

Discrepancies are Virtue: Weak-to-Strong Generalization through Lens of Intrinsic Dimension

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FSML

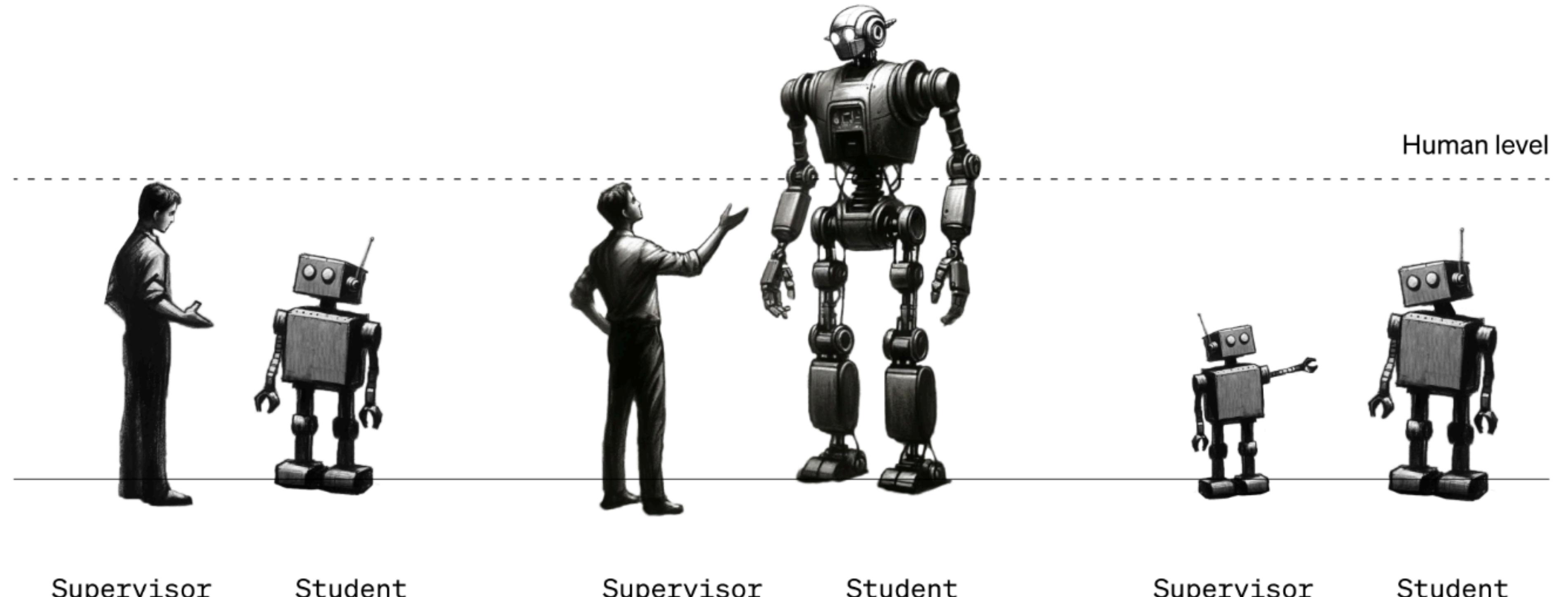
Superalignment → weak-to-strong (W2S) generalization

Traditional ML

Superalignment

W2S

[Burns et al, ICML2024]



When and how does weak-to-strong generalization happen?

