CS 229br: Advanced Topics in the theory of machine learning

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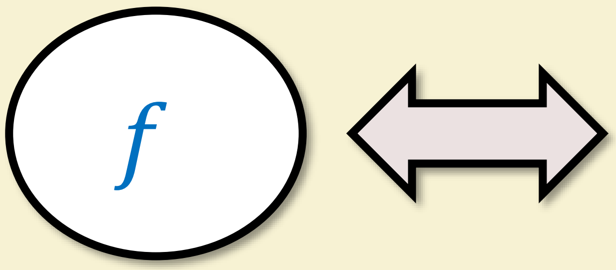
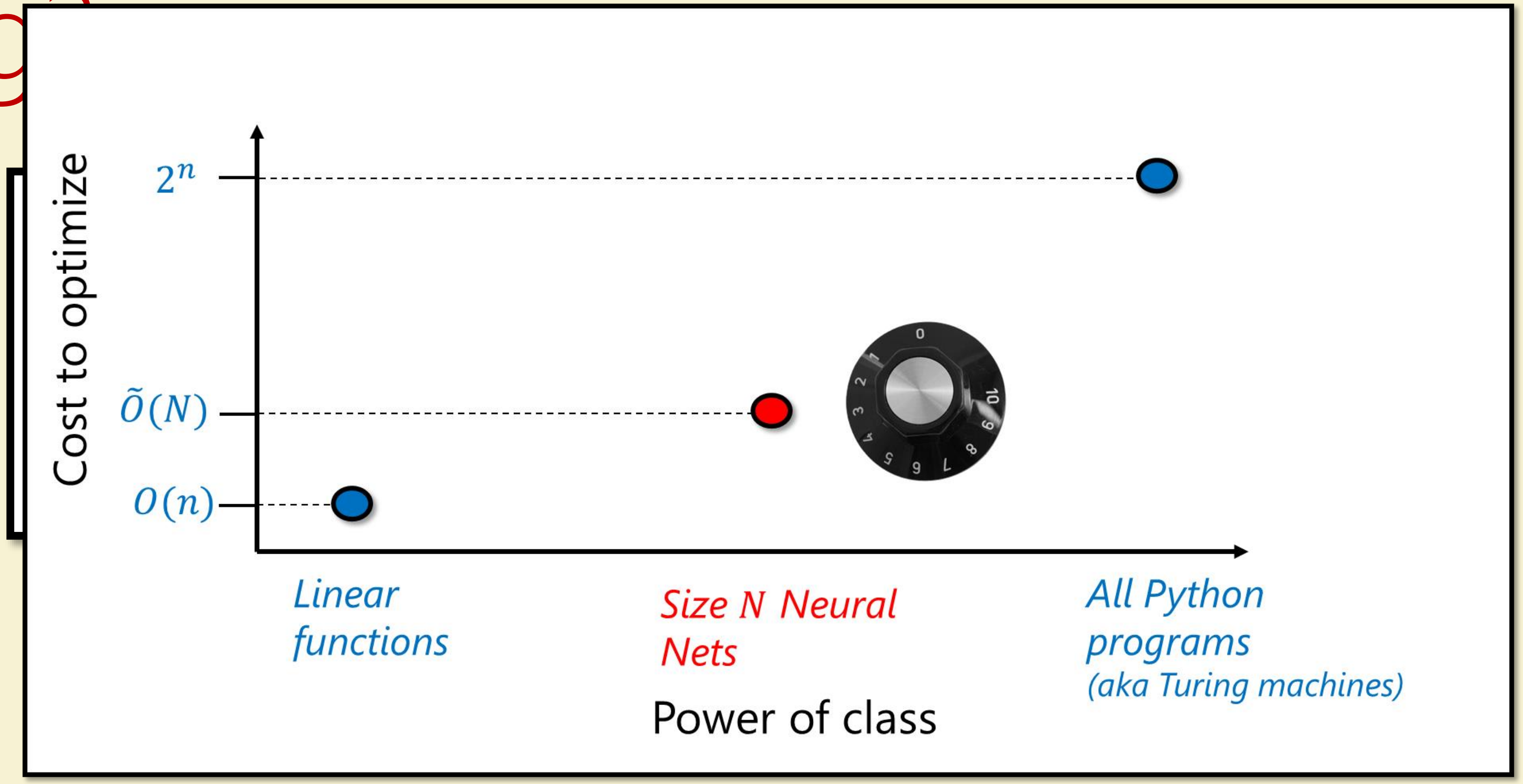
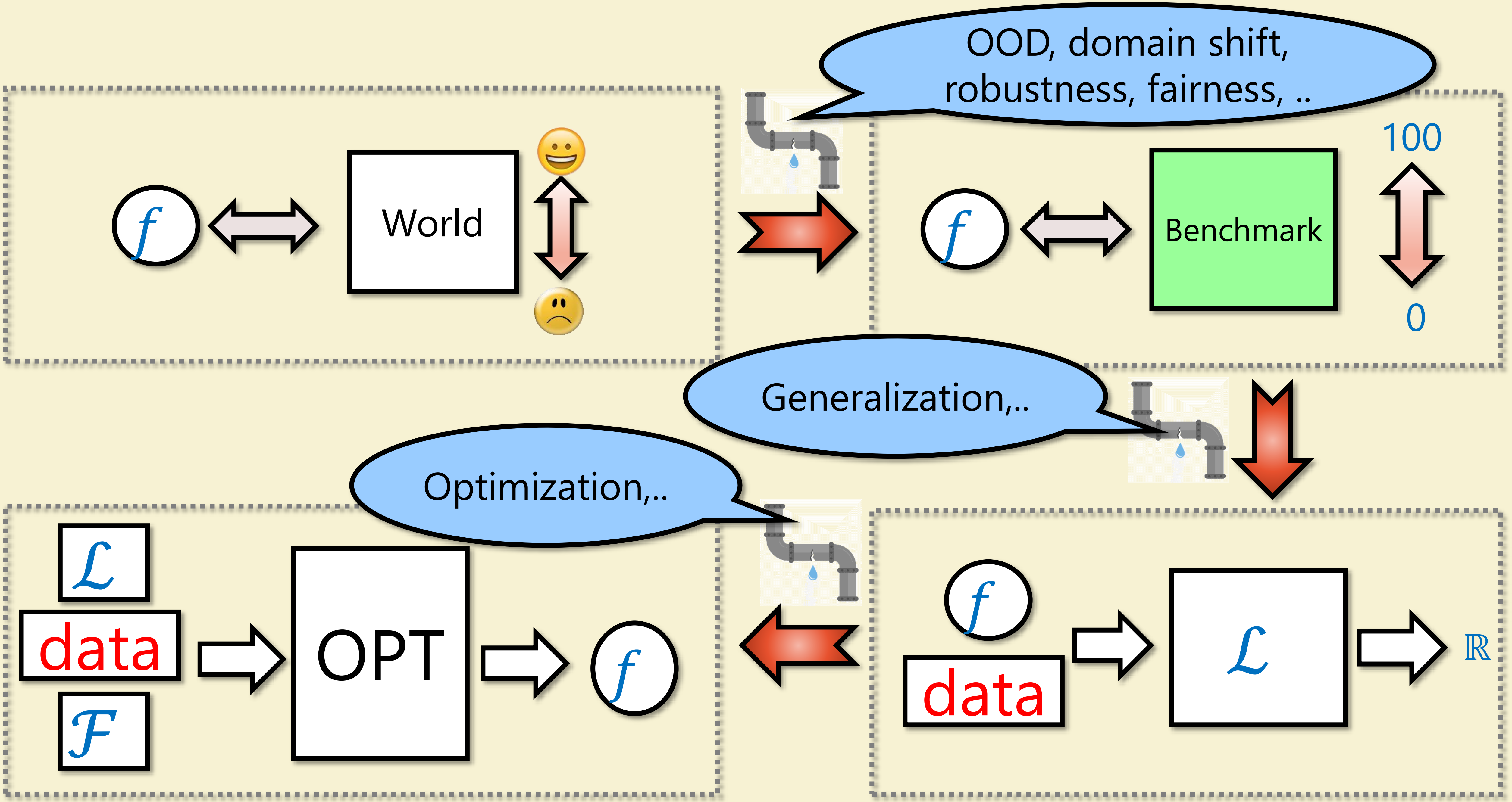
Join slack team and sign in on your devices!

What is learning?

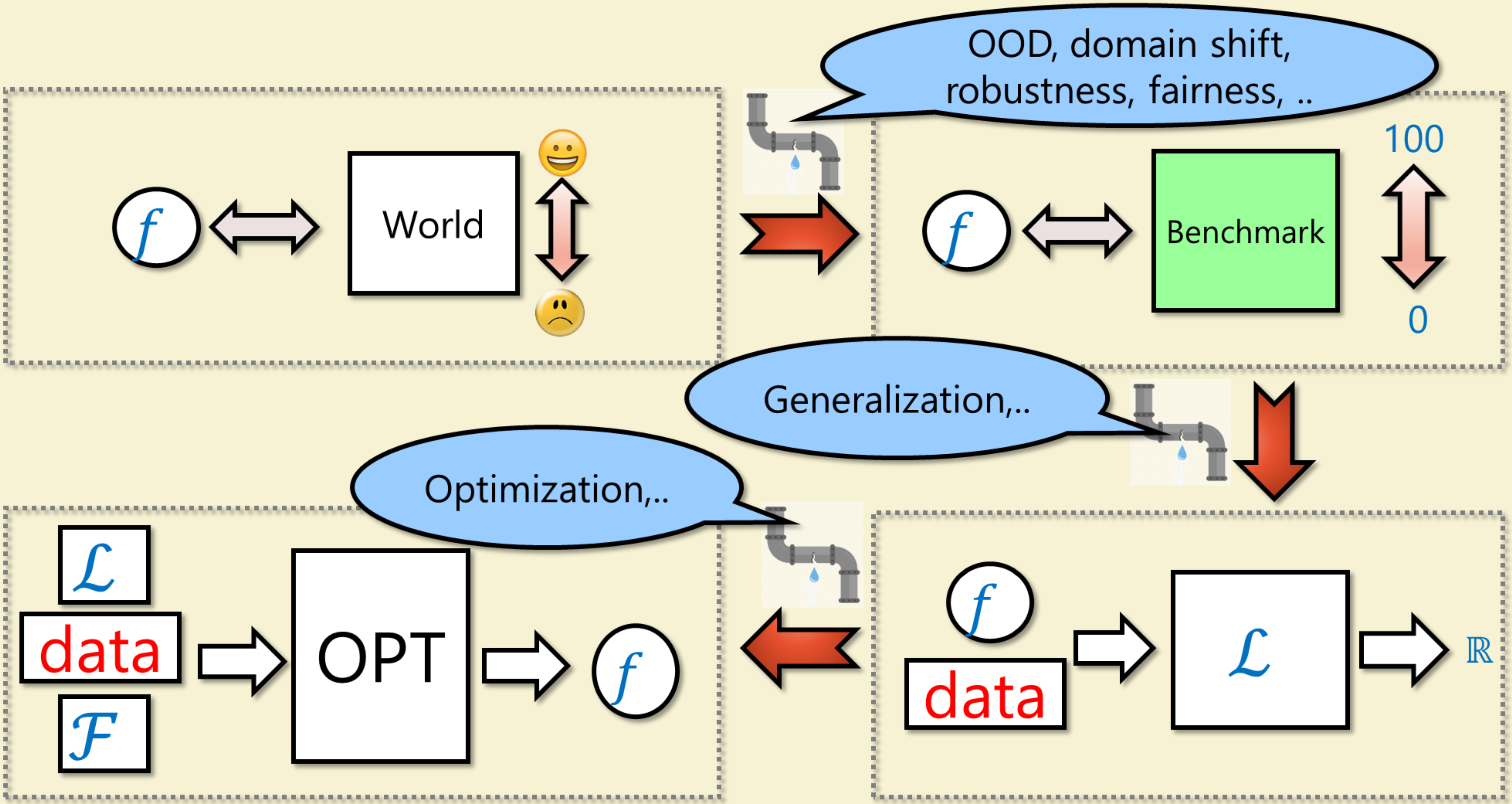




What is deep learning?



