Kernel Methods: From Basics to Modern Applications

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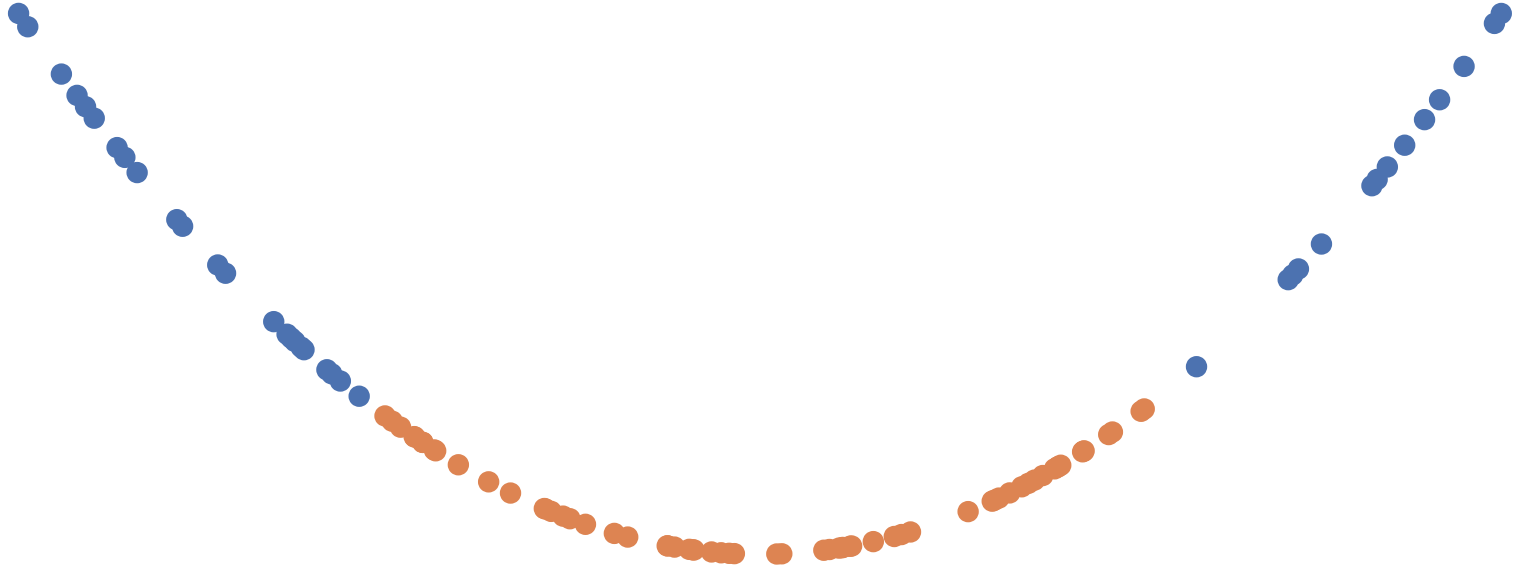