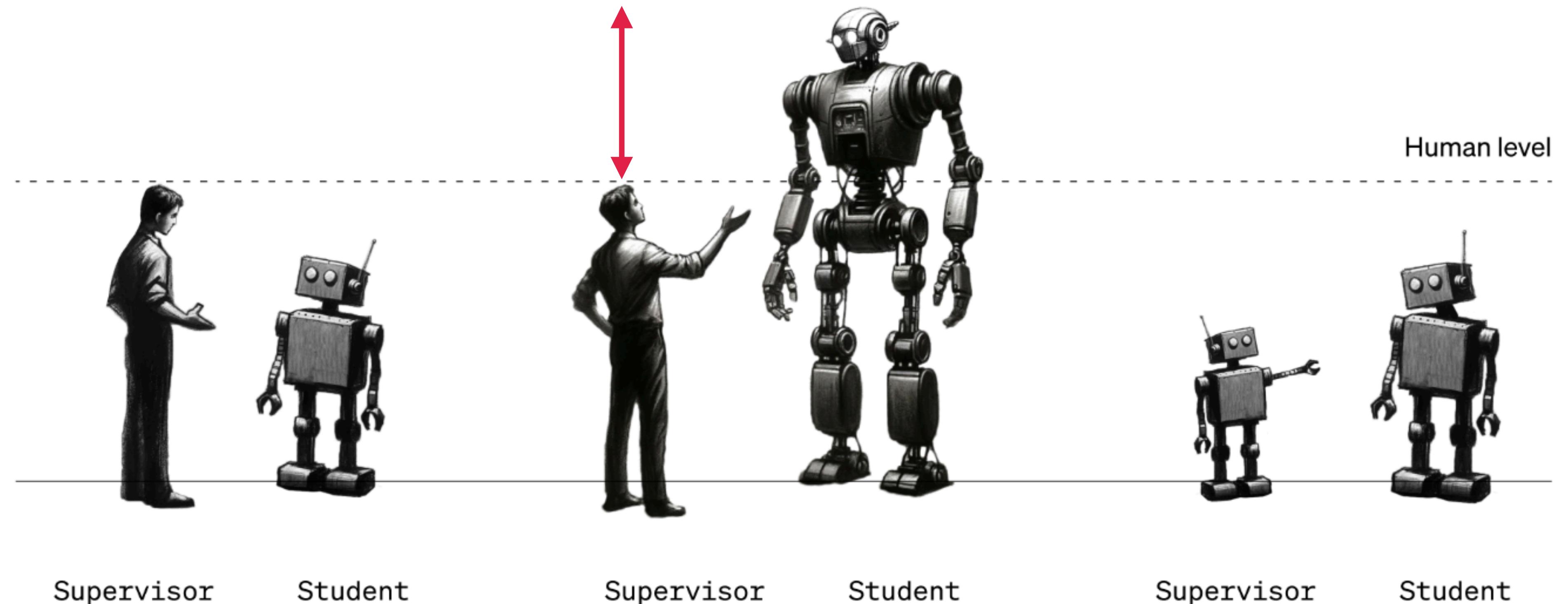
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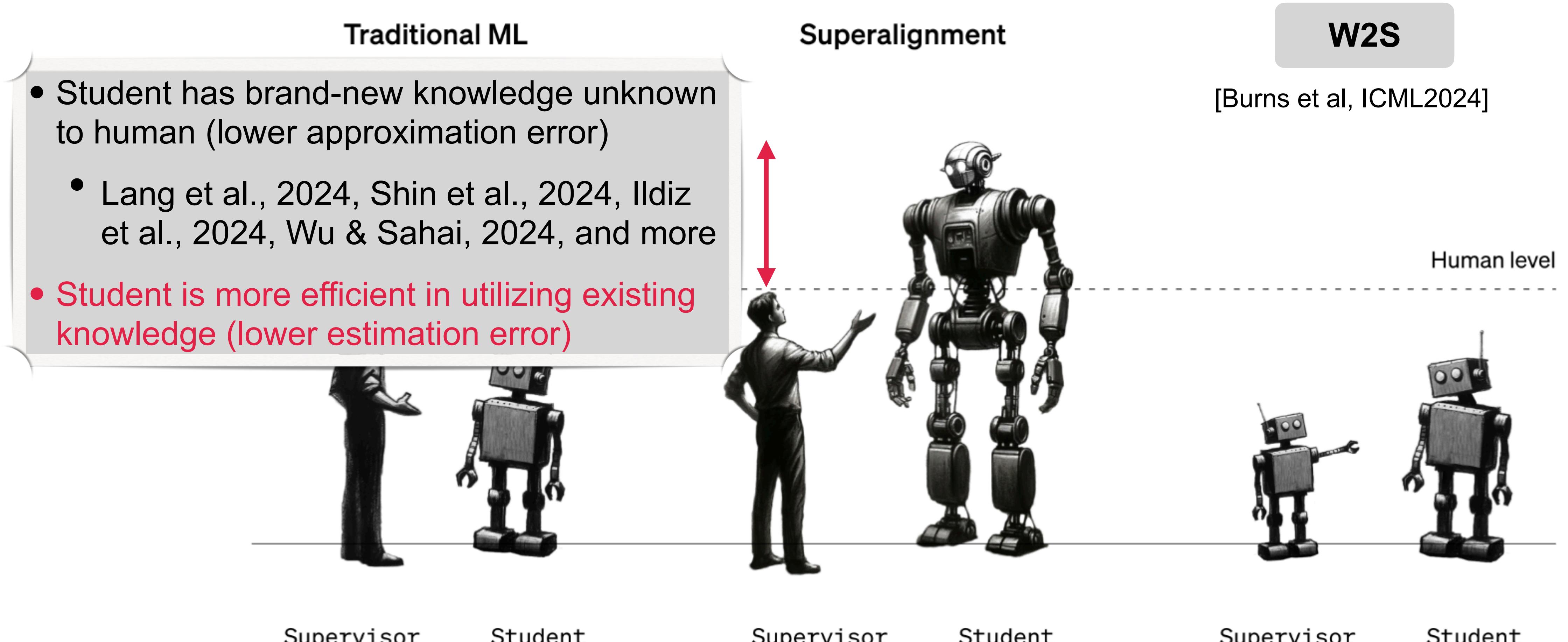
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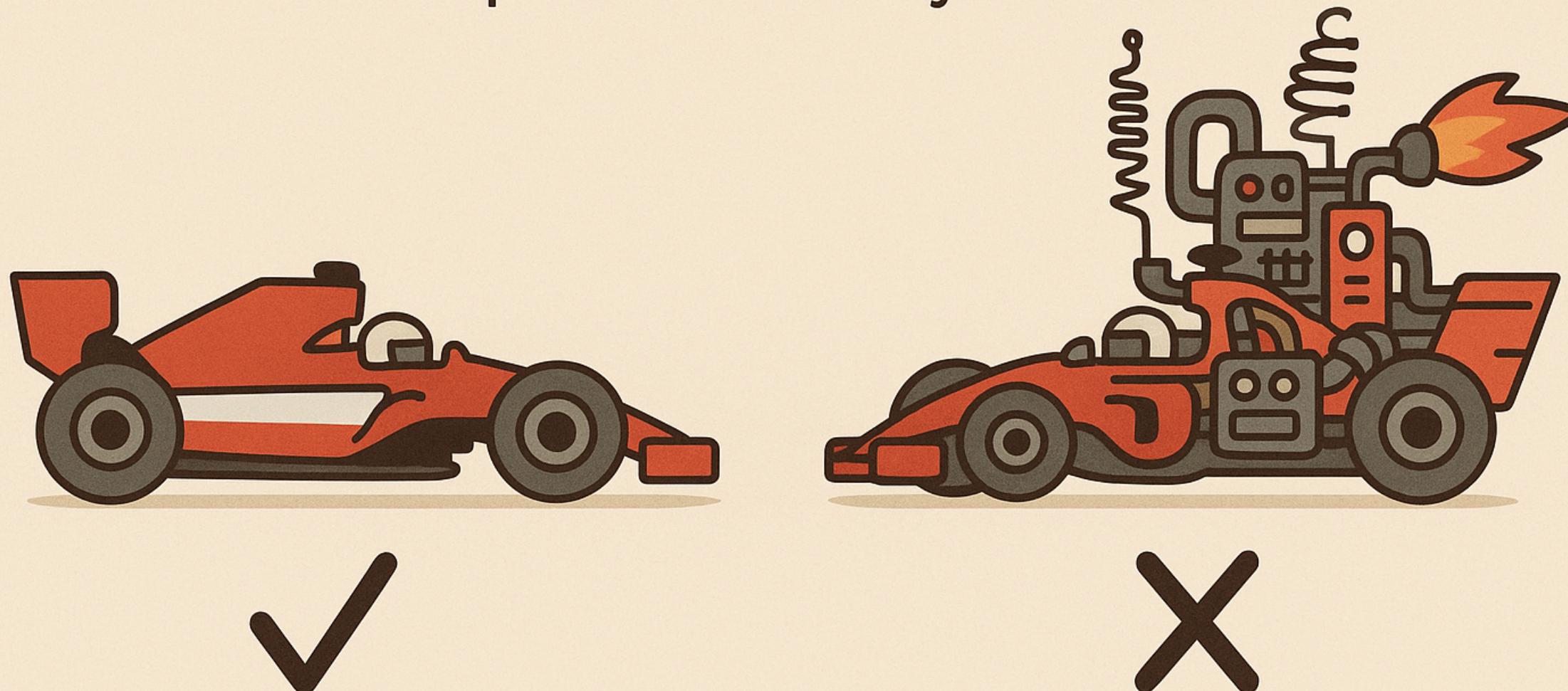


When and how does weak-to-strong generalization happen?

