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A guided tour of machine learning (theory)

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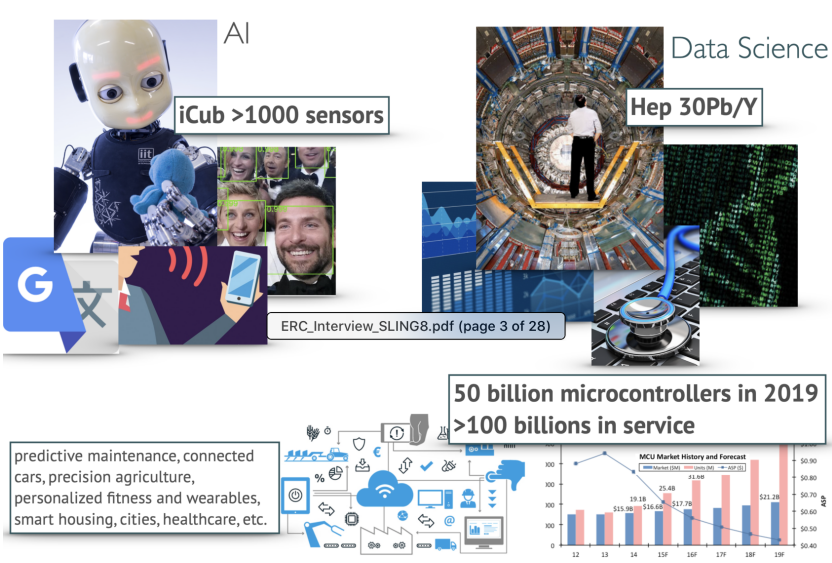
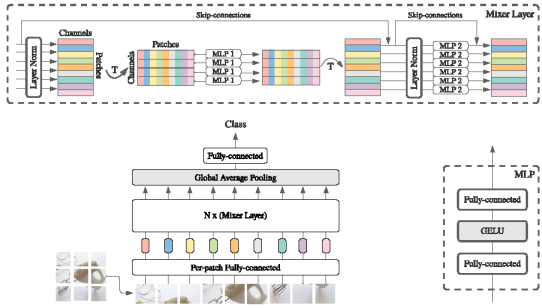
RoMaDS Colloquim, University of Rome Tor Vergata, May 9th 2022

AI everywhere (literally...)



The state of affairs



Rethinking machine learning:

- with statistical mechanics
- with information theory
- with tropical geometry
- ...

Outline

Data driven modeling paradigm

Statistical learning, bias and variance

From statistics to optimization

A theory crisis?

The basic picture

$$(x_i, y_i)_{i=1}^n \quad \mapsto \quad f : X \to Y$$

Fixing a model

$$w \in \mathbb{R}^p \;\mapsto\; f_w$$

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$$f_w(x) = \sum_{j=1}^{p} w^j \phi_j(x)$$

$$f_w(x) = \sum_{j=1}^{p} \beta^j \sigma(a_j^\top x + \alpha_j),$$

Fitting (or overfitting??)

$$\min_{w} \frac{1}{n} \sum_{i=1}^{n} (f_w(x_i) - y_i)^2$$

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Overparametrization

w has often millions of parameters...data are often (much) less!

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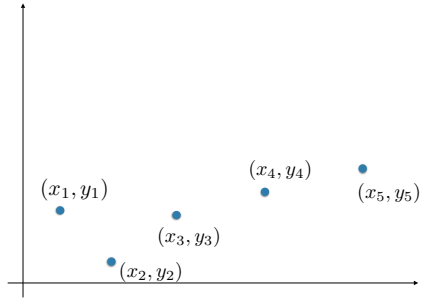
Overparametrization

w has often millions of parameters...data are often (much) less!