OOD, domain shift,
robustness, fairness, ..
f
World
f
Benchmark
100
0
Generalization,..
Optimization,..
$\mathcal{L}$
data
$\mathcal{F}$
OPT
f
f
data
$\mathcal{L}$
$\mathbb{R}$



OOD, domain shift, robustness, fairness, ..
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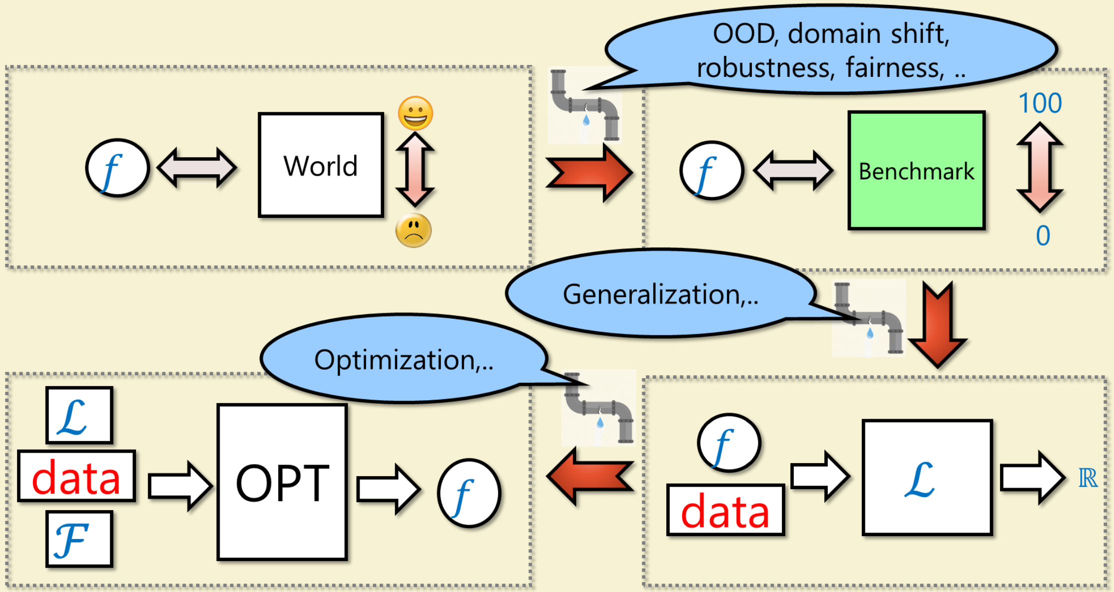


God's view:

$$f = \mathrm{argmax}_f\ \mathbb{E}[\ 😀(f)\ \mid \mathrm{data}\ ]$$

$$f = \mathrm{argmax}_f\ \mathbb{E}[\ 😀(f \leftrightarrow w)\ ]$$
$$w \sim W|\mathrm{data}$$

Perfect A $\Rightarrow$ Perfect B $\neq$ Approx A $\Rightarrow$ Approx B

This seminar

- Taste of research results, questions, experiments, and more
- Goal: Get to state of art research:
  - Background and language
  - Reading and reproducing papers
  - Trying out extensions
- Very experimental and "rough around the edges"
- A lot of learning on your own and from each other
- Hope: Very interactive – in lectures and on slack

CS 229br: Survey of very recent research directions, emphasis on experiments

MIT 18.408: Deeper coverage of foundations, emphasis on theory

Student expectations

Not set in stone but will include:

- Pre-reading before lectures
- Scribe notes / blog posts (adding proofs and details)
- Applied problem sets (replicating papers or mini versions thereof, exploring)
  Note: *Lectures will not teach practical skills – rely on students to pick up using suggested tutorials, other resources, and each other.*
  Unofficial TFs happy to answer questions!
- Some theoretical problem sets.
- Might have you grade each other's work
- Projects – self chosen and directed.

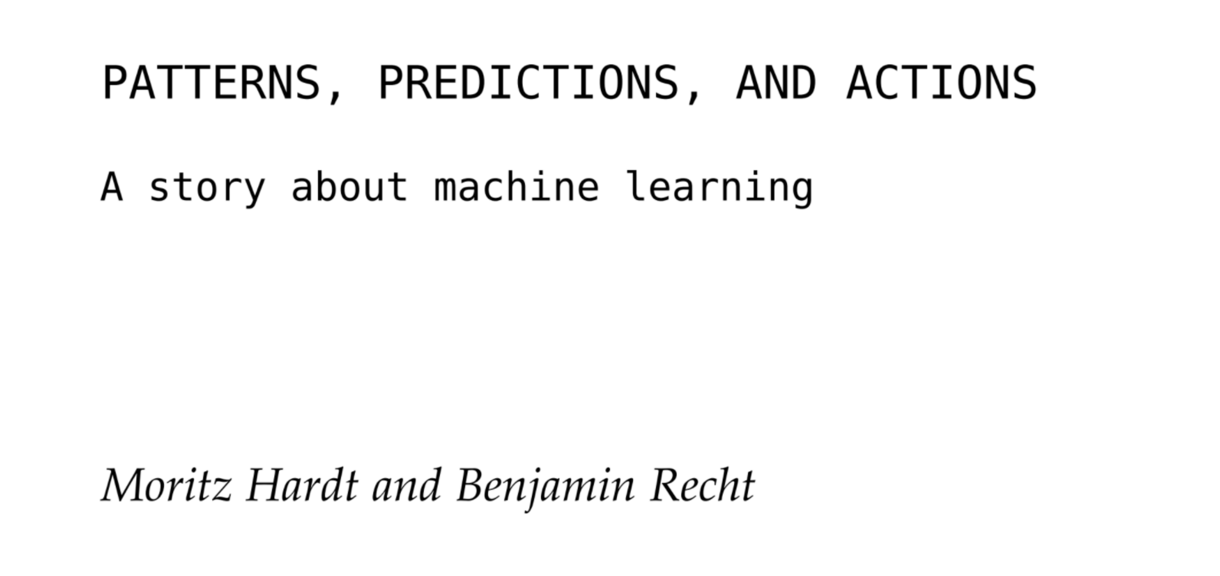
HW0 on slack

Grading: We'll figure out some grade – hope that's not your loss function ☺

Rest of today's lecture:

Blitz through classical learning theory

- Special cases, mostly one dimension
- "Proofs by picture"


PATTERNS, PREDICTIONS, AND ACTIONS

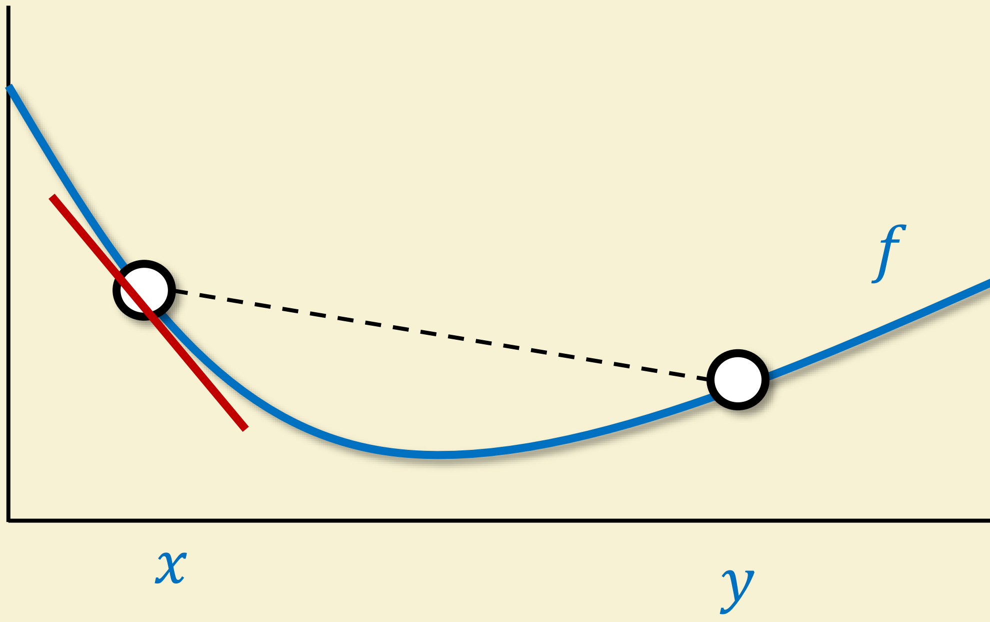
A story about machine learning

Moritz Hardt and Benjamin Recht

Part I: Convexity & Optimization

Convexity

1. Line between $(x, f(x))$ and $(y, f(y))$ above f.
2. Tangent line at x (slope $f'(x)$) below f.
3. $f''(x) > 0$ for all x

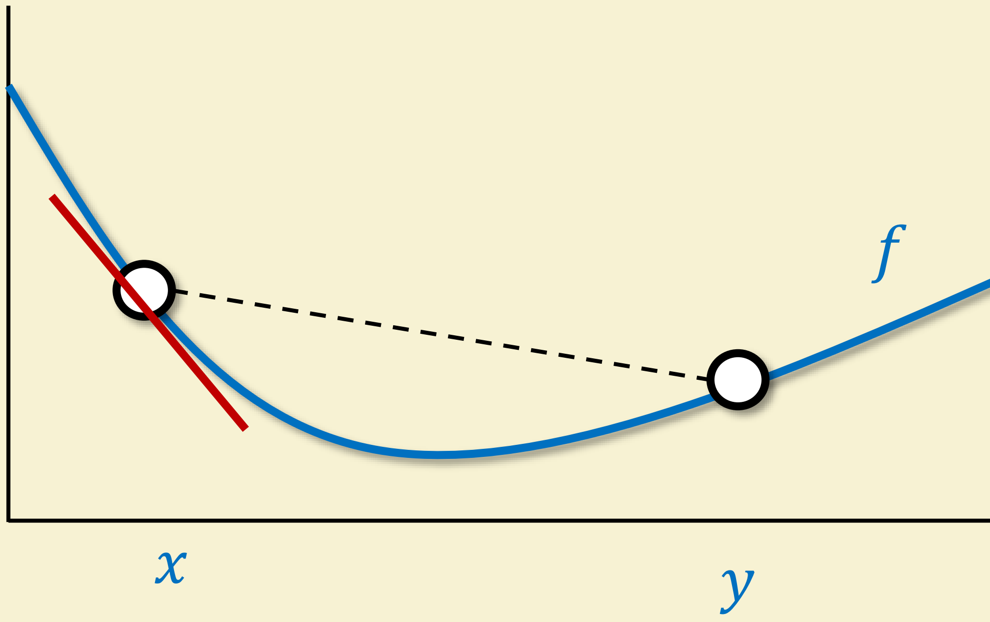


CLAIM: $f''(x) < 0$ implies tangent line at x above f

Proof: $f(x+\delta) = f(x) + \delta f'(x) + \delta^2 f''(x) + O(\delta^3)$ implies f below line

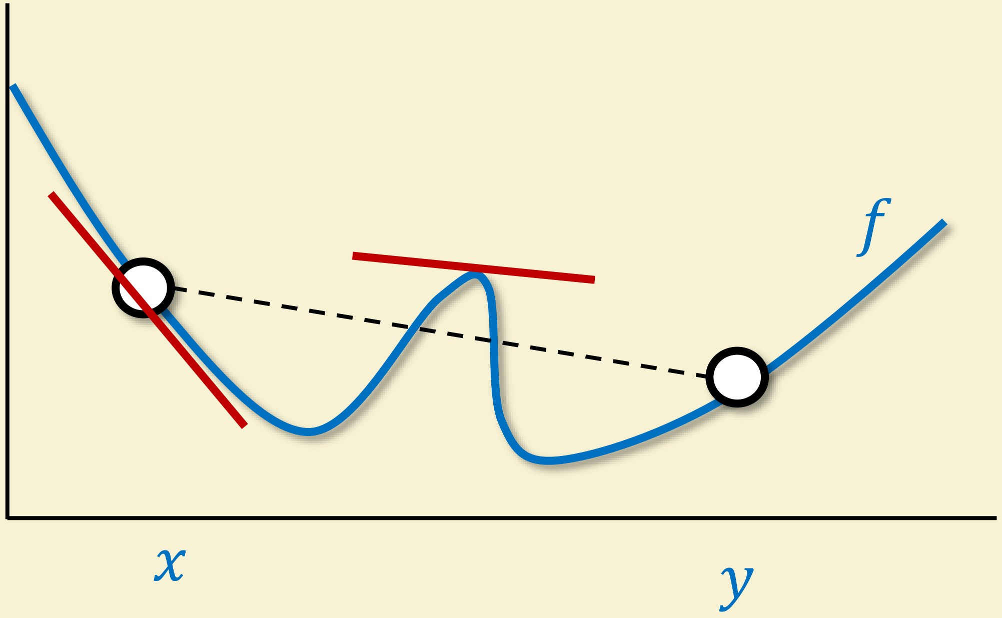
Convexity

1. Line between $(\mathrm{x}, f(x))$ and $(y, f(y))$ above f.
2. Tangent line at x (slope $f'(x)$) below f.
3. $f''(x) > 0$ for all x



CLAIM: If f above $(\mathrm{x}, f(x)) - (y, f(y))$ then exists z with tangent line at z above f

Proof by picture:



Gradient Descent

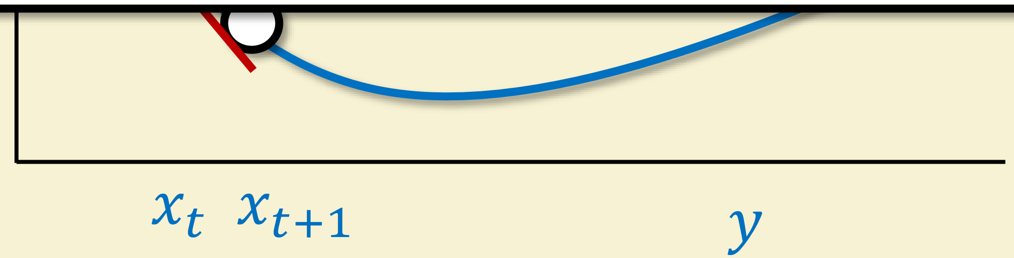
Dimension d:

$f'(x) \to \nabla f(x) \in \mathbb{R}^d$

$f''(x) \to H_f(\mathrm{x}) = \nabla_2 f(x) \in \mathbb{R}^{d \times d}$ (psd)

$\eta \sim 1/\lambda_d$ drop by $\sim \frac{\lambda_1}{\lambda_d} \|\nabla\|^2$

$$x_{t+1} = x_t - \eta f'(x_t)$$



$$f(x_t + \delta) \approx f(x_t) + \delta f'(x_t) + \frac{\delta^2}{2} f''(x_t)$$

$$f(x_{t+1}) \approx f(x_t) - \eta f'(x_t)^2 + \frac{\eta^2 f'(x_t)^2}{2} f''(x_t) \quad = f(x_t) - \eta f'(x_t)^2 \left(1 - \frac{\eta f''(x_t)}{2}\right)$$

- If $\eta < 2/f''(x_t)$ then make progress
- If $\eta \sim 2/f''(x_t)$ then drop by $\sim \eta f'(x_t)^2$

Stochastic Gradient Descent

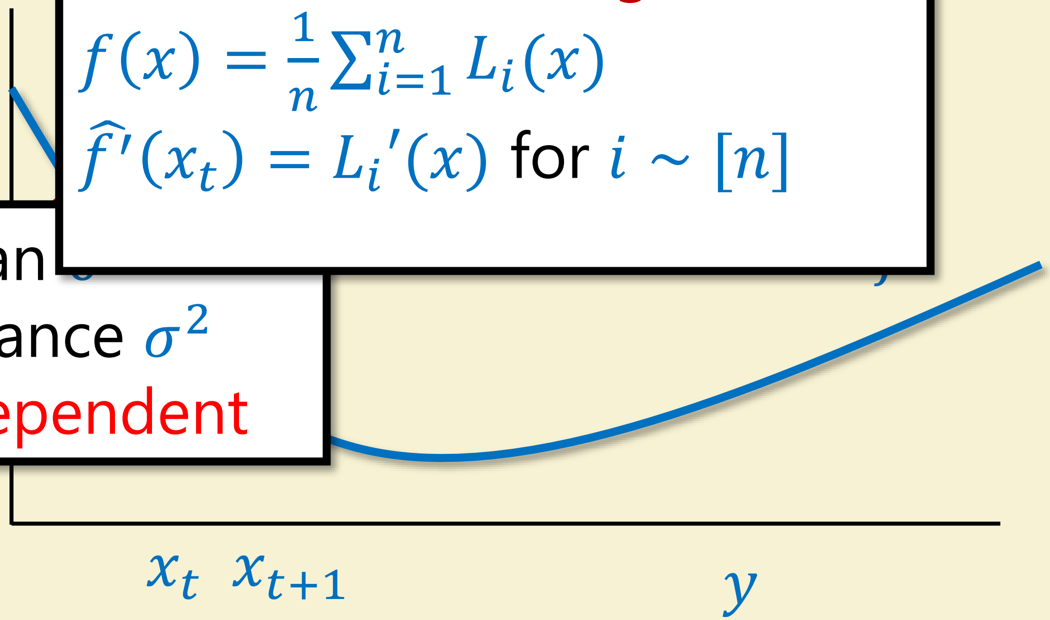
$x_{t+1} = x_t - \eta \widehat{f}'(x_t)$

$\mathbb{E}[\widehat{f}'(x)] = f'(x_t)$, $V[\widehat{f}'(x)] = \sigma^2$

Assume $\widehat{f}'(x) = f'(x) + N$

Mean
Variance σ^2
Independent

In Machine Learning:
$f(x) = \frac{1}{n}\sum_{i=1}^{n} L_i(x)$
$\widehat{f}'(x_t) = L_i{}'(x)$ for $i \sim [n]$



$$f(x_t + \delta) \approx f(x_t) + \delta f'(x_t) + \frac{\delta^2}{2} f''(x_t)$$

$$f(x_{t+1}) \approx f(x_t) - \eta f'(x_t)^2 \left(1 - \frac{\eta f''(x_t)}{2}\right) + \eta^2 \sigma^2 f''(x_t)$$

- If $\eta < 2/f''(x_t)$ and (*) $\eta\sigma^2 \ll f'(x_t)^2/f''(x)$ then make progress
- If $\eta \sim 2/f''(x_t)$ and (*) then drop by $\sim \eta f'(x_t)^2$

Part II: Generalization

Supervised learning

Empirical Risk Minimization (ERM):
$A(S) = \arg\min_{f \in \mathcal{F}} \hat{\mathcal{L}}_S(f)$

Distribution (X, Y) over $\mathcal{X} \times \{\pm 1\}$

$S = (x_i, y_i)_{i=1..n}$

data $\Rightarrow$ Learning Algorithm A $\Rightarrow$ $f \in \mathcal{F}$

$\mathcal{L}(f) = \Pr[f(X) \neq Y]$

Population 0-1 loss

$\hat{\mathcal{L}}_S(f) = \frac{1}{n} \sum_{i=1}^{n} 1_{f(x_i) \neq y_i}$

Empirical 0-1 loss

Generalization gap: $\mathcal{L}(f) - \hat{\mathcal{L}}_S(f)$ for $f = A(S)$

Bias Variance Tradeoff

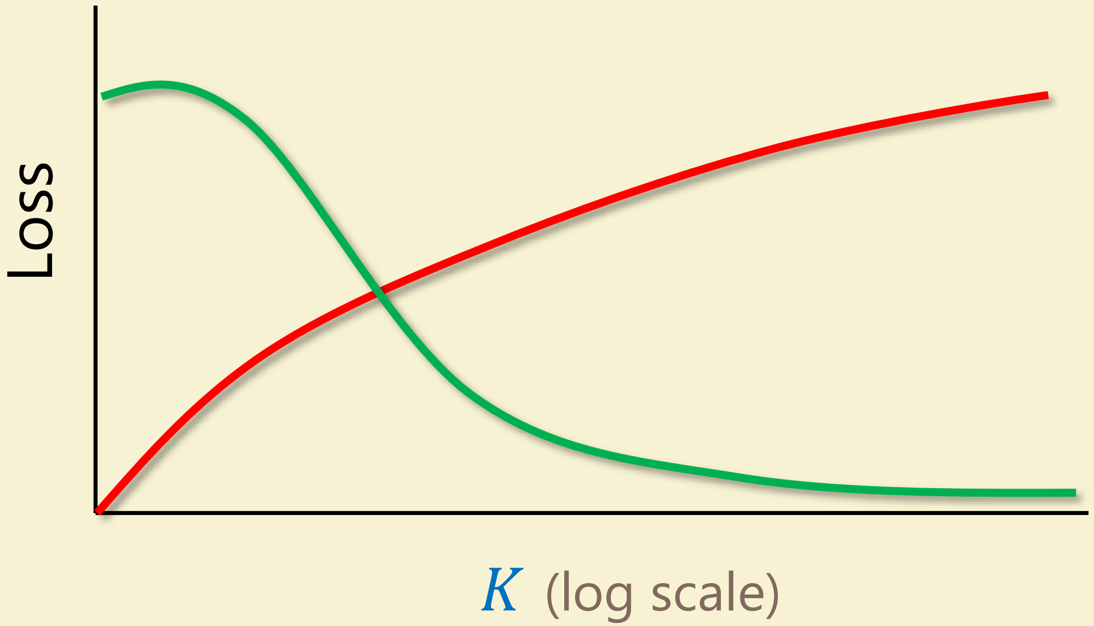
Empirical Risk Minimization (ERM):

$$A(S) = \arg\min_{f\in\mathcal{F}} \hat{\mathcal{L}}_S(f)$$

$S = (x_i, y_i)_{i=1..n}$

Population 0-1 loss $\mathcal{L}(f) = \Pr[f(X) \neq Y]$ bias Emp variance ss $\hat{\mathcal{L}}_S(f) = \frac{1}{n}\sum_{i=1}^{n} 1_{f(x_i)\neq y_i}$

Assume $\mathcal{F}_K = \{f_1, \dots, f_K\}$, $\hat{\mathcal{L}}(f_i) = \mathcal{L}(f_i) + N(0, 1/n)$



$\sim \sqrt{\frac{\log K}{n}}$?

$\sim (\log K)^{-\alpha}$??

Bias Variance Tradeoff

Empirical Risk Minimization (ERM):

$$A(S) = \arg\min_{f \in \mathcal{F}} \hat{\mathcal{L}}_S(f)$$

$S = (x_i, y_i)_{i=1..n}$ → Learning Algorithm A → $f \in \mathcal{F}$

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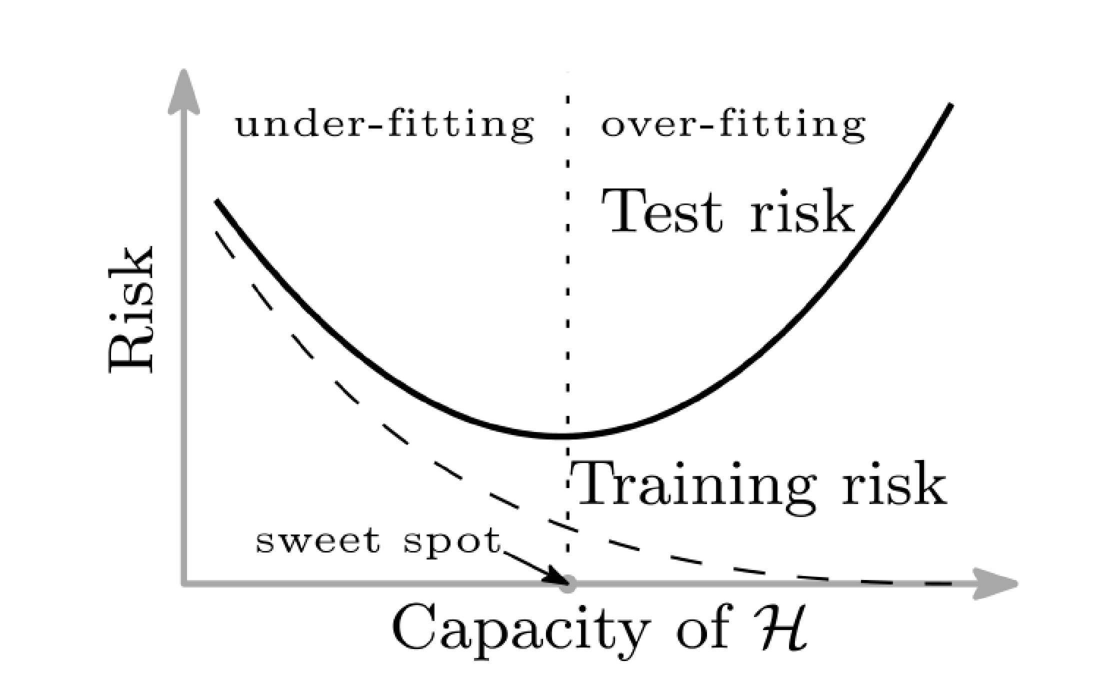
Assume $\mathcal{F}$ ... $) + N(0, 1/n)$



$\sim \sqrt{\frac{\log K}{n}}$?

$\sim (\log K)^{-\alpha}$??