Intrinsic dimension

OCCAM'S RAZOR

When faced with multiple hypotheses,
the simplest is usually the best



Intrinsic dimension = the minimal number of model parameters needed to achieve (nearly) optimal performance on a specific task

Pretrained
initialization

$$\theta^D = \theta_0^D + \Gamma \theta^d$$

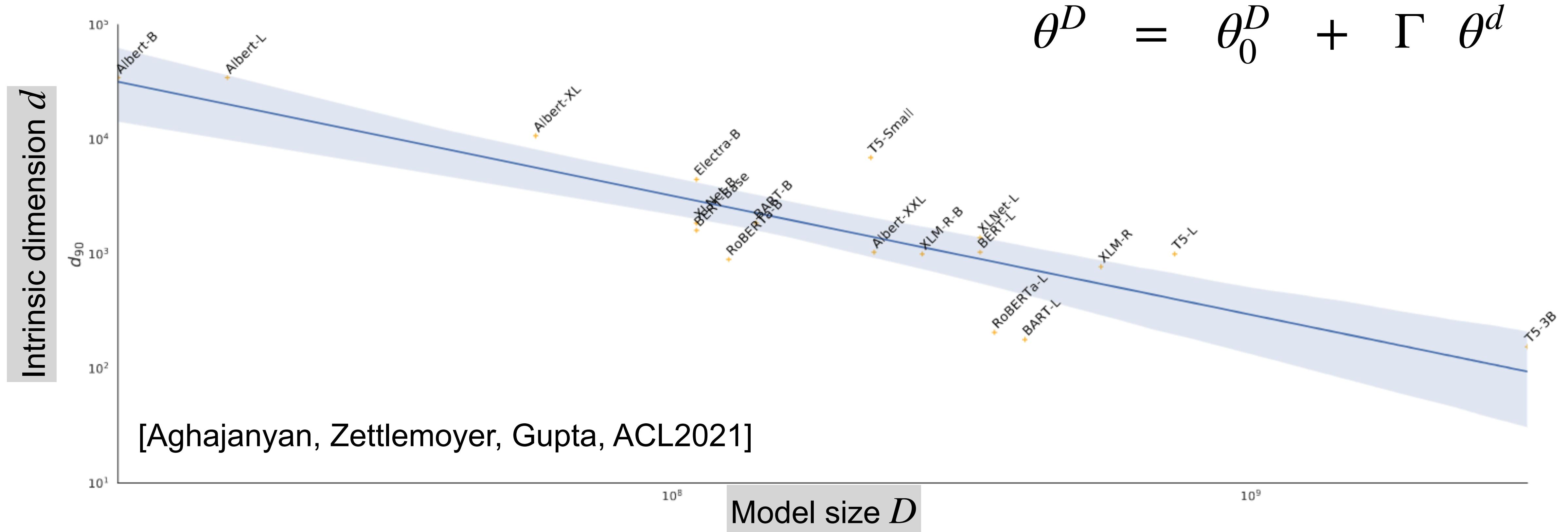
Model parameter of
high dimension D

Finetunable parameter of
intrinsic dimension $d < D$

$$D \times d \text{ random projection}$$

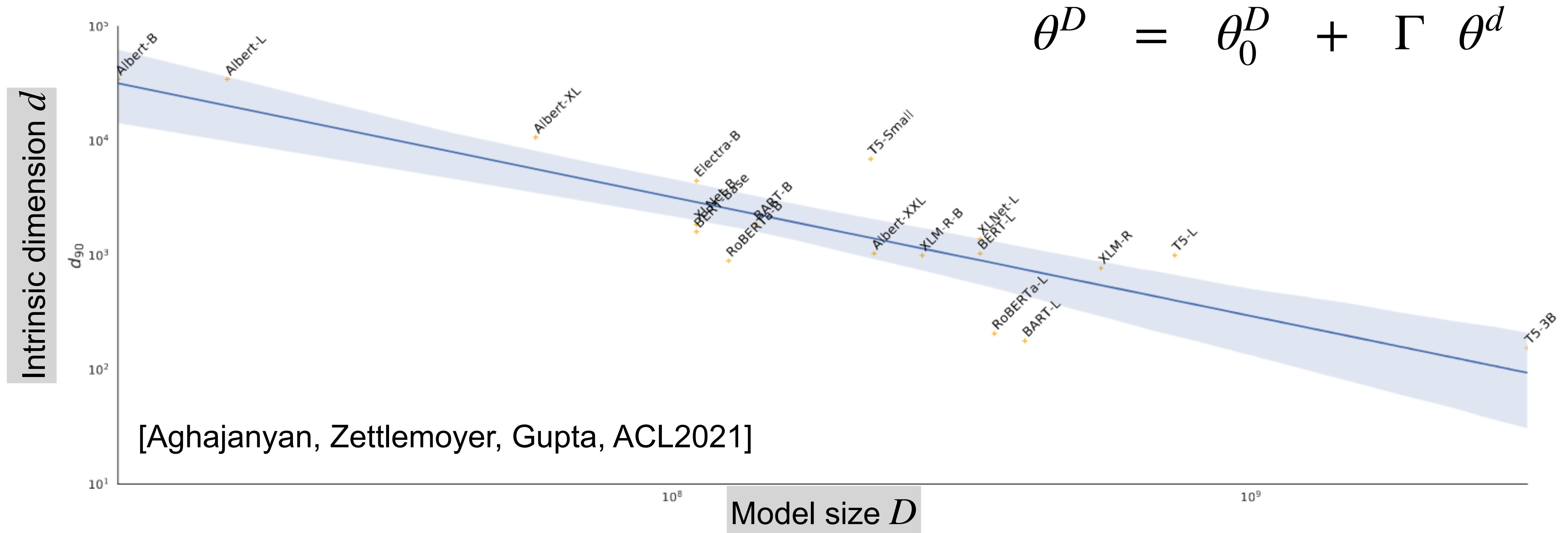
Low intrinsic dimension of finetuning

Learning over a well-pretrained model (e.g. finetuning) usually exhibits **low intrinsic dimensions**.



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Larger pretrained language models have lower intrinsic dimensions on downstream tasks!