> "With four parameters I can fit an elephant, and with five I can make him wiggle his trunk"
>
> von Neumann

Learning is not (just) fitting, but prediction



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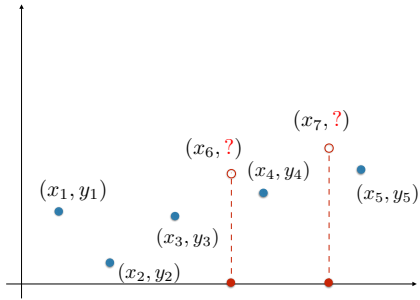

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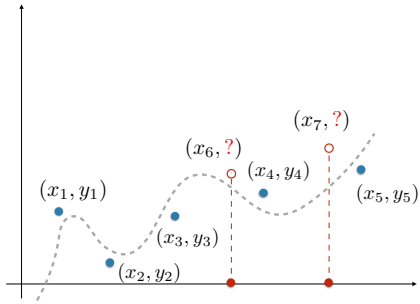

Predictions from random and noisy samples

Learning pipeline

Model fitting (regularized)

$$\widehat{w}_\theta = \underset{\|w\| \leqslant \theta}{\operatorname{argmin}} \frac{3}{n} \sum_{i=1}^{n/3} (f_w(x_i) - y_i)^2$$

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Model tuning

$$\widehat{\theta} = \underset{\theta}{\operatorname{argmin}} \frac{3}{n} \sum_{i=n/3+1}^{2n/3} (f_{\widehat{w}_\theta}(x_i) - y_i)^2$$

Learning pipeline

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Model assessment

$$\frac{3}{n} \sum_{i=2n/3+1}^{n} (f_{\widehat{w}_{\widehat{\theta}\,\theta}}(x_i) - y_i)^2$$

Classic vs data driven modeling

- Paradigm shift in modeling, **driven by data** availability.
- Careful **pipeline** needed.
- **Theoretical** guidance needed.

ML theory

- Representation: ”Which model?”
- Generalization: ”How accurate is my model?”
- Optimization: ”How can I compute my model?”

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Statistical learning, bias and variance

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Statistical machine learning

- $(X, Y) \sim P$ random variables in $\mathbb{R}^d \times \mathbb{R}$, and $(x_1, y_1), \ldots, (x_n, y_n) \sim P^n$.

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- $\ell : \mathbb{R} \times \mathbb{R} \to [0, \infty)$ loss function, e.g. $\ell(f(x), y) = (y - f(x))^2$.

Problem: minimize

$$L(f) = \mathbb{E}[\ell(f(X), Y)],$$

given only $(x_1, y_1), \ldots, (x_n, y_n) \sim P^n$.

ERM and its excess risk

$$\widehat{w}_\theta = \operatorname*{argmin}_{\|w\| \leqslant \theta} \widehat{L}(f_w), \qquad \widehat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

$$\widehat{f}_\theta = f_{\widehat{w}_\theta}$$

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Excess risk

$$L(\widehat{f}_\theta) - \min L(f)$$

Error decomposition

Population algorithm

$$f_\theta = f_{w_\theta}, \qquad w_\theta = \operatorname*{argmin}_{\|w\| \leqslant \theta} L(f_w)$$

Error decomposition

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$$f_\theta = f_{w_\theta}, \qquad w_\theta = \operatorname*{argmin}_{\|w\| \leqslant \theta} L(f_w)$$

$$L(\widehat{f}_\theta) - \min L(f) = \underbrace{L(\widehat{f}_\theta) - L(f_\theta)}_{\text{Estimation error}} + \underbrace{L(f_\theta) - \min L(f)}_{\text{Approximation error}}$$

Approximation error

Assume

$$|\ell(y, f(x)) - \ell(y, f(x))| \leqslant C_\ell |f(x) - f'(x)|$$

Lemma

Let $L(f_*) = \min L(f)$, *then*

$$L(f_\theta) - \min L(f) \leqslant C_\ell \min_{\|w\| \leqslant \theta} \|f_\theta - f_*\|_{L^1(P)}$$

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$$L(f_\theta) - \min L(f) \leqslant C_\ell \min_{\|w\| \leqslant \theta} \|f_\theta - f_*\|_{L^1(P)}$$

Proof.

$$L(f_\theta) - L(f_*) = \min_{\|w\| \leqslant \theta} \int (\ell(f(x), y) - \ell(f_*(x), y)) dP(x, y) \leqslant C_\ell \min_{\|w\| \leqslant \theta} \int |f(x) - f_*(x)| dP(x, y)$$

□

[Cucker, Zhou '93]

Universality

A model is universal if for all f_*

$$\lim_{\theta \to \infty} \|f_\theta - f_*\|_{L^1(P)} = 0.$$

e.g. Kernel methods and neural nets.