Can prove:

GAP $\leq O\left(\sqrt{\frac{\log |\mathcal{F}|}{n}}\right)$

Population 0-1 loss $\mathcal{L}(f) = \Pr[f(X) \neq Y]$ Empirical 0-1 loss $\hat{\mathcal{L}}_S(f) = \sum_{i=1}^{n} 1_{f(x_i) \neq y_i}$

Can prove:

GAP $\leq O\left(\sqrt{\frac{\log |\mathcal{F}|}{n}}\right)$

THM: with high prob over $S \sim (X, Y)^n$, $\max_{f \in \mathcal{F}} \left|\mathcal{L}(f) - \hat{\mathcal{L}}_S(f)\right| \leq O\left(\sqrt{\frac{\log|\mathcal{F}|}{n}}\right)$

Population 0-1 loss $\mathcal{L}(f) = \Pr[f(X) \neq Y]$ Empirical 0-1 loss $\hat{\mathcal{L}}_S(f) = \sum_{i=1}^{n} 1_{f(x_i) \neq y_i}$

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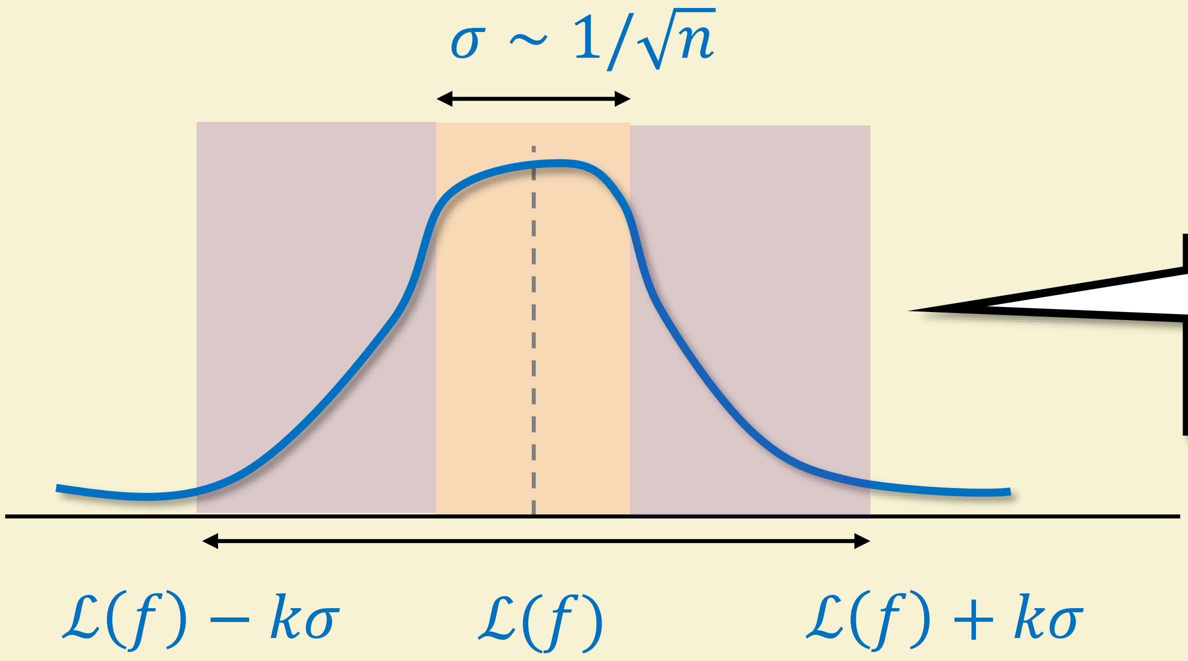
LEM: For every fixed f, $\Pr_S\left[\left|\mathcal{L}(f) - \hat{\mathcal{L}}_S(f)\right| \geq \frac{k}{\sqrt{n}}\right] \leq \exp(-c \cdot k^2)$

PF: Central limit thm / Chernoff / Hoeffding / ….



$\Pr[|X - \mathbb{E}X| \geq k\sigma] \leq \exp(-c \cdot k^2)$

LEM⇒THM: Set $k = 10 \cdot \sqrt{\log|\mathcal{F}|}/c$

Generalization bounds

Can prove:

$$\text{GAP} \leq O\left(\sqrt{\frac{\log|\mathcal{F}|}{n}}\right)$$

$\log|\mathcal{F}|$ can be replaced with dimensionality / capacity of $\mathcal{F}$

VC dimension:
$\max d$ s.t. $\mathcal{F}$ can fit every labels $y \in \{\pm 1\}^d$ on every samples $x_1, \ldots, x_d$

Rademacher complexity:
$\max d$ s.t. $\mathcal{F}$ can fit random labels $y \sim \{\pm 1\}^d$ on random $x_1, \ldots, x_d \sim X$

PAC Bayes:
$d = I(A(S); S)$ where S is training set.

Margin bounds:
$\max d$ s.t. linear classifier satisfies $\langle w_i, x_i \rangle y_i > \|w_i\| \cdot \|x_i\| / \sqrt{d}$ for correct predictions

General form: If $C(f) \ll n$ then $\hat{\mathcal{L}}(f) - \mathcal{L}(f) \approx 0$

Intuition: Can't "overfit" – if you do well on n samples, must do well on population

Challenge: Many modern deep nets and natural C , $C(f) \gg n$

Hope: Find better C?

UNDERSTANDING DEEP LEARNING REQUIRES RE-THINKING GENERALIZATION

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Oriol Vinyals
Google DeepMind
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ICLR 2017

General form: If $C(f) \ll n$ then $\hat{\mathcal{L}}(f) - \mathcal{L}(f) \approx 0$

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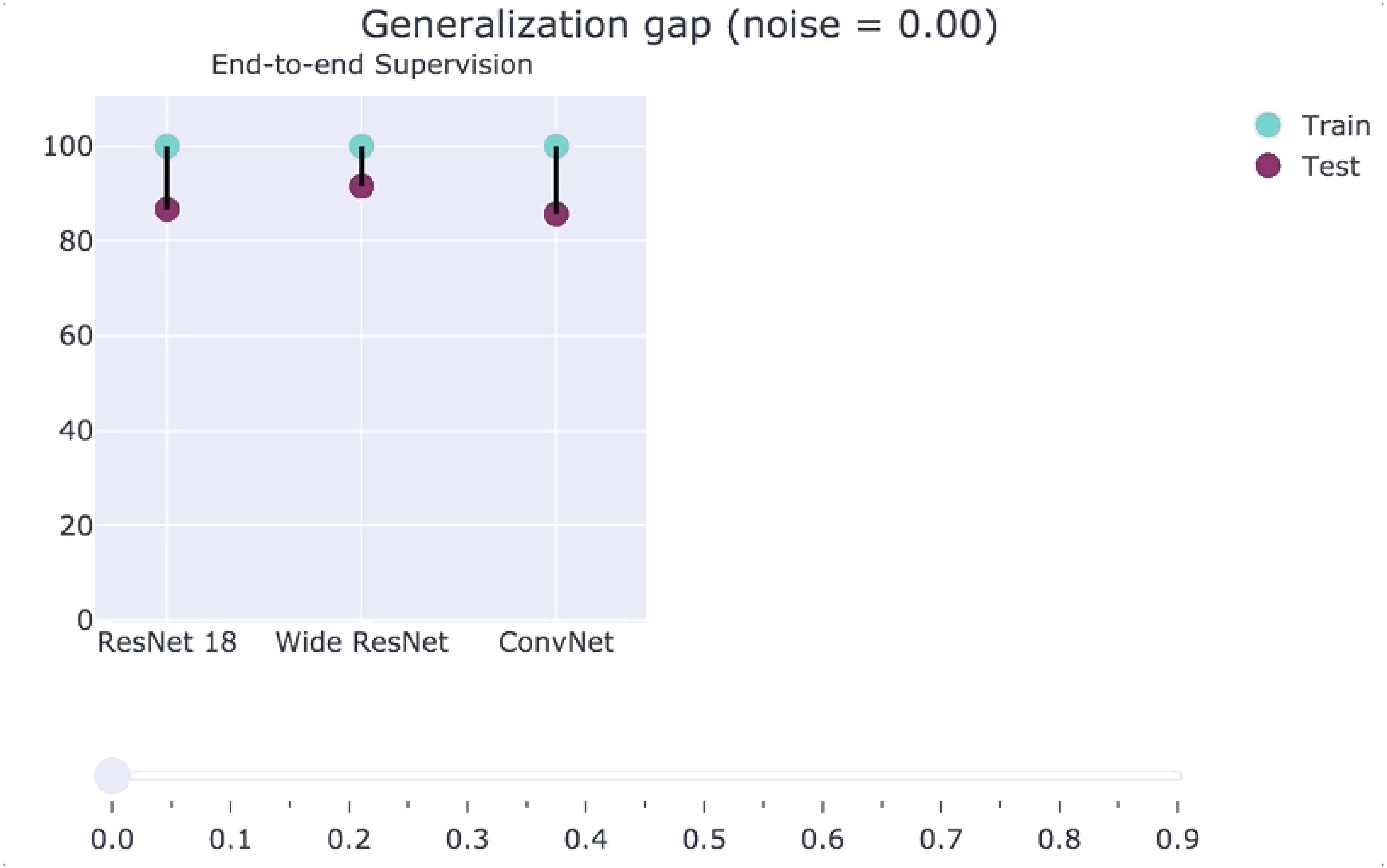
Performance on CIFAR-10

Classifier	Train	Test
Wide ResNet[1]	100%	92%
ResNet 18[2]	100%	87%
Myrtle[3]	100%	86%

Performance on noisy CIFAR-10:*

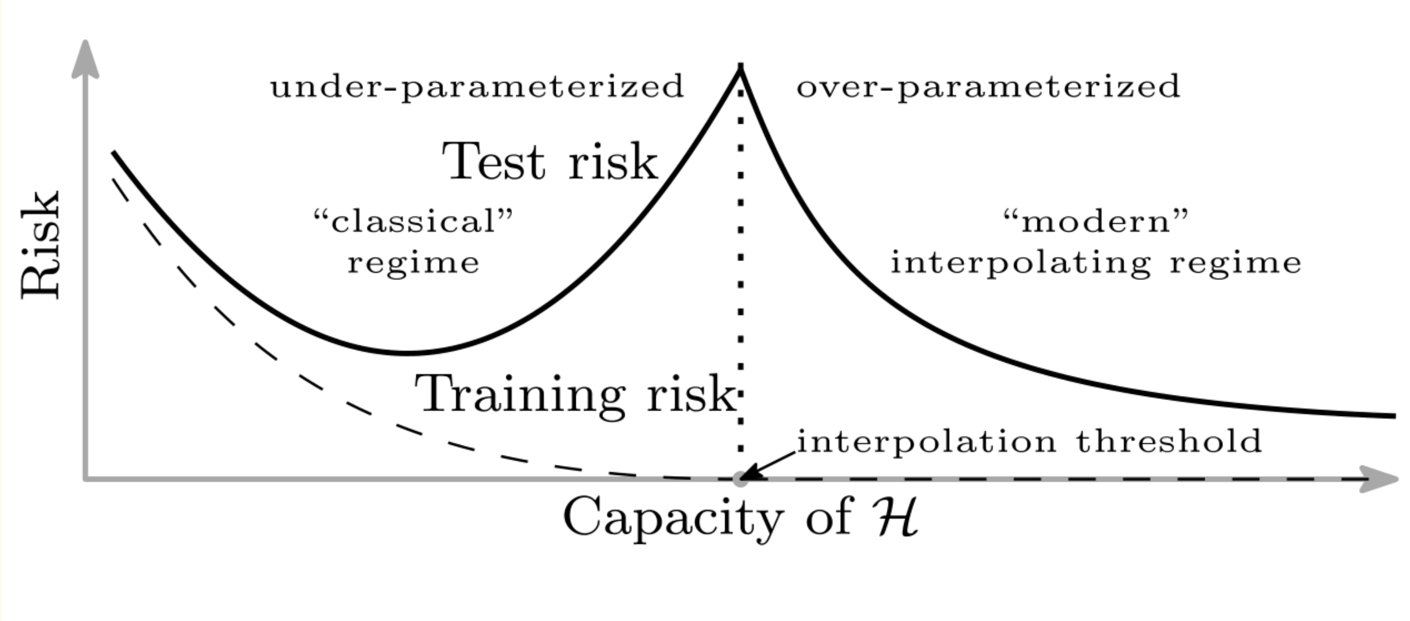
Train	Test
100%	10%
100%	10%
100%	10%

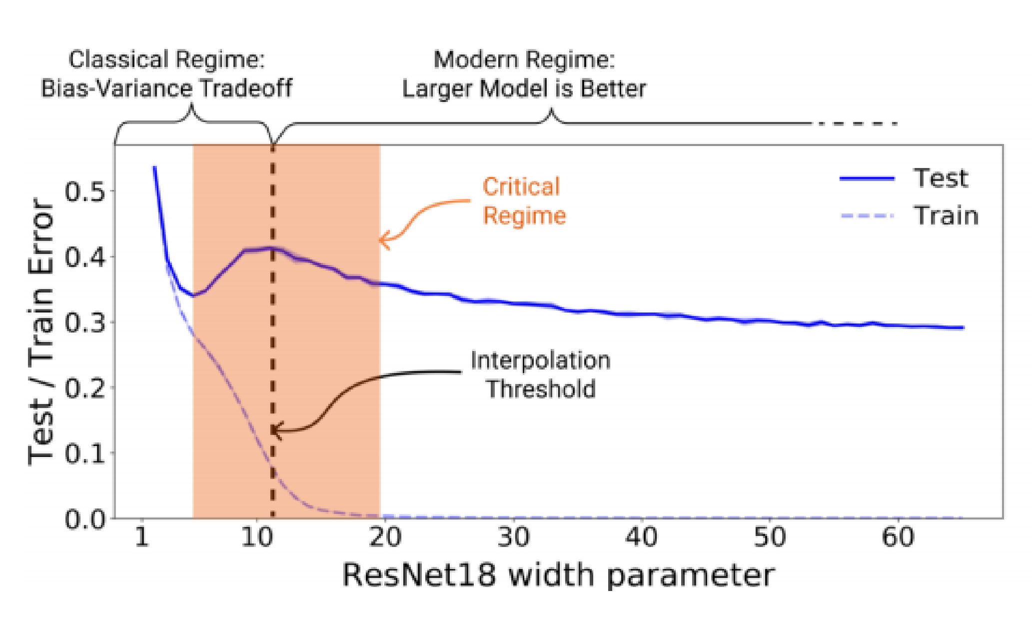
[1] Zagoruyko-Komodakis'16 [2] He-Zhang-Ren-Sun'15 [3] Page '19



Bansal-Kaplun-B, ICLR 2021

"Double descent"





Belkin, Hsu, Ma, Mandal, PNAS 2019.