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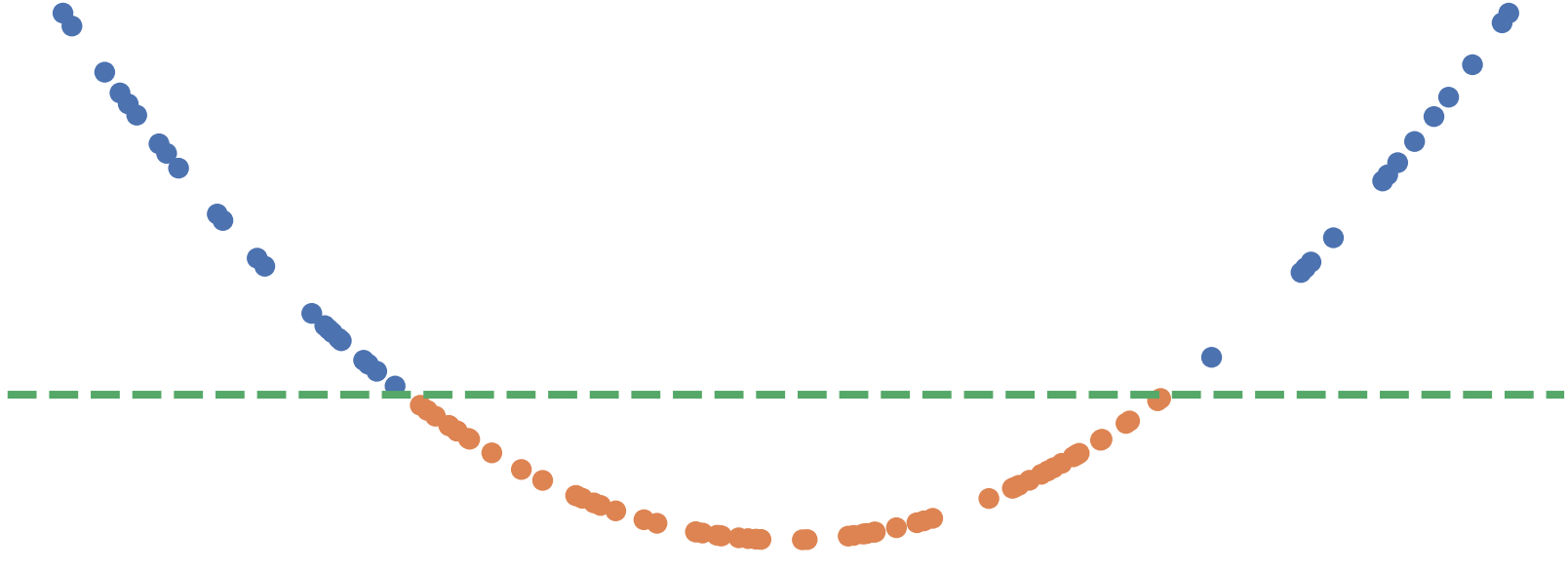

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- ϕ will live in a *reproducing kernel Hilbert space*

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  - $\langle f, g \rangle_{\mathcal{H}} = \langle g, f \rangle_{\mathcal{H}}$
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- Complete: "well-behaved" (Cauchy sequences have limits in $\mathcal{H}$)

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

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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 $k(x, x) = \|\phi(x)\|_{\mathcal{H}}^2 \geq 0$.

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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$$\begin{aligned} \sum_{i=1}^{n} \sum_{j=1}^{n} \langle a_i \phi(x_i), a_j \phi(x_j) \rangle_{\mathcal{H}} &= \left\langle \sum_{i=1}^{n} a_i \phi(x_i), \sum_{j=1}^{n} a_j \phi(x_j) \right\rangle_{\mathcal{H}} \\ &= \left\| \sum_{i=1}^{n} a_i \phi(x_i) \right\|_{\mathcal{H}}^2 \geq 0 \end{aligned}$$

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

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

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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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$$\frac{1}{\sigma^2} x^\mathsf{T} y$$

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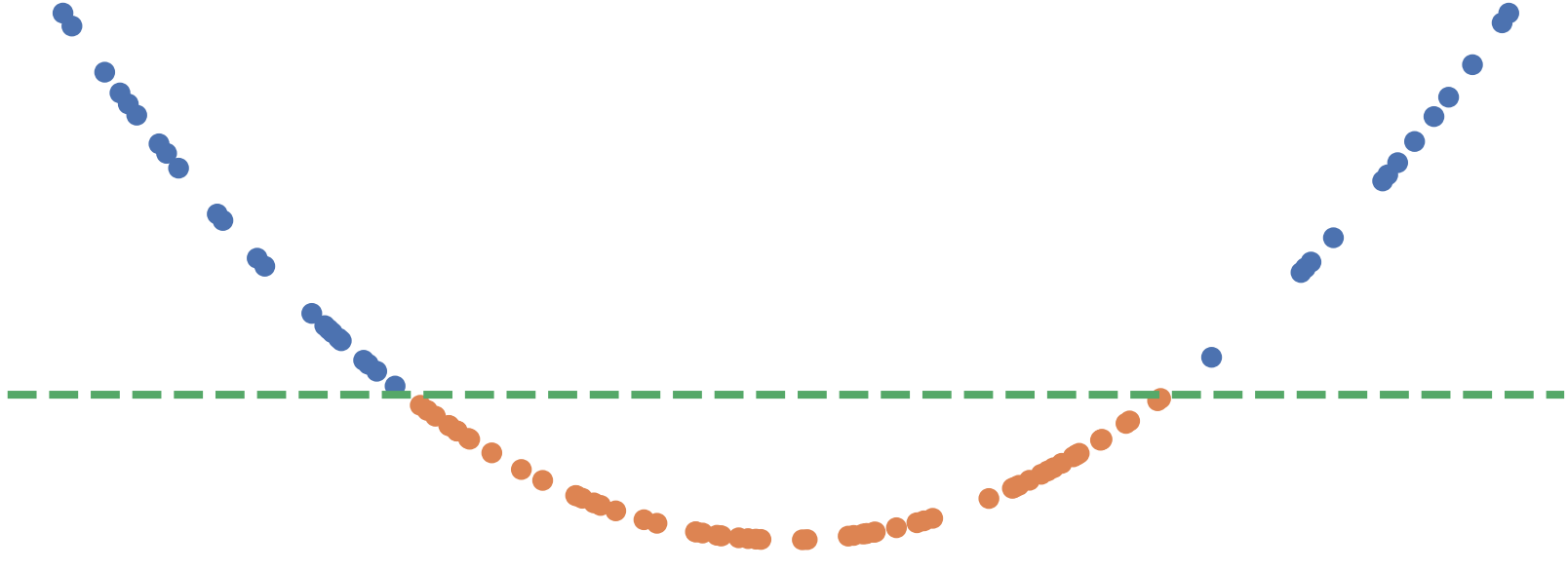