Finetuning with low intrinsic dimensions

Downstream task

- $(x, y) \sim \mathcal{D}(f_*)$ s.t. $y = f_*(x) + z$ with i.i.d. noise $z \sim \mathcal{N}(0, \sigma^2)$ and $|f_*(x)| < 1$ a.s.
- Want to learn the ground truth function $f_* : \mathcal{X} \rightarrow \mathbb{R}$ given access to two datasets:
 - **Labeled** (small) dataset: $\tilde{X} \in \mathcal{X}^n$ with noisy labels $\tilde{y} \in \mathbb{R}^n$
 - **Unlabeled** (large) dataset: $X \in \mathcal{X}^N$ with unknown labels $y \in \mathbb{R}^N$

Finetuning (FT) \approx linear probing on low-rank gradient features

- FT falls in **kernel regime**: $f(x | \theta) = \phi(x)^\top \theta$ with finetunable parameter $\theta \in \mathbb{R}^d$
- Nonlinear case: $\phi(x) = \nabla_\theta f(x | \theta_0)$ = gradient at pretrained initialization $\theta_0 \in \mathbb{R}^d$
- **Weak** model $\phi_w : \mathcal{X} \rightarrow \mathbb{R}^d$ produces $\tilde{\Phi}_w = \phi_w(\tilde{X}) \in \mathbb{R}^{n \times d}$, $\Phi_w = \phi_w(X) \in \mathbb{R}^{N \times d}$
- **Strong** model $\phi_s : \mathcal{X} \rightarrow \mathbb{R}^d$ produces $\tilde{\Phi}_s = \phi_s(\tilde{X}) \in \mathbb{R}^{n \times d}$, $\Phi_s = \phi_s(X) \in \mathbb{R}^{N \times d}$

$$\text{rank}(\Sigma_w) = d_w \ll d \quad \text{rank}(\Sigma_s) = d_s \ll d$$

$$\Sigma_w = \mathbb{E}[\phi_w(x)\phi_w(x)^\top]$$

$$\Sigma_s = \mathbb{E}[\phi_s(x)\phi_s(x)^\top]$$

Weak v.s. strong: model capacity + similarity

Representation efficiency — low intrinsic dimensions:

$$\text{rank}(\Sigma_w) = d_w \ll d \quad \text{rank}(\Sigma_s) = d_s \ll d$$

Representation accuracy — FT approximation error: $0 \leq \rho_s \leq \rho_w \leq 1$ where

$$\rho_s := \min_{\theta \in \mathbb{R}^d} \mathbb{E}[(\phi_s(x)^\top \theta - f_*(x))^2] \quad \text{and} \quad \rho_w := \min_{\theta \in \mathbb{R}^d} \mathbb{E}[(\phi_w(x)^\top \theta - f_*(x))^2].$$

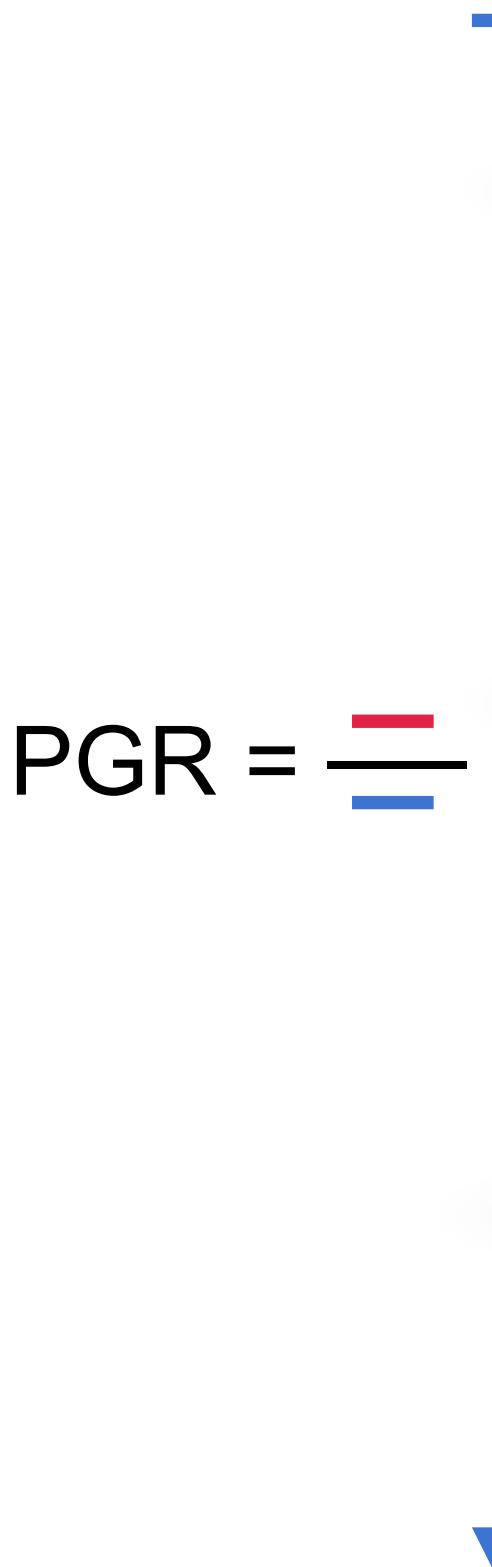
We are interested in the variance-dominated regime $\rho_s + \rho_w \ll \sigma^2$.

Representation similarity — correlation dimension: Consider spectral decompositions

$$\Sigma_s = \begin{matrix} V_s & \Lambda_s & V_s^\top \\ d \times d_s & d_s \times d_s & \end{matrix} \quad \text{and} \quad \Sigma_w = \begin{matrix} V_w & \Lambda_w & V_w^\top \\ d \times d_w & d_w \times d_w & \end{matrix}.$$

The correlation dimension of (ϕ_s, ϕ_w) is $d_{s \wedge w} = \|V_s^\top V_w\|_F^2$ s.t. $0 \leq d_{s \wedge w} \leq \min\{d_s, d_w\}$.

W2S finetuning as regression



Weak teacher $f_w(x) = \phi_w(x)^\top \theta_w$: $\theta_w = \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{n} \|\tilde{\Phi}_w \theta - \tilde{y}\|_2^2 + \alpha_w \|\theta\|_2^2$

W2S

W2S $f_{w2s}(x) = \phi_s(x)^\top \theta_{w2s}$: $\theta_{w2s} = \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{N} \|\Phi_s \theta - \Phi_w \theta_w\|_2^2 + \alpha_{w2s} \|\theta\|_2^2$

Strong SFT $f_s(x) = \phi_s(x)^\top \theta_s$: $\theta_s = \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{n} \|\tilde{\Phi}_s \theta - \tilde{y}\|_2^2 + \alpha_s \|\theta\|_2^2$

Strong ceiling $f_c(x) = \phi_s(x)^\top \theta_c$: $\theta_c = \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{n+N} \left\| \begin{bmatrix} \tilde{\Phi}_s \\ \Phi_s \end{bmatrix} \theta - \begin{bmatrix} \tilde{y} \\ y \end{bmatrix} \right\|_2^2 + \alpha_c \|\theta\|_2^2$