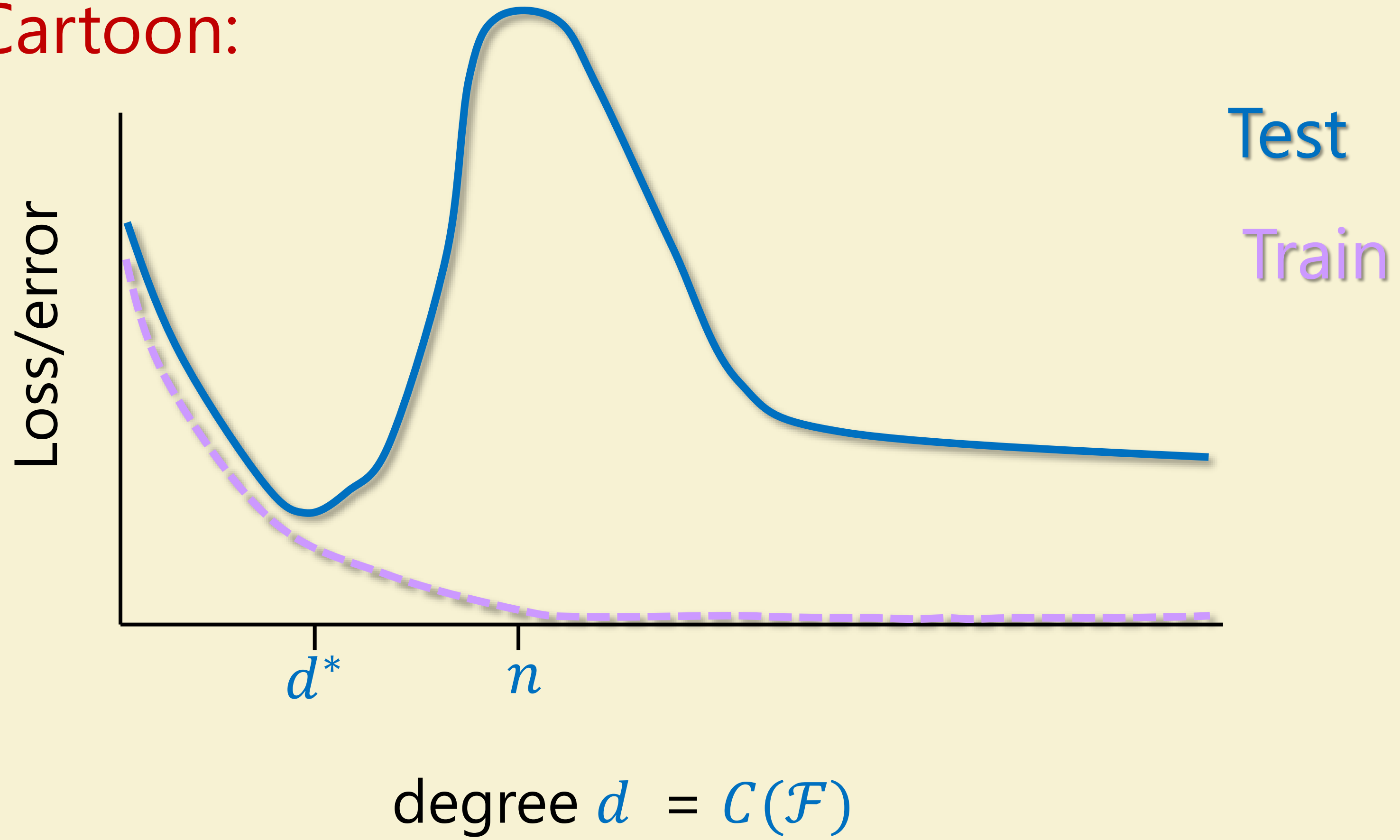
Nakkiran-Kaplun-Bansal-Yang-B-Sutskever, ICLR 2020

Example:

Data: $(x_i, f^*(x_i) + N)$ where f^* degree d^* polynomial

Algorithm: SGD to minimize $\sum(f(x_i) - y_i)^2$ where $f \in \mathcal{F}_d$=degree d polys

Cartoon:



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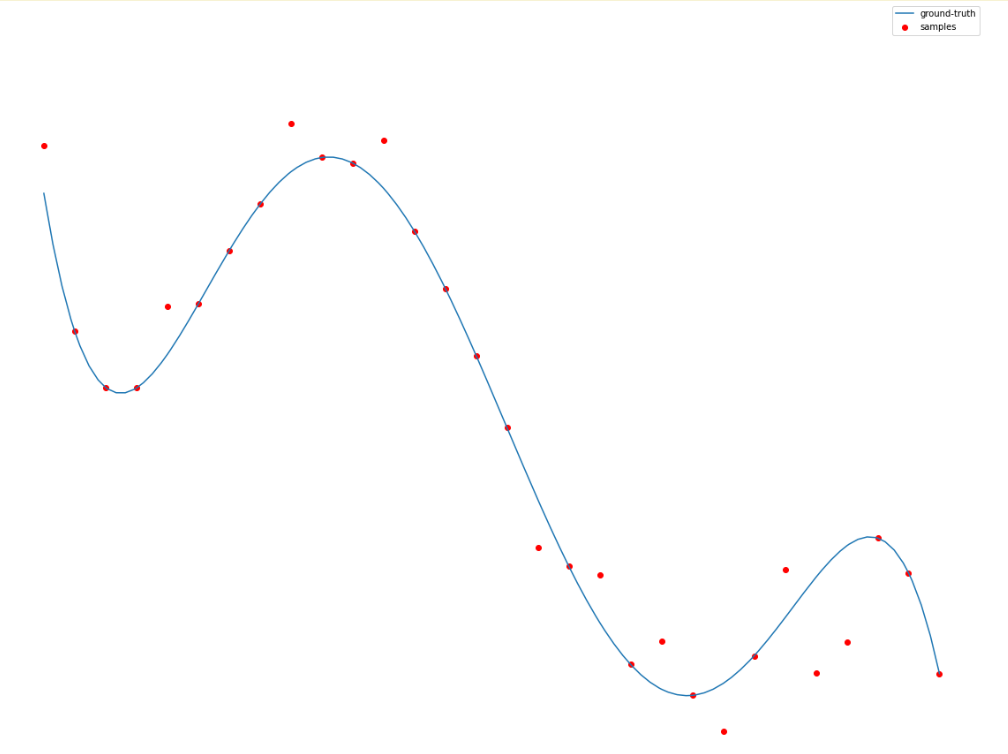

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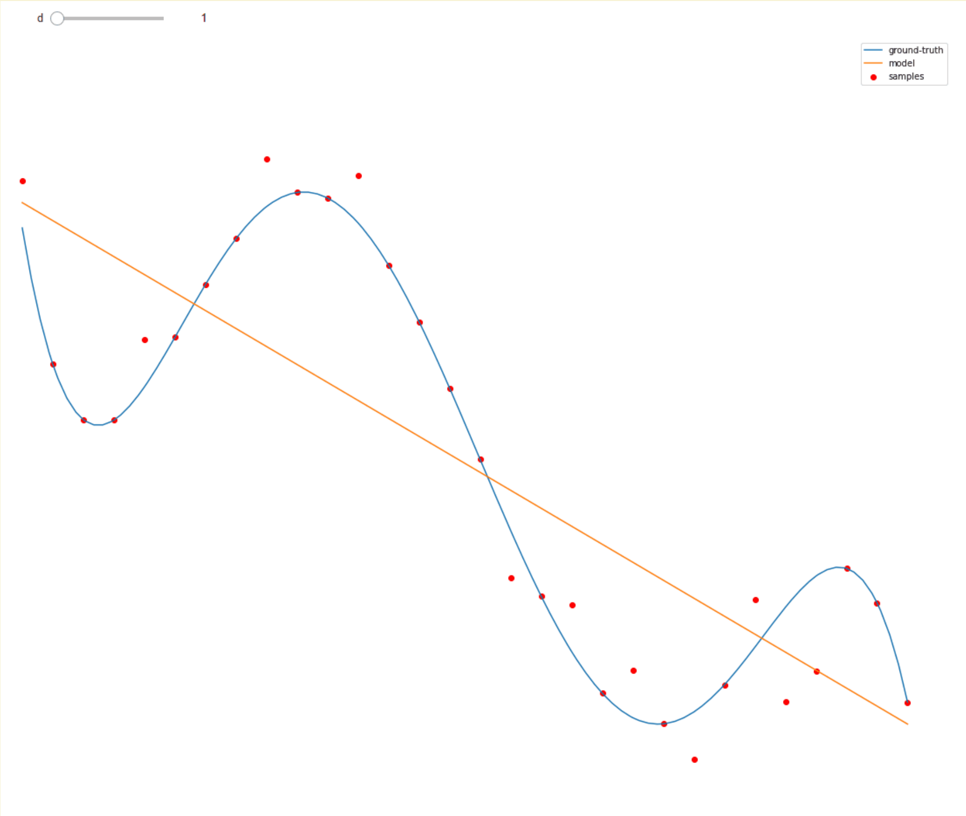
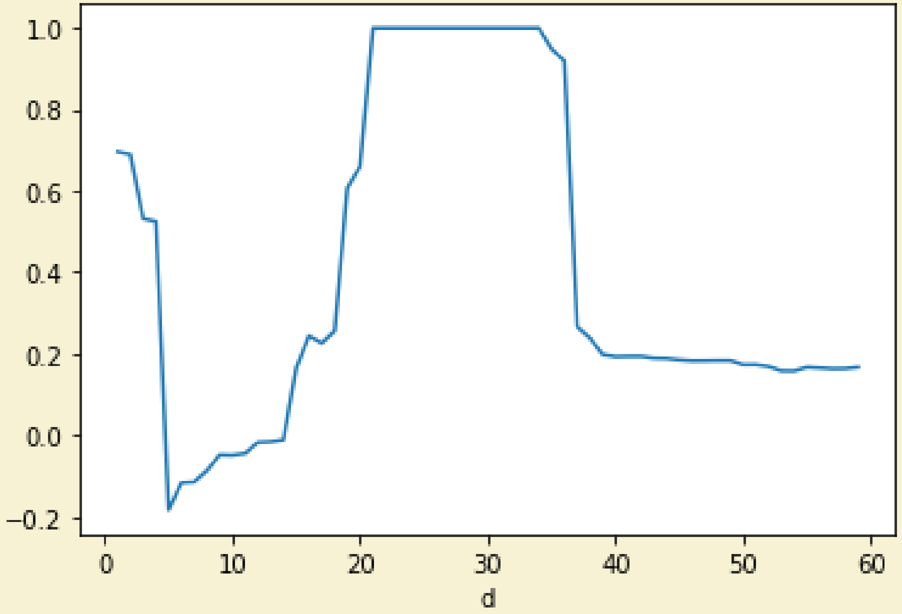
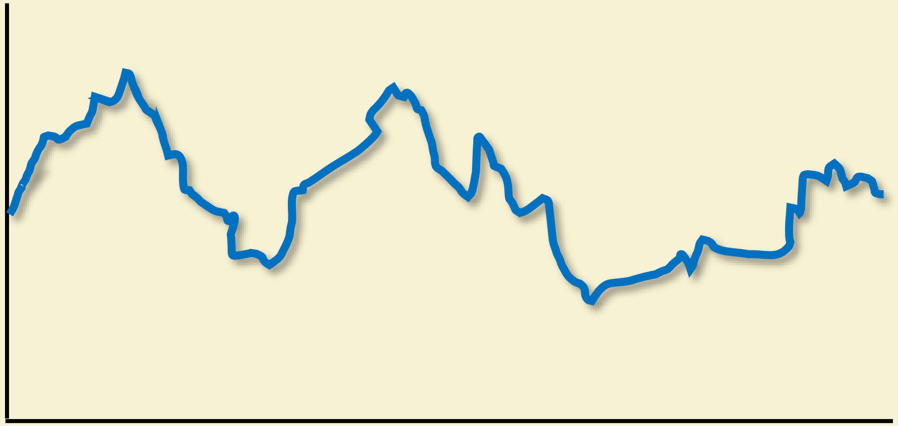
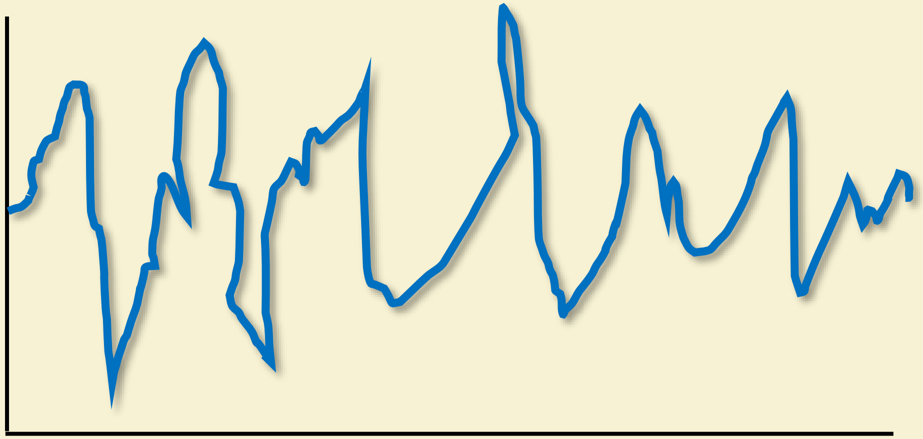