[DeVore, Lorentz '93, Pinkus '99]

Smoohtness conditions

Assume

$$f_* \in \mathcal{H}_s,$$

for some smoothness class $\mathcal{H}_s$. e.g. the Sobolev space $W^{s,2}$.

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Approximation results ensure that

$$\min_{\|w\| \leqslant \theta} \|f_\theta - f_*\|_{L^1(P)} \lesssim a(\theta, s)$$

where $a(\theta, a)$ decays for θ incresing and rate depending on s, e.g. $\theta^{-s/d}$

[DeVore, Lorentz, '93]

Estimation error

Lemma

By definition of ERM, it holds

$$L(\widehat{f}_\theta) - L(f_\theta) \leqslant C_\ell \sup_{\|w\| \leqslant \theta} |\widehat{L}(f_w) - L(f_w)|$$

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Proof.

$$L(\widehat{f}_\theta) - L(f_\theta) = L(\widehat{f}_\theta) - \widehat{L}(\widehat{f}_\theta) + \underbrace{\widehat{L}(\widehat{f}_\theta) - \widehat{L}(f_\theta)}_{\leqslant 0} + \widehat{L}(f_\theta) - L(f_\theta)$$

□

[Vapnilk, Chervonenkis, '77, Gyorfi, Devroye, Lugosi, '96]

Capacity measures

Empirical process

$$\sup_{\|w\| \leqslant \theta} |\widehat{L}(f_w) - L(f_w)|$$

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$$\sup_{\|w\| \leqslant \theta} |\widehat{L}(f_w) - L(f_w)|$$

Lemma (Rademacher complexities)

If $\sigma_i \in \{\pm 1\}, P(1) = P(-1) = 1/2, i = 1, \dots, n$ *(Rademacher random variables), then*

$$\mathbb{E}\left[\sup_{\|w\| \leqslant \theta} |\widehat{L}(f_w) - L(f_w)|\right] \leqslant 2C_\ell \underbrace{\mathbb{E}\left[\frac{1}{n} \sup_{\|w\| \leqslant \theta} \sum_{i=1}^{n} \sigma_i f_w(x_i)\right]}_{\text{Rademacher complexity}},$$

Capacity measures for linear models

$$f_w = \sum_{j=1}^{\infty} w^j \phi_j$$

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Lemma

If

$$\sup_x |\sum_{j=1}^{\infty} \phi_j(x)|^2 \leqslant \kappa^2$$

then

$$\mathbb{E}\left[\frac{1}{n} \sup_{\|w\| \leqslant \theta} \sum_{i=1}^{n} \sigma_i f_w(x_i)\right] \leqslant \frac{\theta\kappa}{\sqrt{n}}$$

Results for nonlinear models can be similarly derived.

The bias-variance trade-off

$$L(\widehat{f}_\theta) - \min L(f) \lesssim \frac{\theta}{\sqrt{n}} + a(\theta, s)$$

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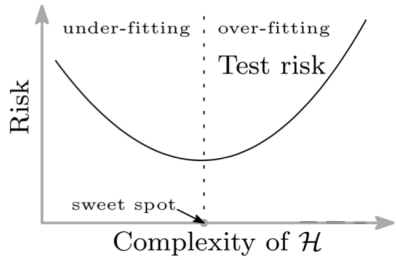

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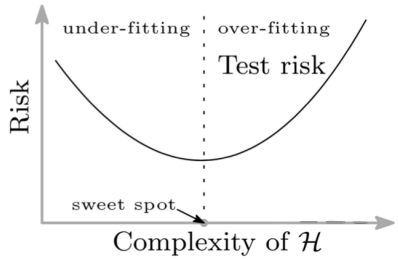

$$\theta_* = \theta(s, n) \quad \Longrightarrow \quad L(\widehat{f}_{\theta_*}) - \min L(f) \lesssim \epsilon(n, s)$$

where $\epsilon(\theta, a)$ decays with n increasing and rate depending on s, e.g. $n^{-\frac{2s}{2s+d}}$

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Enter optimization

$$\min_{\|w\| \leqslant \theta} \widehat{L}(f_w)$$

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Gradient methods

$$\widehat{w}_{\theta,t+1} = P_\theta \left(\widehat{w}_{\theta,t} - \gamma_t \nabla \widehat{L}(f_{\widehat{w}_{\theta,t}}) \right)$$

Hard to prove convergence unless the model is linear...