W2S v.s. SFT

Is the additional compute of W2S worthwhile?
(Outperformance ratio/OPR)

W2S generalization: ridgeless regression ($\alpha \rightarrow 0$)

$\text{ER}(f) = \text{Var}(f) + \text{Bias}(f)$ where

$$\text{Var}(f) = \mathbb{E}_{X,y} \left[\frac{1}{N} \|f(X) - \mathbb{E}_{y|X}[f(X)]\|_2^2 \right]$$

$$\text{Bias}(f) = \mathbb{E}_X \left[\frac{1}{N} \|\mathbb{E}_{y|X}[f(X)] - f_*(X)\|_2^2 \right]$$

Proposition [DLLLL25].

$$\text{Var}(f_w) = \frac{\sigma^2 d_w}{n - d_w - 1}, \quad \text{Bias}(f_w) \lesssim \rho_w$$

$$\text{Var}(f_s) = \frac{\sigma^2 d_s}{n - d_s - 1}, \quad \text{Bias}(f_s) \lesssim \rho_s$$

$$\text{Var}(f_c) = \sigma^2 \frac{d_s}{n + N}, \quad \text{Bias}(f_c) \leq \rho_s$$

Theorem [DLLLL25]. Assume $\phi_s(x)$ is zero-mean subgaussian and $\phi_w(x) \sim \mathcal{N}(0_d, \Sigma_w)$ (can be relaxed to subgaussian), for $n > d_w + 1$:

$$\text{Var}(f_{w2s}) = \frac{\sigma^2}{n - d_w - 1} \left(d_{s \wedge w} + \frac{d_s}{N} (d_w - d_{s \wedge w}) \right)$$

$$\text{Bias}(f_{w2s}) \leq \text{Bias}(f_w) + \rho_s \leq O(\rho_w) + \rho_s$$

$$\mathcal{V}_s = \text{Range}(\Sigma_s), \quad \mathcal{V}_w = \text{Range}(\Sigma_w)$$

$$\text{Var}(f_{w2s}) \asymp \boxed{\frac{d_{s \wedge w}}{n}} + \boxed{\frac{d_s}{N}} \boxed{\frac{d_w - d_{s \wedge w}}{n}}$$

Var. in $\mathcal{V}_w \cap \mathcal{V}_s$ W2S Var. in $\mathcal{V}_w \setminus \mathcal{V}_s$

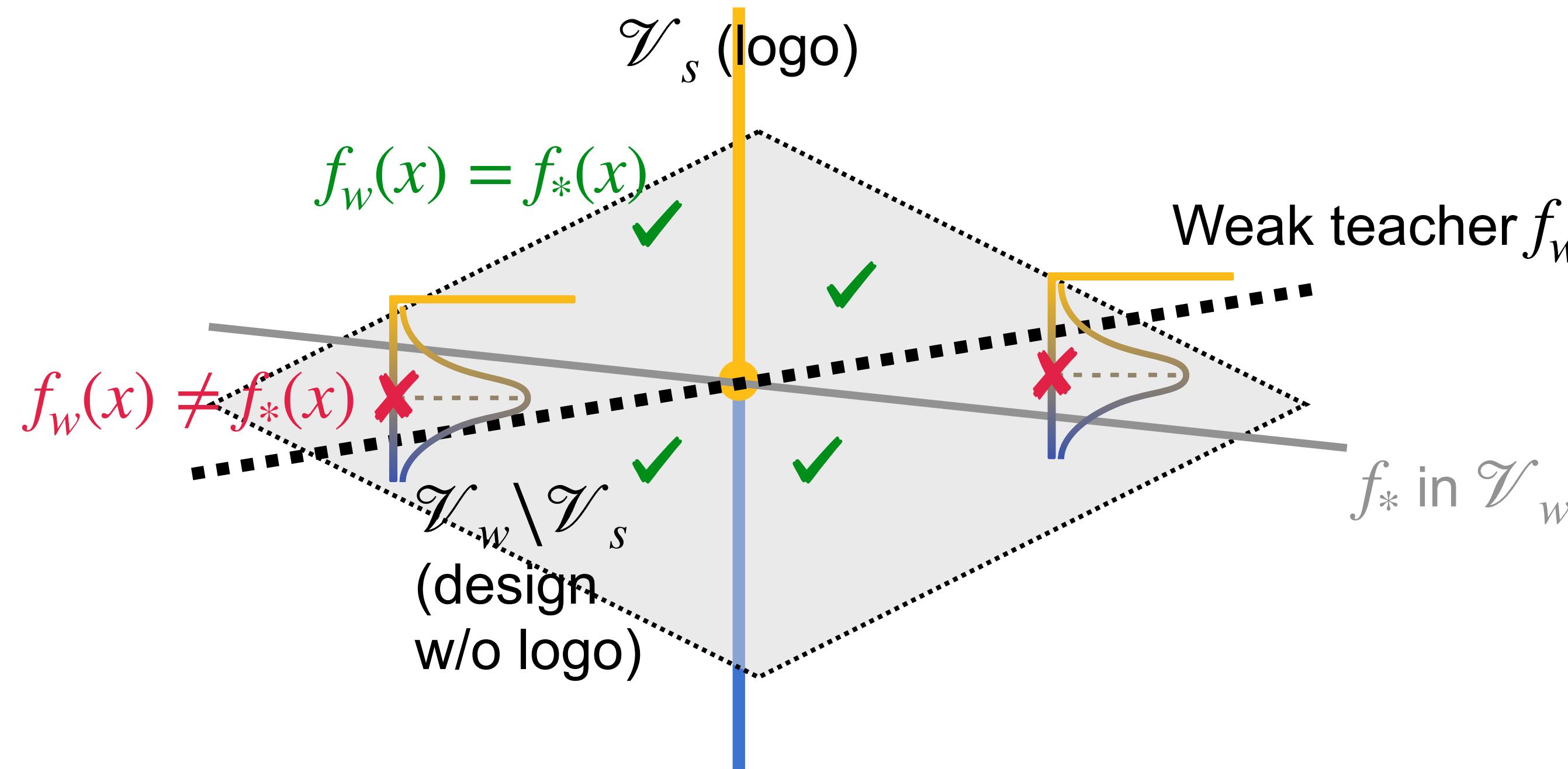
Intuition: How does variance reduction in W2S happen?

$$\mathcal{V}_s = \text{Range}(\Sigma_s), \mathcal{V}_w = \text{Range}(\Sigma_w)$$

$$\text{Var}(f_{w2s}) \asymp \frac{d_{s \wedge w}}{n} + \frac{d_s}{N} \frac{d_w - d_{s \wedge w}}{n}$$

Var. in $\mathcal{V}_w \cap \mathcal{V}_s$ W2S Var. in $\mathcal{V}_w \setminus \mathcal{V}_s$

Task: Determine the make of a car



Pseudolabel error in $\mathcal{V}_w \setminus \mathcal{V}_s$ can be viewed as **independent label noise** w.r.t. the orthogonal strong features \mathcal{V}_s , variance from which reduces proportionally to d_s/N .