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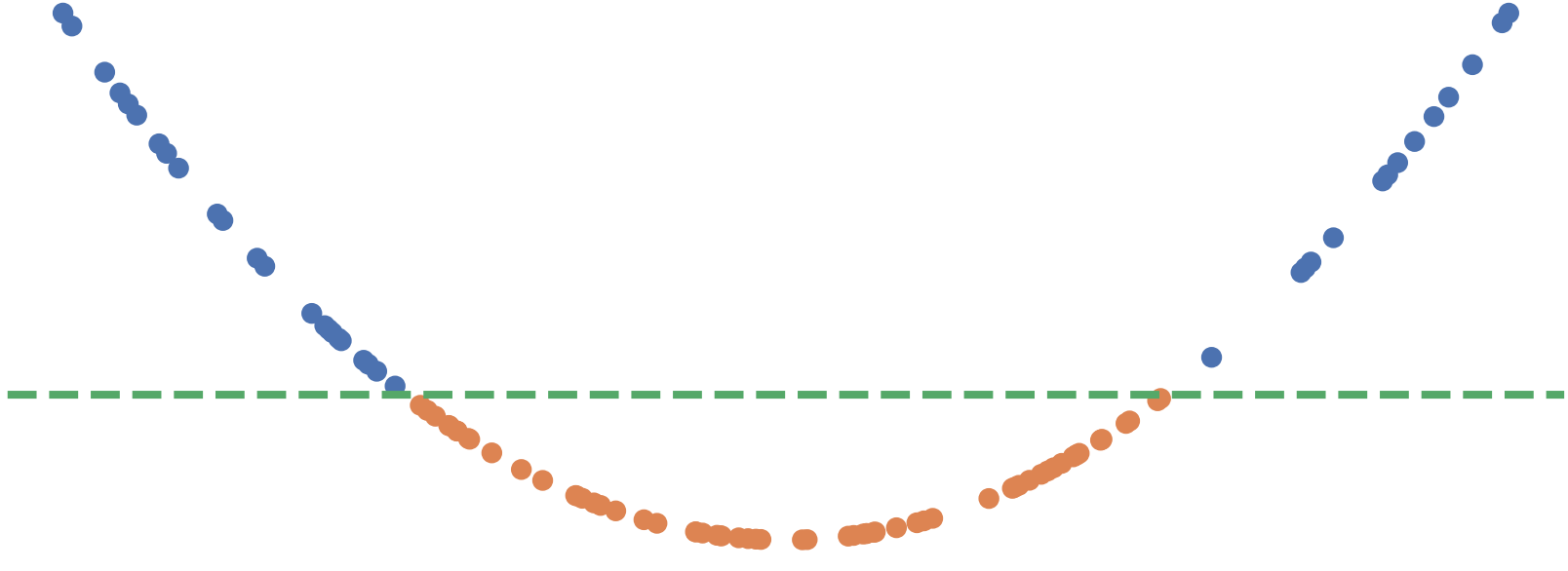

