}^d$: $k(x, y) = \langle x, y \rangle_{\mathbb{R}^d}$

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$$= \langle \varphi_1(x), \varphi_1(y) \rangle_{\mathcal{H}_1} + \langle \varphi_2(x), \varphi_2(y) \rangle_{\mathcal{H}_2}$$

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- Is $k_1(x, y) - k_2(x, y)$ necessarily a kernel?
    - Take $k_1(x, y) = 0$, $k_2(x, y) = xy$, $x \neq 0$.
    - Then $k_1(x, x) - k_2(x, x) = -x^2 < 0$
    - But $k(x, x) = \|\phi(x)\|^2_{\mathcal{H}} \geq 0$.

Positive definiteness

- A symmetric function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is *positive semi-definite (psd)* if for all $n \geq 1$, $a_1, \ldots, a_n \in \mathbb{R}^n$, $x_1, \ldots, x_n \in \mathcal{X}^n$,

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- Equivalently: *kernel matrix* K is PSD

$$K := \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \ldots & k(x_1, x_n) \\ k(x_2, x_1) & k(x_2, x_2) & \ldots & k(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \ldots & k(x_n, x_n) \end{bmatrix}$$

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- Hilbert space kernels are psd
- psd functions are Hilbert space kernels
  - Moore-Aronszajn Theorem; we'll come back to this

Some more ways to build kernels

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  - Let $V \sim \mathcal{N}(0, K_1)$, $W \sim \mathcal{N}(0, K_2)$ be independent
  - $\operatorname{Cov}(V_i W_i, V_j W_j) = \operatorname{Cov}(V_i, V_j) \operatorname{Cov}(W_i, W_j) = k_\times(x_i, x_j)$
  - Covariance matrices are psd, so $k_\times$ is too

Schur's Theorem

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  $\left(x^\mathsf{T} y + c\right)^n$, the **polynomial kernel**

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    - $k_{\exp}(x, y) = \lim_{N\to\infty} \sum_{n=0}^{N} \frac{1}{n!} k(x, y)^n$

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    - Use the feature map $x \mapsto f(x)\phi(x)$

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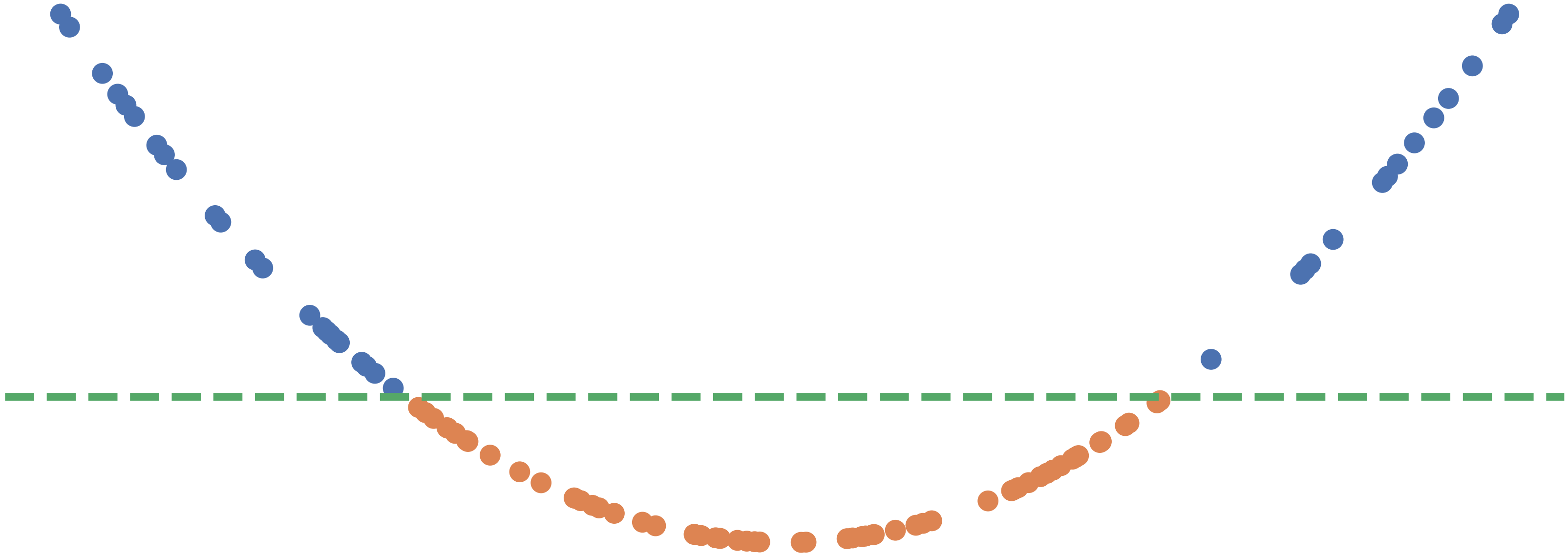