Suitable regularization is essential for W2S: ridge regression

- Positive-definite covariances: $\Sigma_w, \Sigma_s, \Sigma_* > 0$
- $f_*(x) = \phi_*(x)^\top \theta_*$, $\theta_* \in \mathbb{R}^d$, $\mathbb{E}[\phi_*(x)\phi_*(x)^\top] = \Sigma_*$
- Normalized features: $\|\Sigma_w\|_2 \asymp \|\Sigma_s\|_2 \asymp \|\Sigma_*\|_2 \asymp 1$
- Intrinsic dimensions: $\text{tr}(\Sigma_w) \asymp d_w$, $\text{tr}(\Sigma_s) \asymp d_s \ll d$

Theorem [DLLLL25]. Let $Q_w = \|\Sigma_w^{-1/2} \Sigma_*^{1/2} \theta_*\|_2^2$, $Q_s = \|\Sigma_s^{-1/2} \Sigma_*^{1/2} \theta_*\|_2^2$. Set $\alpha_w = \frac{\sigma^2 \text{tr}(\Sigma_s \Sigma_w)}{4nN} \frac{Q_s}{Q_w^2}$ and $\alpha_{w2s} = \frac{\sigma^2 \text{tr}(\Sigma_s \Sigma_w)}{4nN} \frac{Q_w}{Q_s^2}$. When $N \geq \frac{\text{tr}(\Sigma_s) \text{tr}(\Sigma_w)}{\text{tr}(\Sigma_s \Sigma_w)}$,

$$\text{ER}(f_{w2s}) \leq 3 \left(\frac{3\sigma^2}{4nN} Q_s Q_w \text{tr}(\Sigma_s \Sigma_w) \right)^{1/3}.$$

Choose some suitable $\alpha_w, \alpha_{w2s} > 0$ s.t.

$$\theta_w = \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{n} \|\widetilde{\Phi}_w \theta - \tilde{y}\|_2^2 + \alpha_w \|\theta\|_2^2$$

$$\theta_{w2s} = \arg \min_{\theta \in \mathbb{R}^d} \frac{1}{N} \|\Phi_s \theta - \Phi_w \theta_w\|_2^2 + \alpha_{w2s} \|\theta\|_2^2$$

- **Multiplicative sample complexity:**

$$nN \asymp \sigma^2 \text{tr}(\Sigma_s \Sigma_w) Q_s Q_w$$

- **Representation similarity (" $d_{s \wedge w}$ "):**

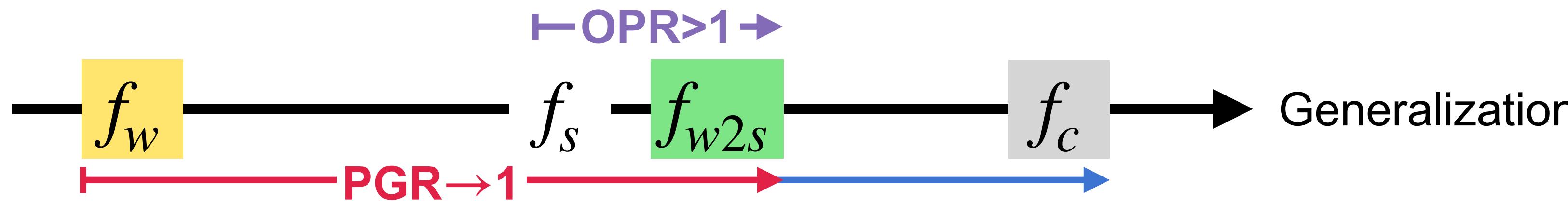
$$\text{tr}(\Sigma_s \Sigma_w) \lesssim \min\{\text{tr}(\Sigma_s), \text{tr}(\Sigma_w)\}$$

- **Representation accuracy:** Q_w, Q_s are small if the dominating eigenspaces of Σ_w, Σ_s cover that of Σ_*

Larger discrepancy (lower $d_{s \wedge w}$) \rightarrow better W2S

Performance gap recovery: $PGR = \frac{ER(f_w) - ER(f_{w2s})}{ER(f_w) - ER(f_c)}$