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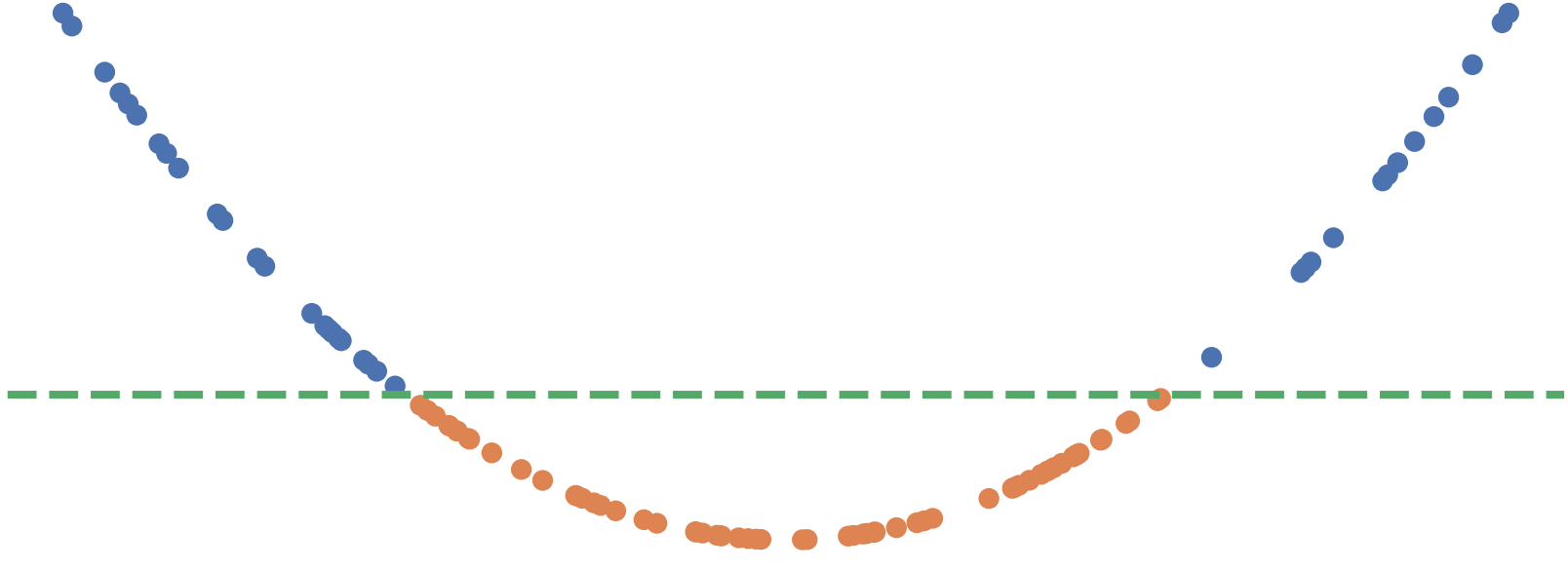

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Reproducing kernel Hilbert space (RKHS)

- 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
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- Combining the two, we sometimes write $k(x, \cdot) = \phi(x)$
- $k(x, \cdot)$ 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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  - Can also show uniqueness
- Theorem: k is psd iff it's the reproducing kernel of an RKHS