Linear models

$$f_w = \sum_{j=1}^{\infty} w^j \phi_j \quad + \quad \ell \quad \text{convex}$$

$$\Longrightarrow \min_{\|w\| \leqslant \theta} \widehat{L}(f_w) \quad \text{convex problem!}$$

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$$\Longrightarrow \min_{\|w\| \leqslant \theta} \widehat{L}(f_w) \quad \text{convex problem!}$$

Optimization results ensures that $\widehat{f}_{\theta,t} = f_{\widehat{w}_{\theta,t}}$

$$\widehat{L}(\widehat{f}_{\theta,t}) - \min_{\|w\| \leqslant \theta} \widehat{L}(f) \leqslant \delta_t$$

with δ_t decaying in t.

[Nesterov, '03]

Estimation + optimization error

Lemma

$$L(\widehat{f}_{\theta,t}) - L(f_\theta) \leqslant C_\ell \sup_{\|w\| \leqslant \theta} |\widehat{L}(f_w) - L(f_w)| + \delta_t$$

Estimation + optimization error

Lemma

$$L(\widehat{f}_{\theta,t}) - L(f_\theta) \leqslant C_\ell \sup_{\|w\| \leqslant \theta} |\widehat{L}(f_w) - L(f_w)| + \delta_t$$

Proof.

$$L(\widehat{f}_{\theta,t}) - L(f_\theta) = L(\widehat{f}_{\theta,t}) - \widehat{L}(\widehat{f}_{\theta,t}) + \underbrace{\widehat{L}(\widehat{f}_{\theta,t}) - \widehat{L}(f_\theta)}_{\leqslant \delta_t} + \widehat{L}(\widehat{f}_\theta) - L(f_\theta)$$

□

The statistical-optimization trade-off

$$L(\widehat{f}_{\theta,t}) - \min L(f) \lesssim \frac{\theta}{\sqrt{n}} + a(\theta, s) + \delta_t$$

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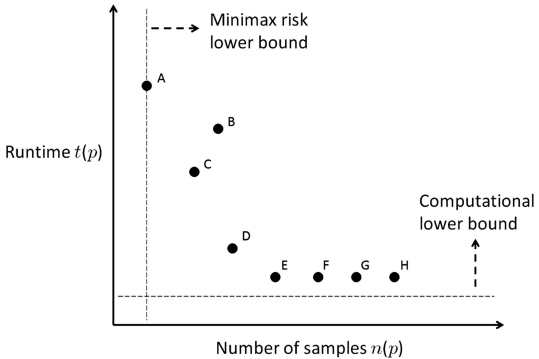

[Bousquet, Bottou '07, Chendrasekaran Jordan, '12]

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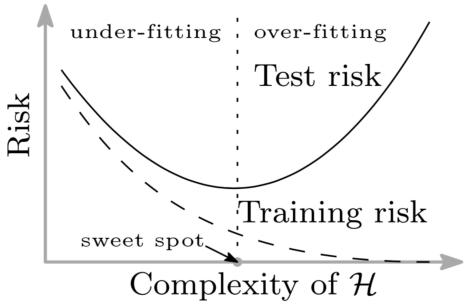
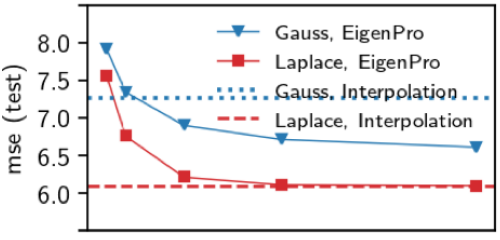
Was it all wrong?