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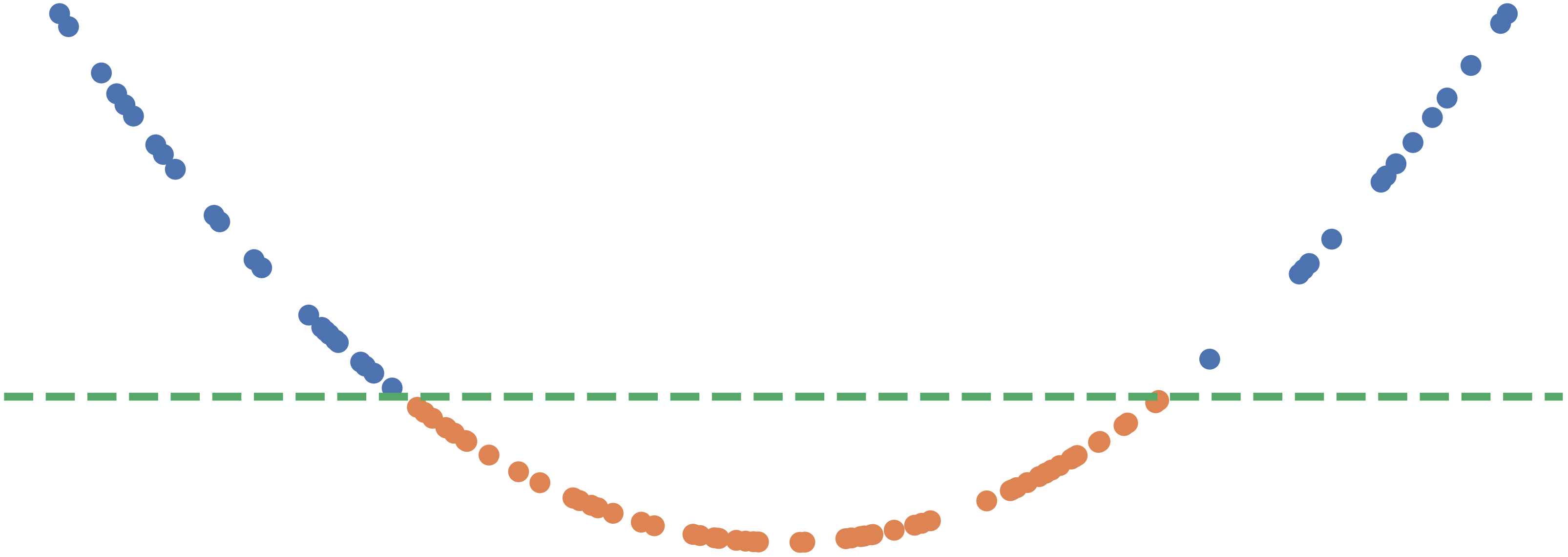