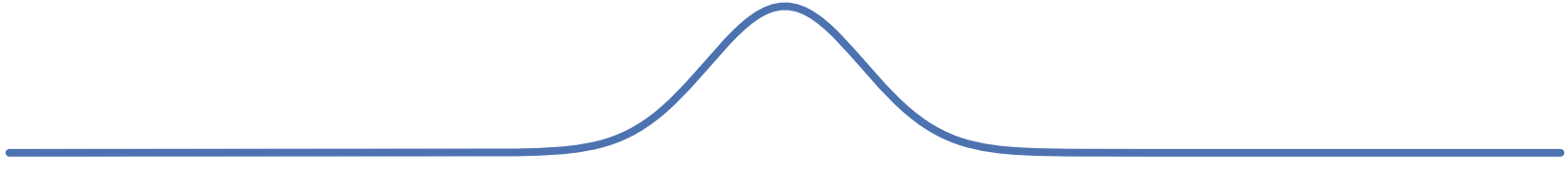
A quick check: linear kernels

- $k(x, y) = x^\mathsf{T} y$ on $\mathcal{X} = \mathbb{R}^d$
- If $f(y) = \sum_{i=1}^{n} a_i k(x_i, y)$, then $f(y) = [\sum_{i=1}^{\infty} a_i x_i]^\mathsf{T} y$
- 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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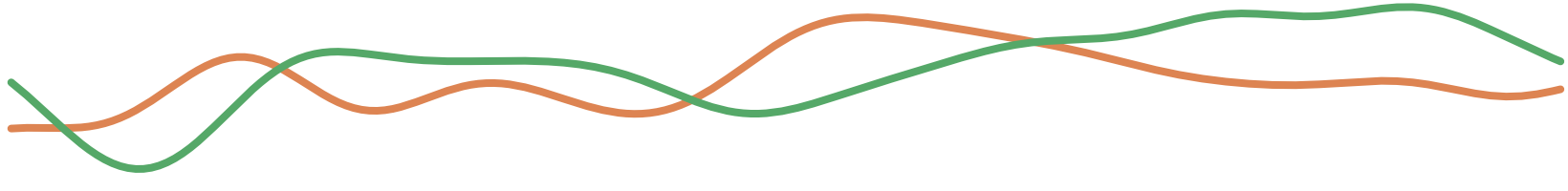

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- Can say lots more with Fourier properties

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Linear kernel gives normal ridge regression:

$$\hat{f}(x) = \hat{w}^{\mathsf{T}} x; \quad \hat{w} = \operatorname*{arg\,min}_{w \in \mathbb{R}^d} \sum_{i=1}^{n} (w^{\mathsf{T}} x_i - y_i)^2 + \lambda \|w\|^2$$

Nonlinear kernels will give nonlinear regression!

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- Minimizer needs $f_\perp = 0$, and so $\hat{f} = \sum_{i=1}^n \alpha_i k(x_i, \cdot)$

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How to find $\hat{f}$? **Representer Theorem**: $\hat{f} = \sum_{i=1}^{n} \hat{\alpha}_i k(x_i, \cdot)$

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\hat{\alpha} &= \arg\min_{\alpha \in \mathbb{R}^n} \alpha^\mathsf{T} K^2 \alpha - 2 y^\mathsf{T} K \alpha + y^\mathsf{T} y + n\lambda \alpha^\mathsf{T} K \alpha \\
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Setting derivative to zero gives $K(K + n\lambda I)\hat{\alpha} = Ky$,

satisfied by $\hat{\alpha} = (K + n\lambda I)^{-1} y$

Other kernel algorithms

- Representer theorem applies if R strictly increasing:

$$\min_{f \in \mathcal{H}} L(f(x_1), \cdots, f(x_n)) + R(\|f\|_{\mathcal{H}})$$

- Classification algorithms:
  - Support vector machines: L is hinge loss
  - Kernel logistic regression: L is logistic loss
- Principal component analysis, canonical correlation analysis
- Many, many more...

Some theory

- If $\mathcal{H}$ *universal*, $f \in \mathcal{H}$ can approximate any continuous func
  - $\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, y) \, \mathrm{d}\mu(x) \, \mathrm{d}\mu(y) > 0$ for all nonzero finite signed measures μ
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  - Norm may go to ∞ as approximation gets better
- If RKHS norm is small, can learn quickly
  - e.g. Rademacher complexity of $\{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq B\}$ is at most $\sqrt{\frac{B^2}{m} \sup_{x \in \mathcal{X}} k(x, x)}$

Limitations of kernel-based learning

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- Generally bad at learning *sparsity*
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- Provably slower than deep learning for a few problems
  - e.g. to learn a single ReLU, $\max(0, w^\mathsf{T} x)$, need norm exponential in d [Yehudai/Shamir NeurIPS-19]
  - Also some hierarchical problems, etc [Kamath+ COLT-20]

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    - SVMs with NTK can be great on small data
  - Inspiration: learn the kernel model end-to-end
    - Ongoing area; good results in two-sample testing, GANs, density estimation, meta-learning, semi-supervised learning, ...