Part III: Approximation and Representation

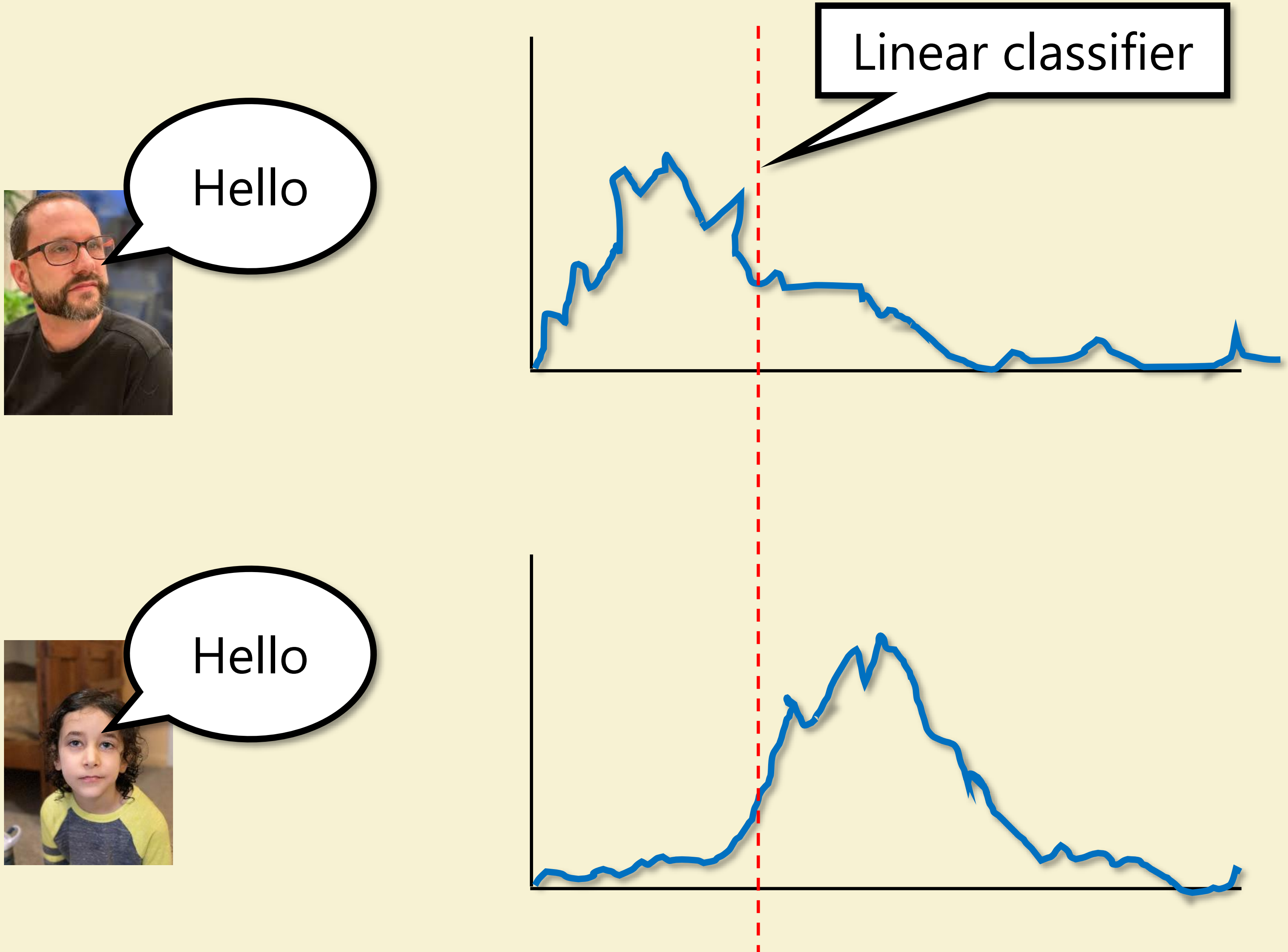
Example:





Example:

After Fourier Transform



Fourier Transform

$$\int_0^1 |f - g| < \epsilon$$

Every continuous $f: [0,1] \to \mathbb{R}$ can be arbitrarily approximated by g of form

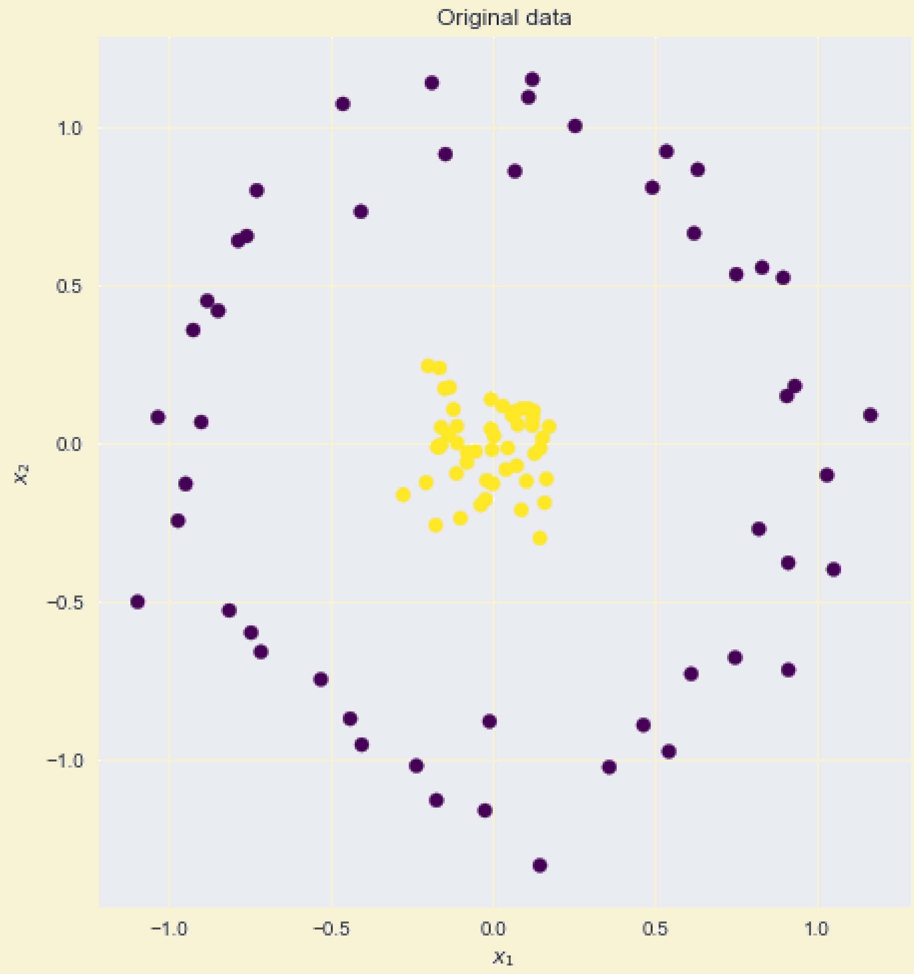
$$g(x) = \sum \alpha_j e^{-2\pi i\, \beta_j x}$$

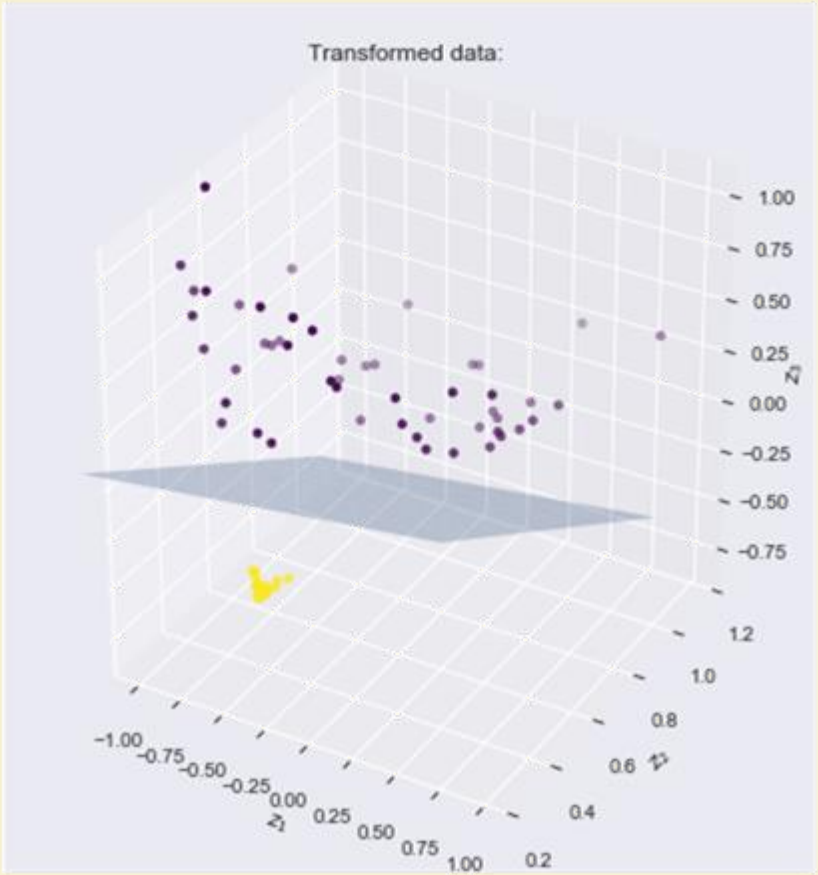
i.e., $f \ \approx$ linear in $\varphi_1(x), \dots, \varphi_N(x)$ where $\varphi_j(x) = e^{-2\pi i\, \beta_j x}$

$\varphi: \mathbb{R} \to \mathbb{R}^N$ embedding

For some natural data, representation φ is "nice" (e.g. sparse, linearly separable,…)

Tasks become simpler after transformation $x \to \varphi(x)$





$$\varphi(x, y) = (xy, x^2, y^2)$$

Xavier Bourret Sicotte, https://xavierbourretsicotte.github.io/Kernel_feature_map.html