Explicit regularization

$$\min_{\|w\| \leqslant \theta} \widehat{L}(f_w) \qquad \widehat{w}_{\theta,t+1} = P_\theta \left(\widehat{w}_{\theta,t} - \gamma_t \nabla \widehat{L}(f_{\widehat{w}_{\theta,t}}) \right)$$

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Implicit regularization

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \nabla \widehat{L}(f_{\widehat{w}_t})$$

Can we characterize $\widehat{f}_t = f_{\widehat{w}_t}$

$$L(\widehat{f}_t) - L(f_*)$$

Inexact optimization with linear models

Linear models: $f_w = \sum_{j=1}^{\infty} w^j \phi_j$, ℓ convex and

$$w_{t+1} = w_t - \gamma_t \nabla L(f_{w_t}),$$

then for $f_t = f_{w_t}$

$$L(f_t) - L(f_*) \leqslant \delta_t.$$

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then for $f_t = f_{w_t}$

$$L(f_t) - L(f_*) \leqslant \delta_t.$$

Idea: consider

$$\widehat{w}_{t+1} = \widehat{w}_t - \gamma_t \left(\nabla L(f_{\widehat{w}_t}) + e_t\right)$$

with

$$e_t = \widehat{\nabla L}(f_{\widehat{w}_{\theta,t}}) - \nabla L(f_{\widehat{w}_{\theta,t}}).$$

[Rockafellar, '76, Salzo, Villa '11, Schmidt, Le Roux, Bach '11]

Excess risk control with inexact gradient

Lemma

$$L(\widehat{f}_t) - L(f_*) \leqslant \delta_t + \sum_{j=1}^{t} \left\langle e_t, \widehat{f}_t - f_* \right\rangle .$$

Excess risk control with inexact gradient

Lemma

$$L(\widehat{f}_t) - L(f_*) \leqslant \delta_t + \sum_{j=1}^{t} \left\langle e_t, \widehat{f}_t - f_* \right\rangle .$$

Need to control:

- gradient error e_t,
- path $(\widehat{f}_j)_j$ around f_*.

Gradient concentration

$$\mathbb{E}\left[\sup_{\|w\|\leqslant\theta}\|\nabla\widehat{L}(f_w)-\nabla L(f_w)\|\right]\lesssim\frac{\theta}{\sqrt{n}}$$

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Path control

For $j\lesssim\sqrt{n}$

$$\|\widehat{f}_t-f_*\|\lesssim\|f_*\|.$$

[Stankewitz, Mücke, R. '21, see also Lin R. '17]

Excess risk control with inexact gradient

Theorem (Stankewitz, Mücke, R. '21)

] For $t \lesssim \sqrt{n}$,

$$\mathbb{E}\left[L(\widehat{f}_t) - L(f_*)\right] \lesssim \frac{1}{\sqrt{n}}$$

Same as explicit regularization: implicit regularization a *new* algorithmic idea[1].

[1] In inverse problem the idea is known since the '50s as iterative regularization …

”Looking for the lost keys under the lamp, because that’s where the light is.”, Yann Lecun

- Can we explain the lack of variance? Learning & interpolation?
- **Are linear model of any practical use?**
- Can linear model explain deep learning?

ML meets large scale computing

Scalable implementations needed $\mapsto$ FALKON

Function `Falkon`$(X \in \mathbb{R}^{n\times d}, y \in \mathbb{R}^n, \lambda, m, t)$**:**

$X_m \leftarrow$ `RamdomSubsample`(X, m);

$T, A \leftarrow$ `Preconditioner`(X_m, λ);

Function `LinOp`(β)**:**

$v \leftarrow A^{-1}\beta$;

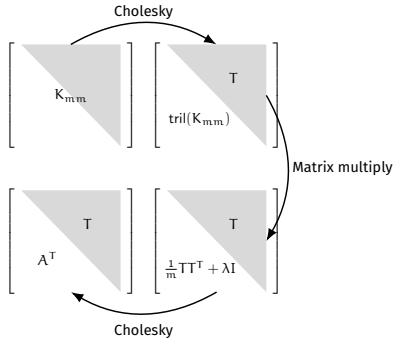
$c \leftarrow k(X_m, X)k(X, X_m)T^{-1}v$;

return $A^{-\top}T^{-\top}c + \lambda n v$;

rhs $\leftarrow A^{-\top}T^{-\top}k(X, X_m)y$;

$\beta \leftarrow$ `ConjugateGradient`$($`LinOp`, rhs, $t)$;