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  - More common reason: comparing distributions

Maximum Mean Discrepancy

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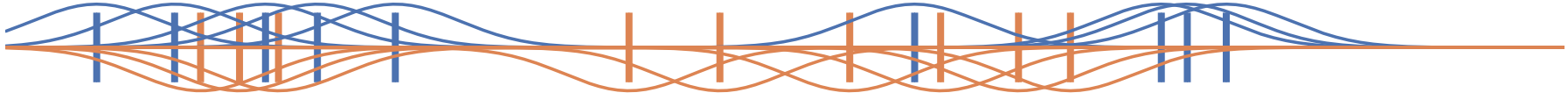

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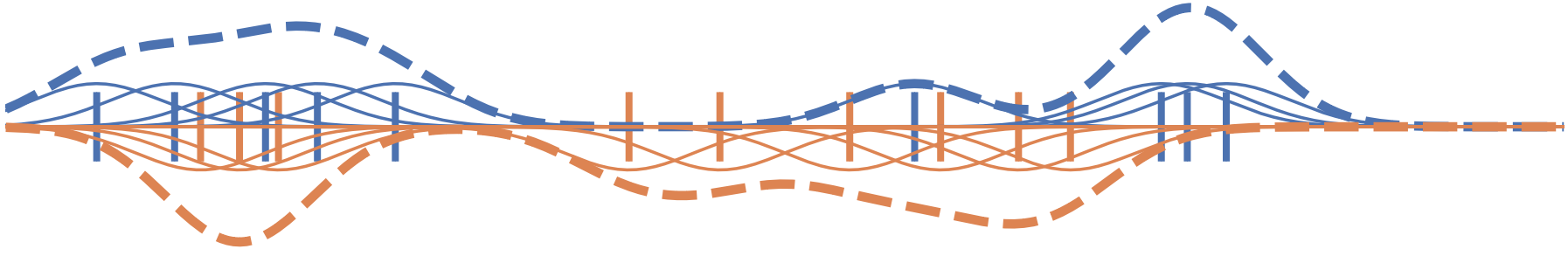

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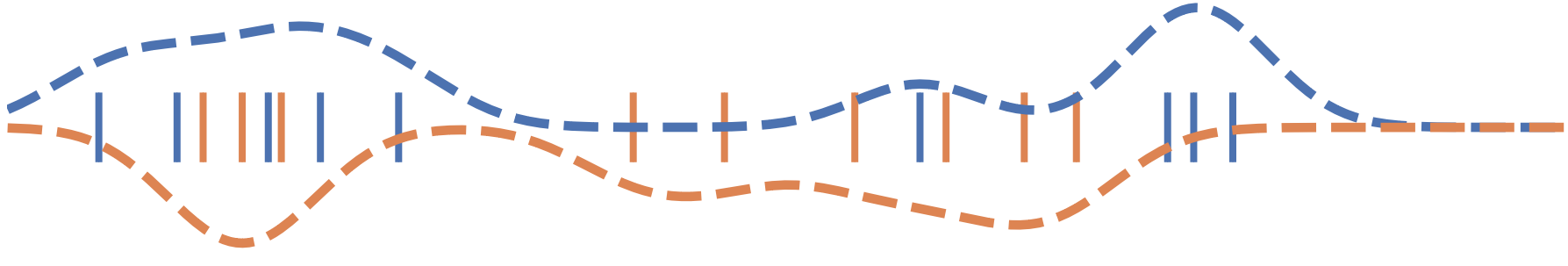

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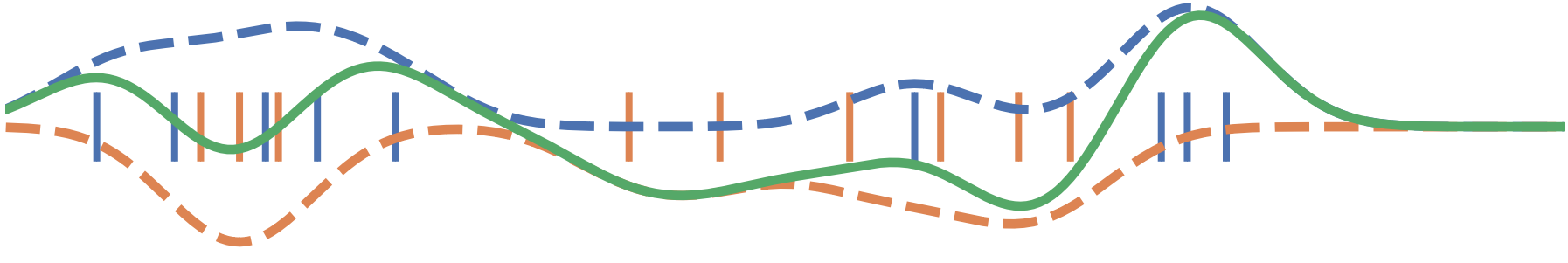