More approximation

$$ReLU(x) = \max(x, 0)$$

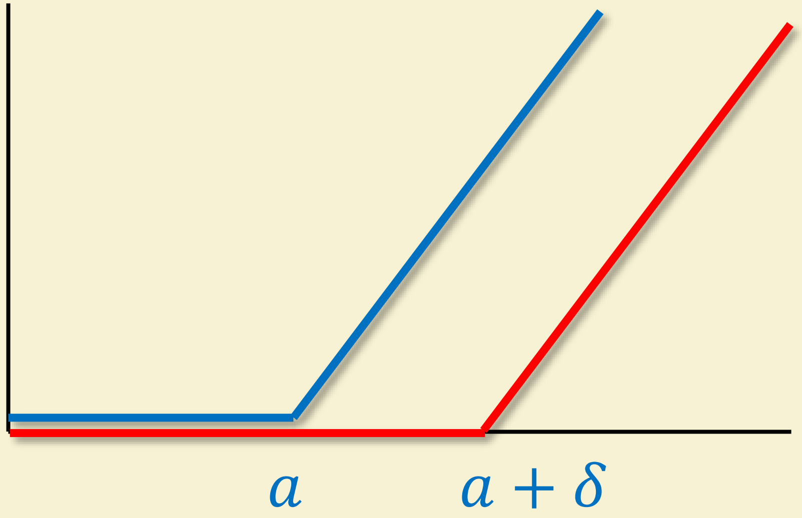
Every continuous $f: [0,1] \to \mathbb{R}$ can be arbitrarily approximated by g of form

$$g(x) = \sum \alpha_i \, ReLU(\beta_i x + \gamma_i)$$

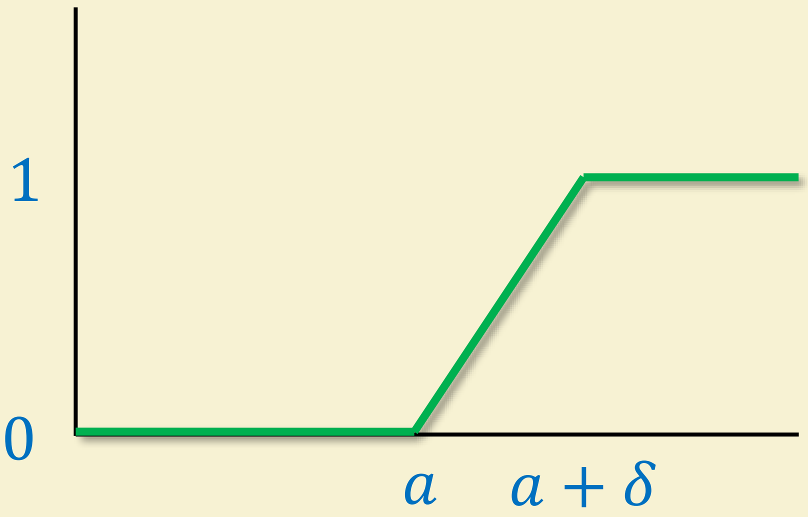
Proof by picture:

$g_a(x) = ReLU(x/\delta - a)$

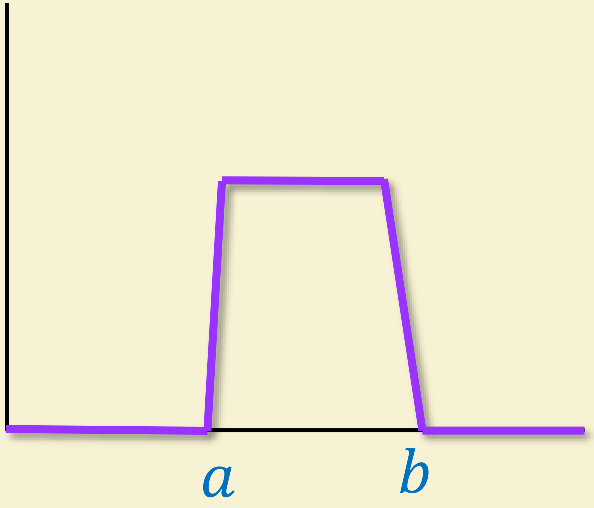
$g_{a+\delta}(x) = ReLU(x/\delta - a - \delta)$



$h_a = g_a - g_{a+\delta}$



$I_{a,b} = h_a - h_b$



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Proof by picture:

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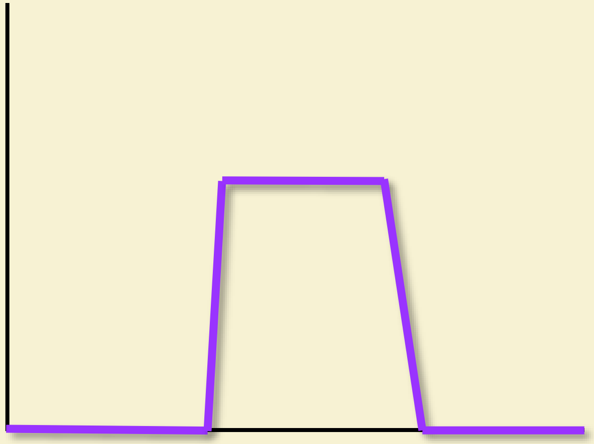
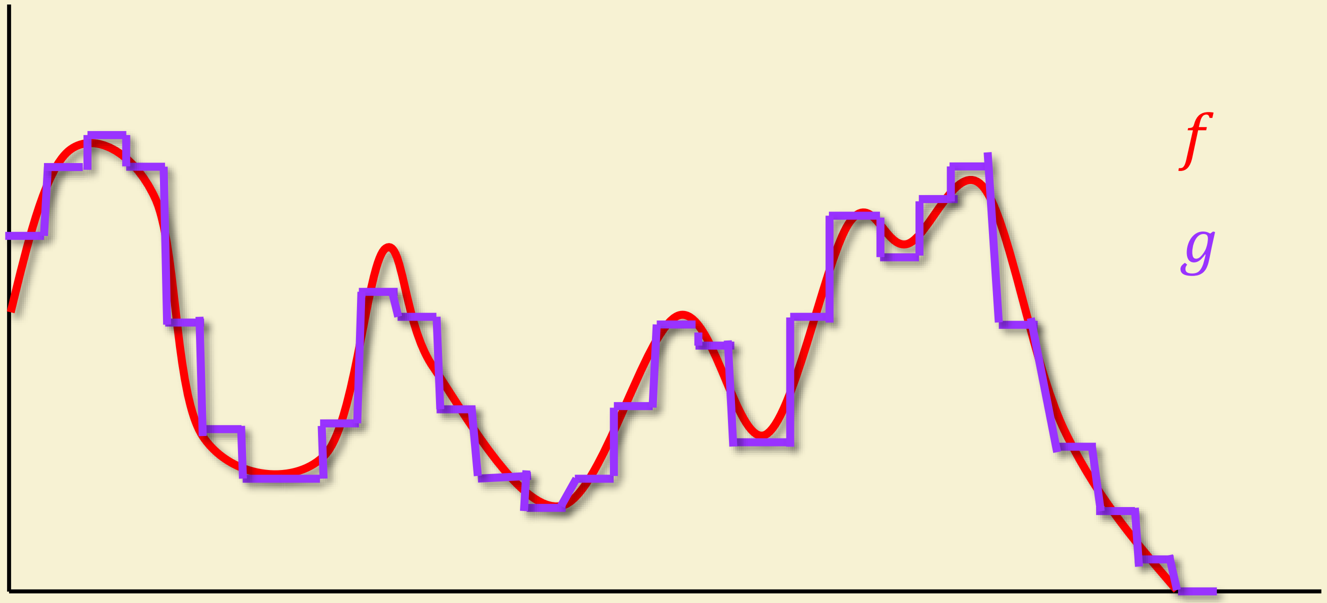
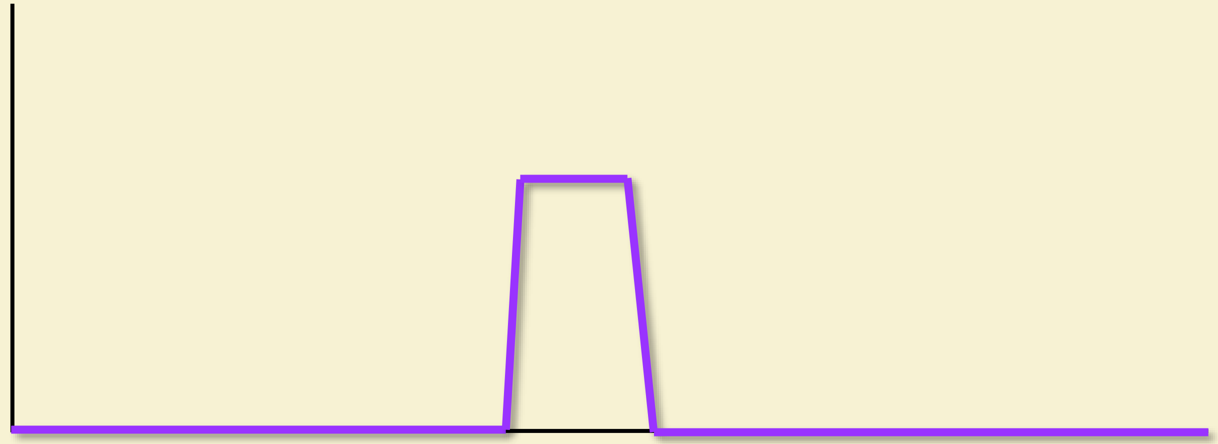