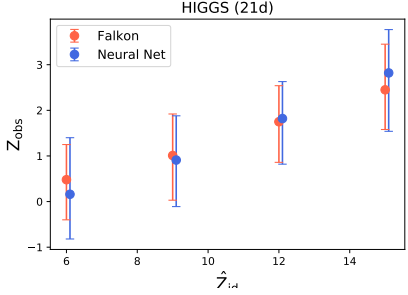
return $T^{-1}A^{-1}\beta$;



[Meanti, Carratino, R., Rudi '20, Meanti, Carratino, De Vito, R. '21]

Efficient linear models in practice: HEP

[Wulzer, D'Agnolo '18]



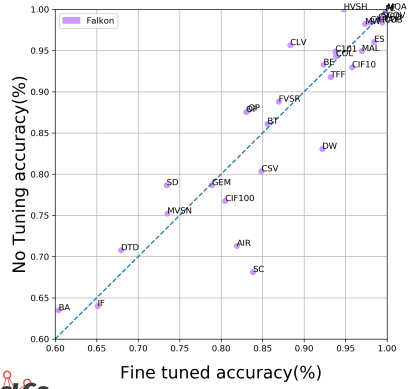
Model	DIMUON	SUSY	HIGGS
Falkon	(53.8 ± 1.9) s	(44.8 ± 1.5) s	(88.7 ± 2.2) s
Neural Net	(4.23 ± 0.73) h	(73.1 ± 10) h	(112 ± 9) h

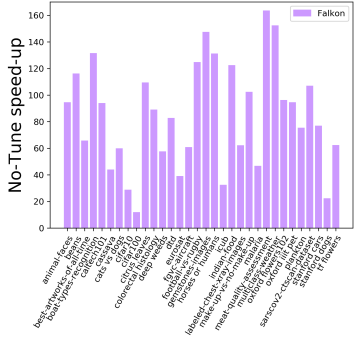
Table 4: Average training times per single run with standard deviations.

[Letizia et al. '21]

Efficient linear models in practice: vision

$$f(x) = \langle w, \Phi(x) \rangle, \quad x \mapsto \underbrace{\Phi_L}_{\text{Efficient linear learning}} \circ \underbrace{\Phi_{L-1} \cdots \circ \Phi_1(x)}_{\text{Pre-trained layers}}$$





[Alfano, Pastore, Odone, R. '21]

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Neural nets as a linear model?

$$f(x) = \sum_{j=1}^{p} \beta^j \sigma(a_j{}^\top x + \alpha_j)$$

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Key idea: Let $\rho(x, \underbrace{(a, \alpha)}_{\xi}) = \sigma(a_j{}^\top x + \alpha_j)$.

$$f_\mu(x) = \int \rho(x, \xi) d\mu(\xi), \qquad \mu = \sum_{j=1}^{q} \delta_{\xi_j} \beta_j$$

[Bach '14, Montanari et al. 18, ...]

Optimality of neural nets

$$f_\mu(x) = \int \rho(x, \xi) d\mu(\xi) = \langle \rho(x, \cdot), \mu \rangle \,, \qquad \|f\|_{\mathcal{B}} = \|\mu\|_{TV}$$

Optimality of neural nets

$$f_\mu(x) = \int \rho(x, \xi) d\mu(\xi) = \langle \rho(x, \cdot), \mu \rangle, \qquad \|f\|_{\mathcal{B}} = \|\mu\|_{TV}$$

Theorem (Bartolucci, De Vito, R., Vigogna, '21)

The problem

$$\min_{f \in \mathcal{B}} \widehat{L}(f) + \|f\|_{\mathcal{B}}$$

has a solution of the form

$$f(x) = \sum_{i=1}^{u} \beta^j \rho(x, \lambda_i), \quad u \leqslant n.$$

see also [Bredies and Carioni '20, Unser et al. '17, Unser '20, Parhi and Nowak '20].

Wrapping up

- From bias-variance…
- …to statistics-optimization trade-off.
- Statistical learning 2.0?

What's next?

- Physics (equation?) informed ML.
- ML for Inverse problems.
- BIGGER linear models: ML meets scientific computing/HPC.

Multiple post-docs/PhD positions @MaLGa!

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