Outperformance ratio: $OPR = \frac{ER(f_s)}{ER(f_{w2s})}$

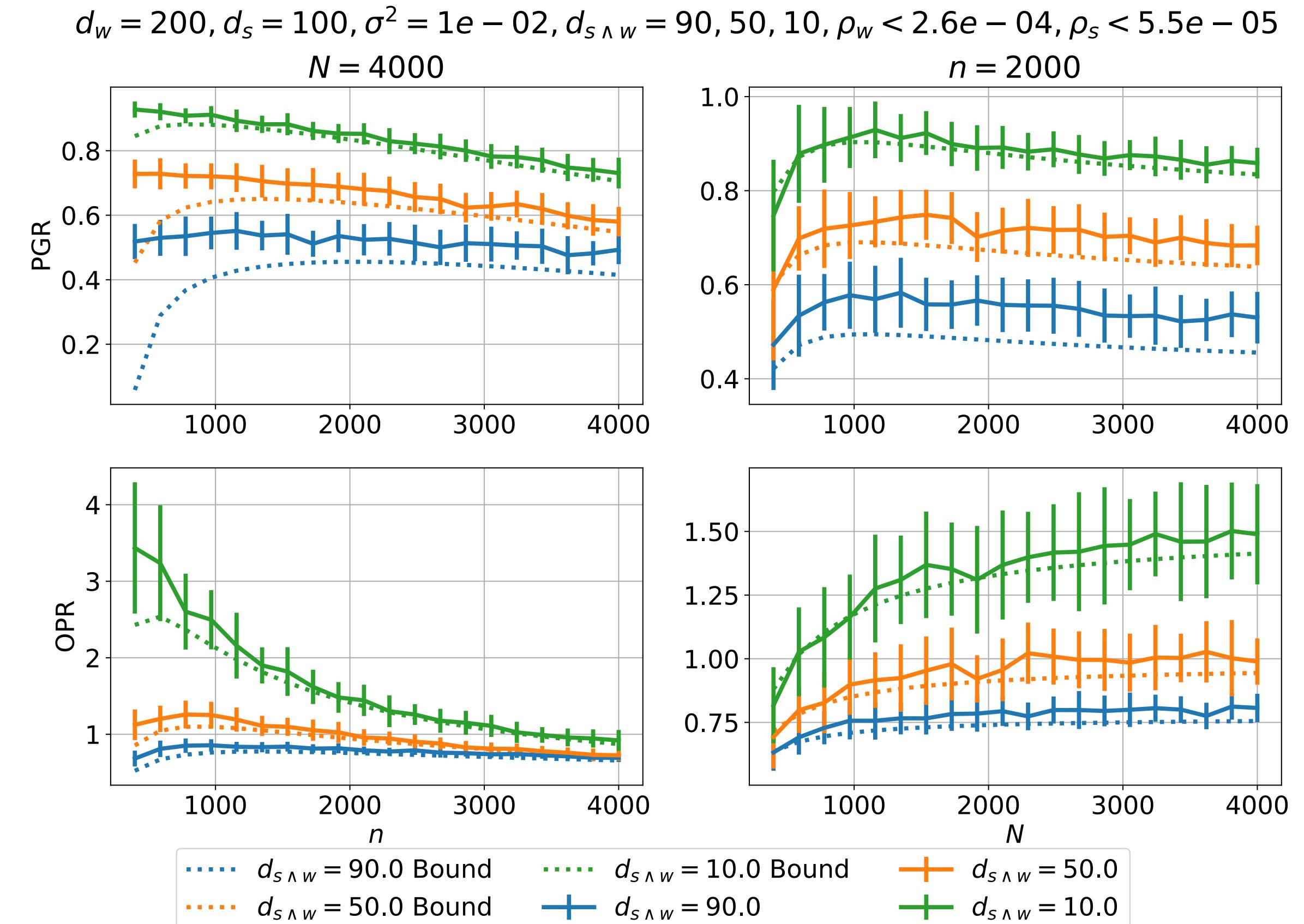
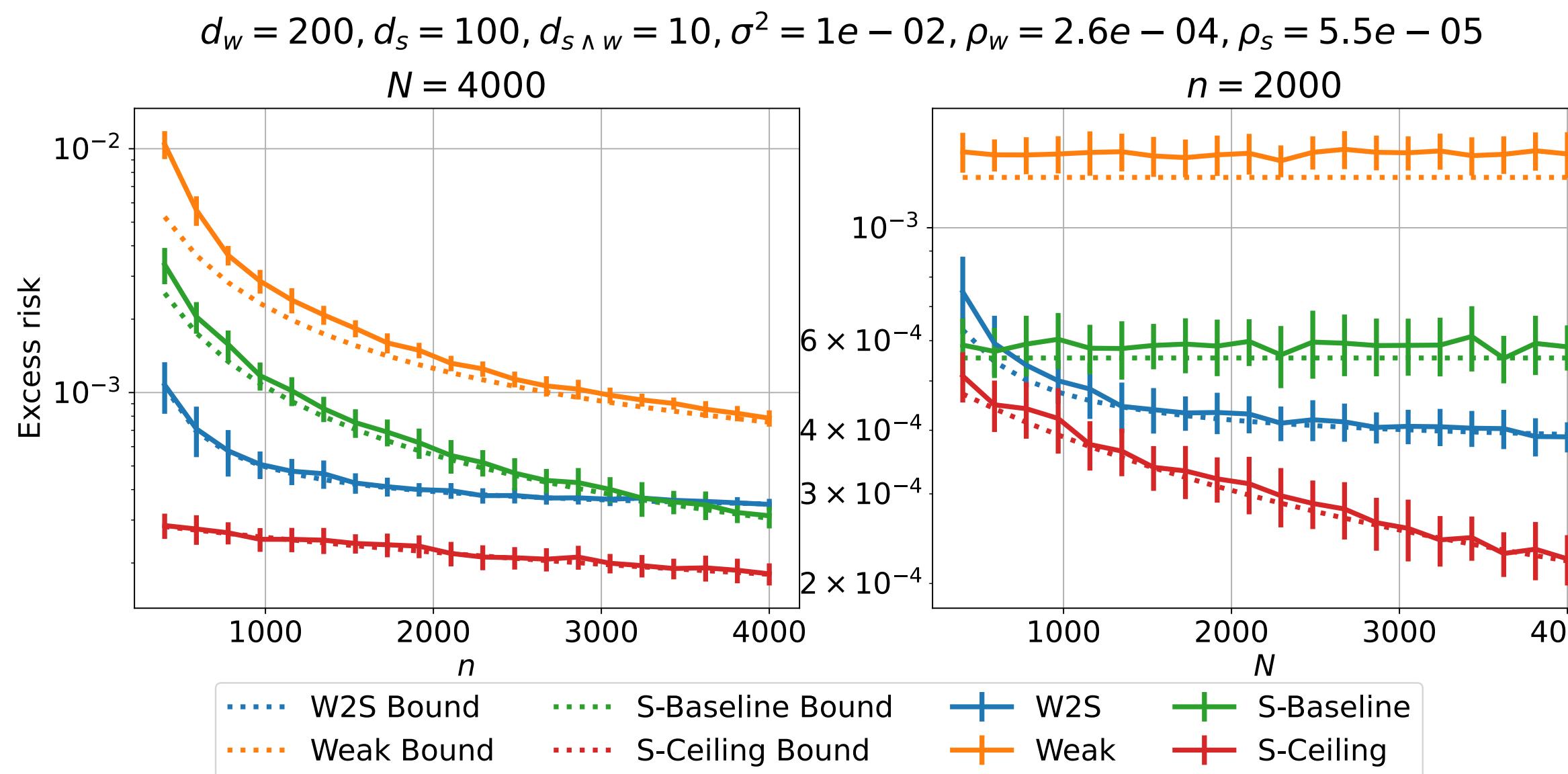


With negligible FT approximation error $(\rho_w + \rho_s)/\sigma^2 \rightarrow 0$,
when $n \gtrsim d_w$ and $N \gtrsim d_s(d_w/d_{s \wedge w} - 1)$, we have

$$PGR \geq 1 - O(d_{s \wedge w}/d_w) \quad \text{and} \quad OPR \geq \Omega(d_s/d_{s \wedge w})$$