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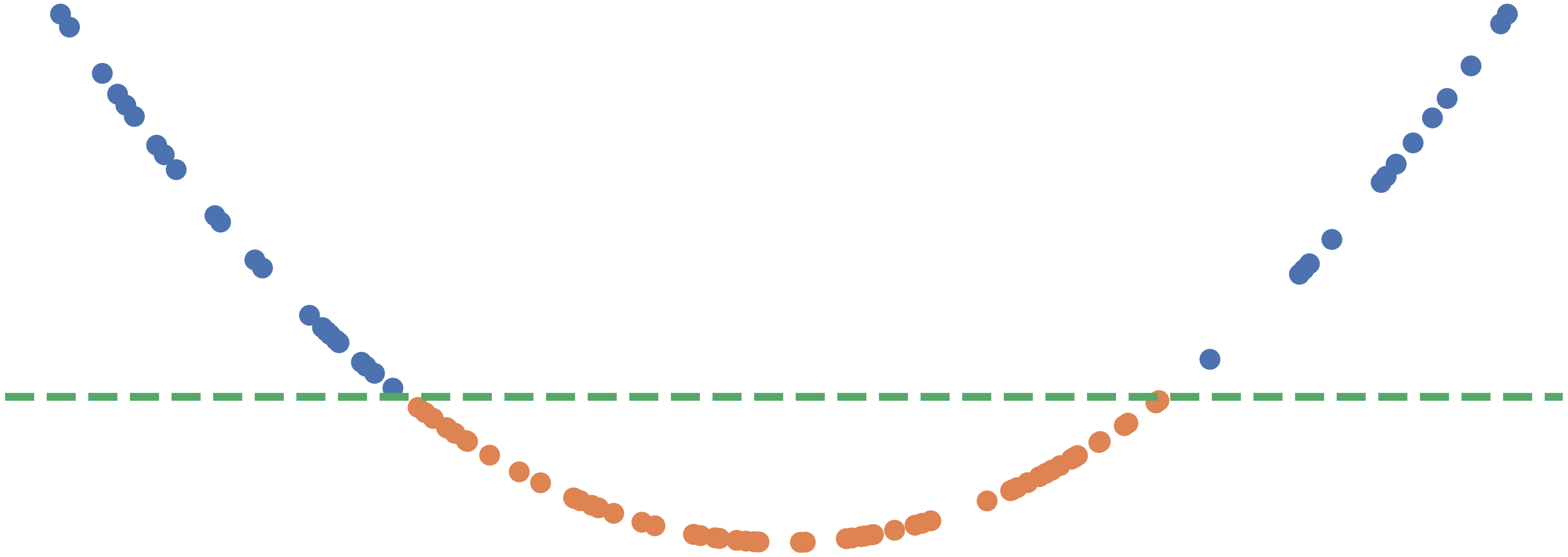

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Reproducing kernel Hilbert space (RKHS)

- Every psd kernel k on $\mathcal{X}$ defines a (unique) Hilbert space, its RKHS $\mathcal{H}$, and a map $\phi : \mathcal{X} \to \mathcal{H}$ where
    - $$k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$$
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- $k(x, \cdot)$ is the **evaluation functional**

  An RKHS is defined by it being *continuous*, or

  $$|f(x)| \leq M_x \|f\|_{\mathcal{H}}$$

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- Theorem: k is psd iff it's the reproducing kernel of an RKHS

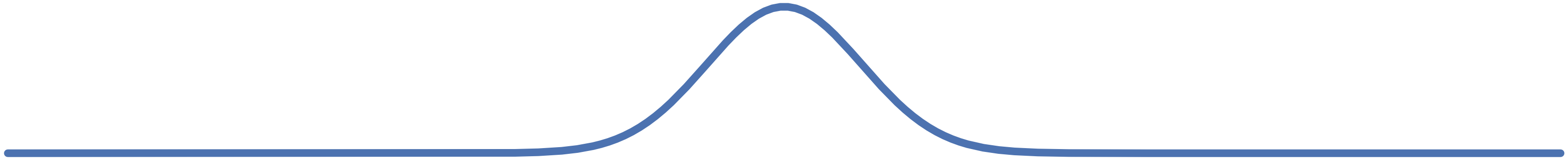
A quick check: linear kernels

- $k(x, y) = x^{\top} y$ on $\mathcal{X} = \mathbb{R}^d$
- If $f(y) = \sum_{i=1}^{n} a_i k(x_i, y)$, then $f(y) = \left[\sum_{i=1}^{n} a_i x_i\right]^{\top} y$
- Closure doesn't add anything here, since $\mathbb{R}^d$ is closed
- So, linear kernel gives you RKHS of linear functions
- $\|f\|_{\mathcal{H}} = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j k(x_i, x_j)} = \|\sum_{i=1}^{n} a_i x_i\|$

More complicated: Gaussian kernels

$$k(x, y) = \exp(\frac{1}{2\sigma^2}\|x - y\|^2)$$

- $\mathcal{H}$ is *infinite-dimensional*



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$\langle k(x+\xi \cdot) - k(x;\cdot), f \rangle_{\mathcal{H}}$

$$f(x+t) - f(x) \leq \|k(x+t,\cdot) - k(x',\cdot)\|_{\mathcal{H}}\|f\|_{\mathcal{H}}$$

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- Can say lots more with Fourier properties