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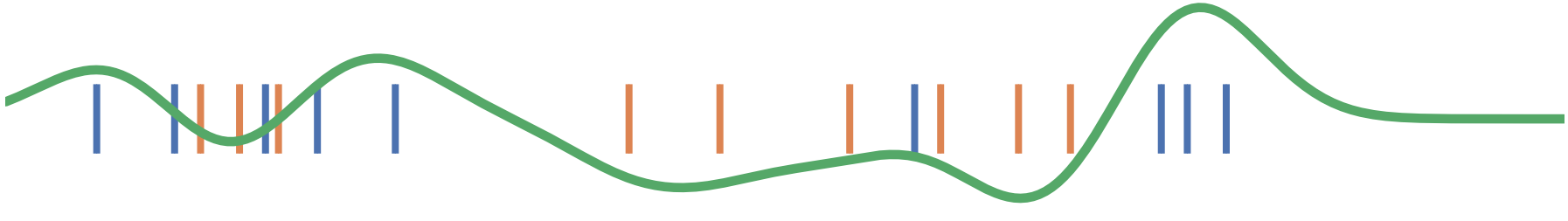

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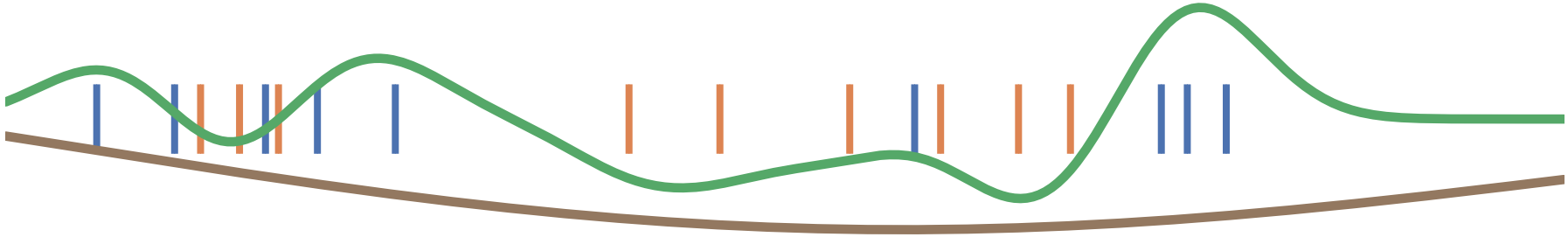

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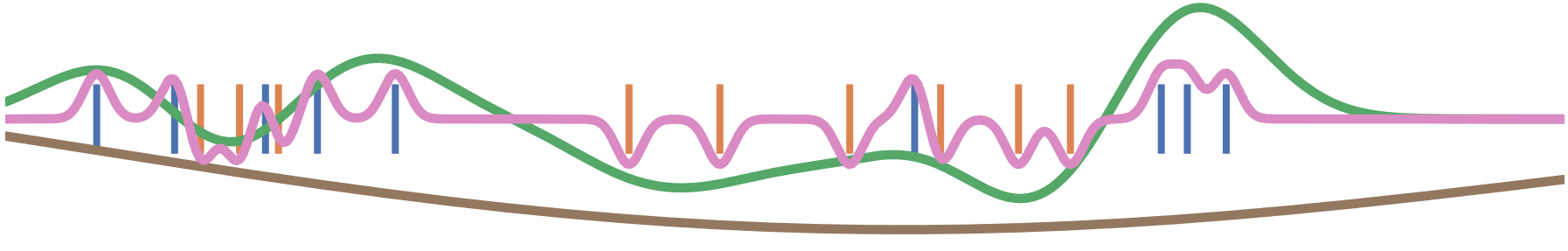

More!

- Foundations: Berlinet and Thomas-Agnan, *RKHS in Probability and Statistics*
- Hardcore theoretical details: Steinwart and Christmann, *Support Vector Machines*
- Close connections to Gaussian processes [Kanagawa+ 'GPs and Kernel Methods' 2018]
- Mean embeddings: survey of [Muandet+ 'Kernel Mean Embedding of Distributions']
- The practical sessions! Some pointers in there