Higher dimension

$r(x) = \max(\langle \alpha, x \rangle + \beta, 0)$, $d + 1$ parameters

$I(x)$

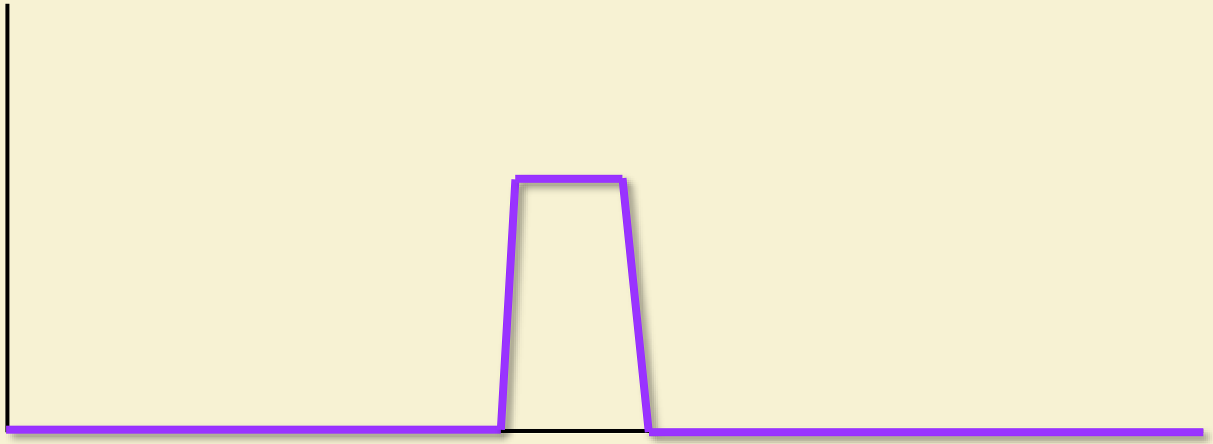


$J_{(1,0)}(x, y) = I(x)$

Higher dimension

$r(x) = \max(\langle \alpha, x \rangle + \beta, 0)$, $d + 1$ parameters

$I(x)$



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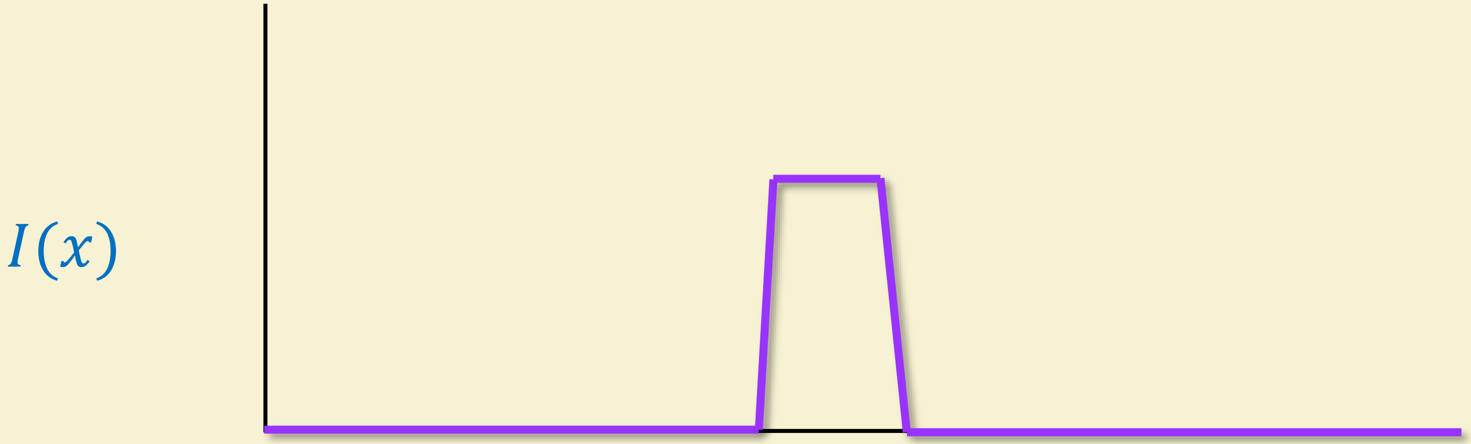
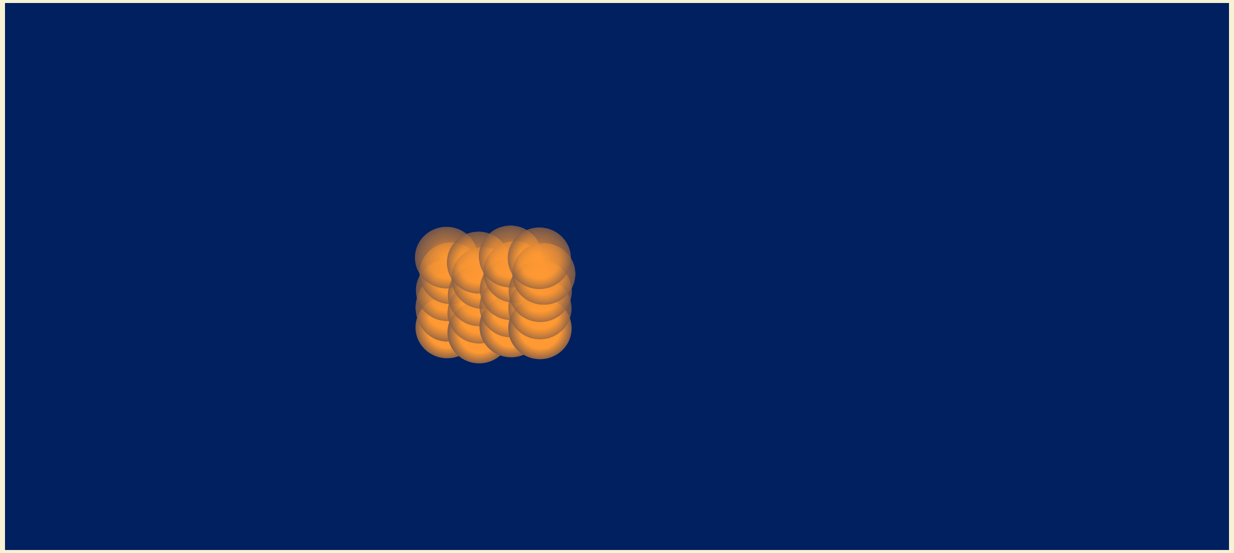




How many ReLU's

Every $f: [0,1]^d \to \mathbb{R}$ can be approximated as sum of $r_{\alpha,\beta}(x) = \max(\langle \alpha, x \rangle + \beta)$

Can discretize $\mathbb{R}^{d+1}$ to $O(1)^d$ points – need at most $O(1)^d = 2^{O(d)}$ ReLUs

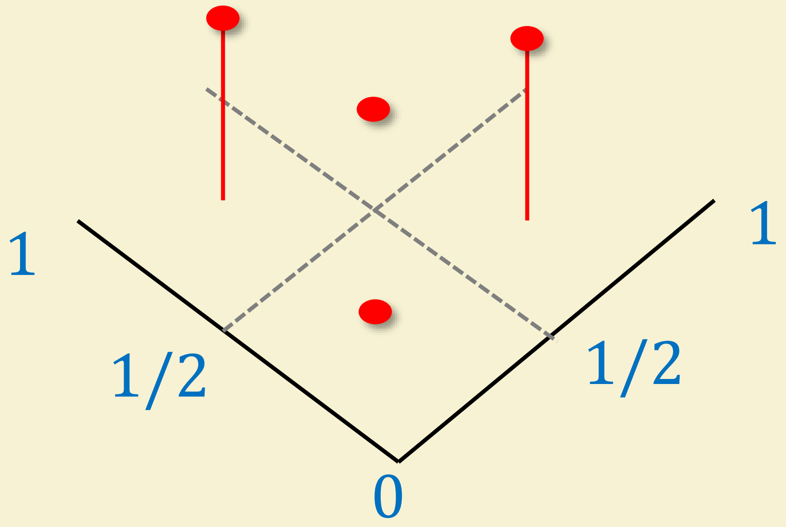
(For formal proofs, see Cybenko '89, Hornik '91, Barron '93; MIT 18.408)

THM: For some f's , $2^{c \cdot d}$ ReLU's are necessary

Random $f: [0,1]^d \to \mathbb{R}$

Choose $f(x) \in \{0,1\}$ independently at random
for $\mathrm{x} \in \{1/4, 3/4\}^d$

Extend linearly



LEMMA: For every fixed $g: [0,1]^d \to \mathbb{R}$, $\Pr\left[\, \int |f - g| < 0.1 \,\right] \leq 2^{-\epsilon \cdot 2^d}$

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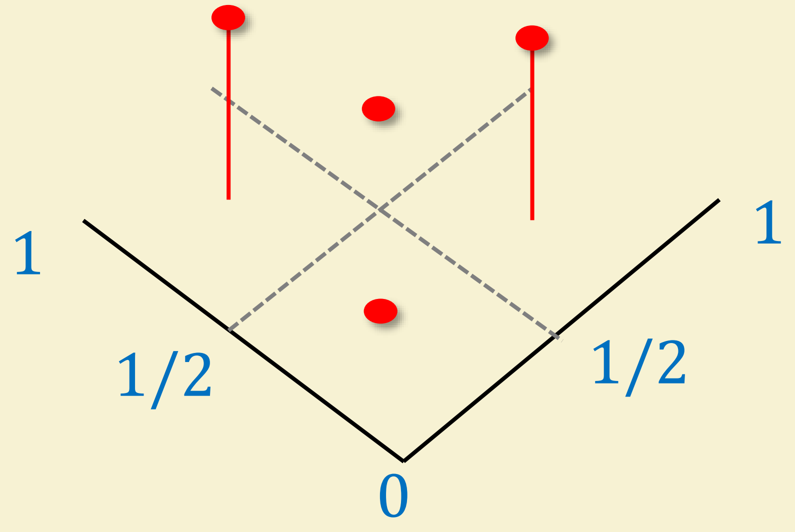


LEMMA: For every fixed $g: [0,1]^d \to \mathbb{R}$, $\Pr[\int |f-g| < 0.1] \leq 2^{-\epsilon\cdot 2^d}$

LEMMA ⇒ THEORM: Need $2^{\epsilon\cdot 2^d}$ distinct g's ⇒ need $\approx 2^d$ distinct ReLUs

PROOF OF LEMMA:
For $x \in \{1/4,3/4\}^d$ let $Z_x = 1$ iff $\int |g(y) - f(y)| dy > 0.2$ over $y \in [-1/4, +1/4]^d + x$

Each Z_x is independent with expectation at least $1/2$

$\Rightarrow \Pr[\frac{1}{2^d}\sum Z_x < 1/4] \leq 2^{-0.1\cdot 2^d}$ $\quad\quad$ $\frac{1}{2^d}\sum Z_x \geq 1/4 \Rightarrow \int |g-f| \geq 1/20$ $\blacksquare$

Bottom line

For every* function $f: \mathbb{R}^d \to \mathbb{R}$ many choices of $\varphi: \mathbb{R}^d \to \mathbb{R}^N$ s.t.

$$f \approx Linear_f \circ \varphi$$

Want to find φ that is useful for many interesting functions f

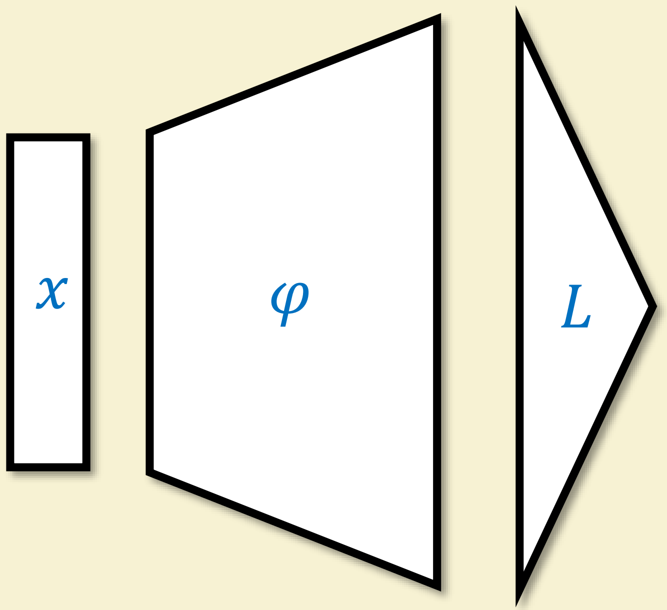
Or f's such that $\psi \circ f$ interesting for some non-linear $\psi: \mathbb{R} \to \mathbb{R}$

useful:

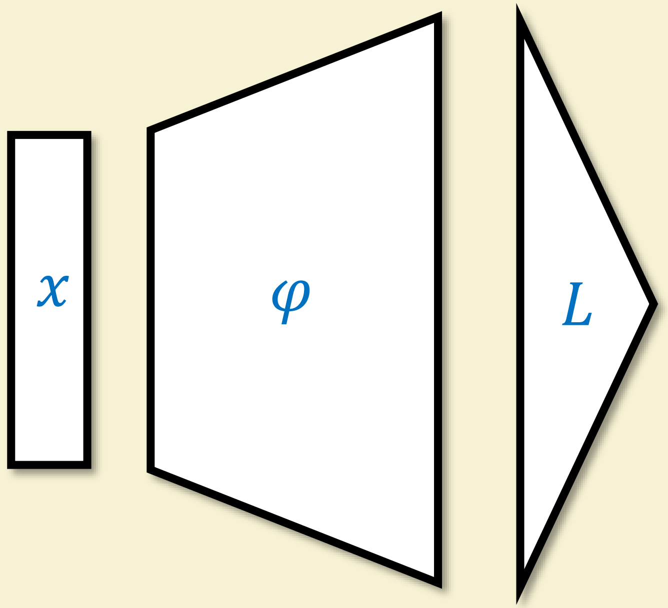
- N is not too big
- Efficiently compute $\varphi(x)$ or $\langle \varphi(x), \varphi(y) \rangle$
- $\langle \varphi(x), \varphi(y) \rangle$ large $\Leftrightarrow$ x and y are "semantically similar"
- For interesting f's, coefficients of $Linear_f$ are *structured*.
- …

Part IV: Kernels

Neural Net



Kernel



Definitely NN

Definitely Kernel

φ trained end-to-end for task at hand	φ pretrained with same data	φ pretrained on different data	φ pretrained on synthetic data	φ hand-crafted based on neural architectures	φ hand-crafted before 1990s

Kernel methods (intuitively)

Distance measure $K(x, x')$

Input: $(x_1, y_1), \dots, (x_n, y_n)$ s.t. $f^*(x_i) \approx y_i$

To approx $f^*(x)$ output y_i for x_i closest to x

or output $\sum \alpha_i y_i$ with α_i depending on $K(x, x_i)$

Hilbert Space

Linear space: $v + u$, $c \cdot v$

Dot product: $\langle u, v + c \cdot w \rangle = \langle u, v \rangle + c\langle u, w \rangle$, $\langle u, v \rangle = \langle v, u \rangle$, $\langle v, v \rangle \geq 0$

Can solve linear equations of form $\{ \langle v_i, x \rangle = b_i \}$ knowing only $\langle v_i, v_j \rangle$

Also do least-square minimization $\min_x \sum (\langle v_i, x \rangle - b_i)\hat{}2$ knowing only $\langle v_i, v_j \rangle$

DEF: Sym matrix $K \in \mathbb{R}^{n \times n}$ is p.s.d. if $v^T K v \geq 0$ for all $v \in \mathbb{R}^n$

Equivalently $\lambda_1(K), \ldots, \lambda_n(K) \geq 0$

CLAIM: K is p.s.d. iff* $u^T K v$ is inner product

PROOF ($\Rightarrow$): $u^T K v = \psi(u) \cdot \psi(v)$ where $\psi(u_1, \ldots, u_n) = (\sqrt{\lambda_1} u_1, \ldots, \sqrt{\lambda_n} u_n)$, expressed in eigenbasis

Kernel Methods

Goal: Solve linear equations, least-square minimization, etc. under φ

Observation: Enough to compute $\mathrm{K}(\mathrm{x}, \mathrm{x}') = \langle \varphi(x), \varphi(x') \rangle$

Let $\hat{x} = \varphi(x)$, given $\{\hat{x}_i, y_i\}_{i=1..n}$ want to find $\widehat{w} \in \mathbb{R}^n$ s.t. $\langle \hat{x}_i, \widehat{w} \rangle \approx y_i \ \forall i$

can compute $\widehat{w} = \sum \alpha_i \ \hat{x}_i$ using $K(x_i, x_j)$

To compute prediction on new x using $\widehat{w}$, can compute $\hat{x} = \sum \beta_i \ \hat{x}_i$ using $K(x, x_i)$