Synthetic experiments

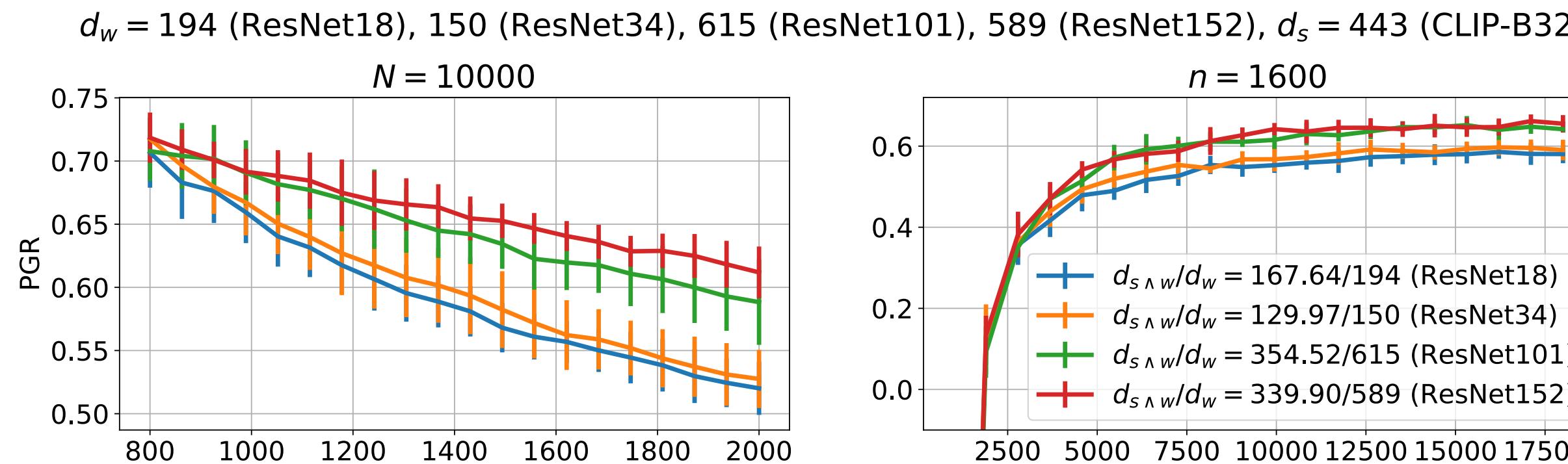
- High-dimensional Gaussian features: $d = 20000$
- $f_*(x) = x^\top \Lambda_*^{1/2} \theta_*$ where $\Lambda_* = \text{diag}(\lambda_1^*, \dots, \lambda_d^*)$
- $\lambda_i^* = i^{-1}$ for $1 \leq i \leq 300$, $\lambda_i^* = 0$ for $i > 300$



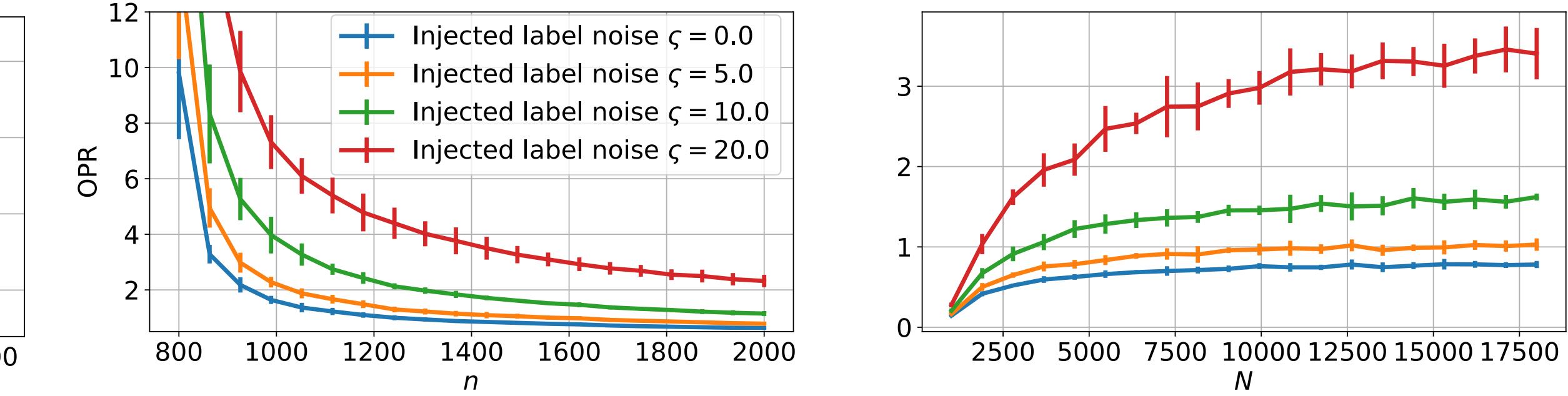
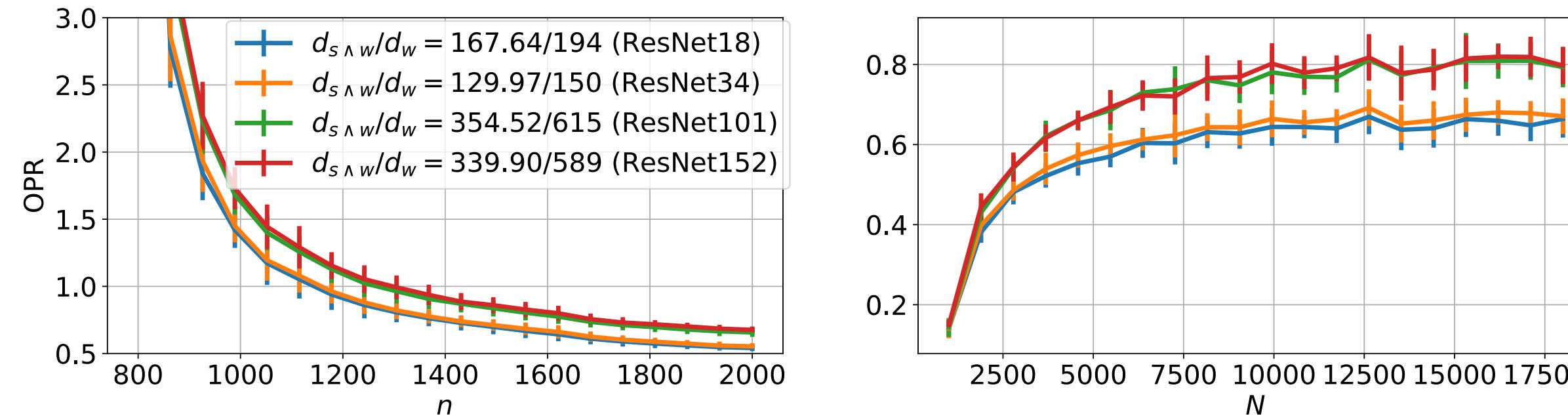
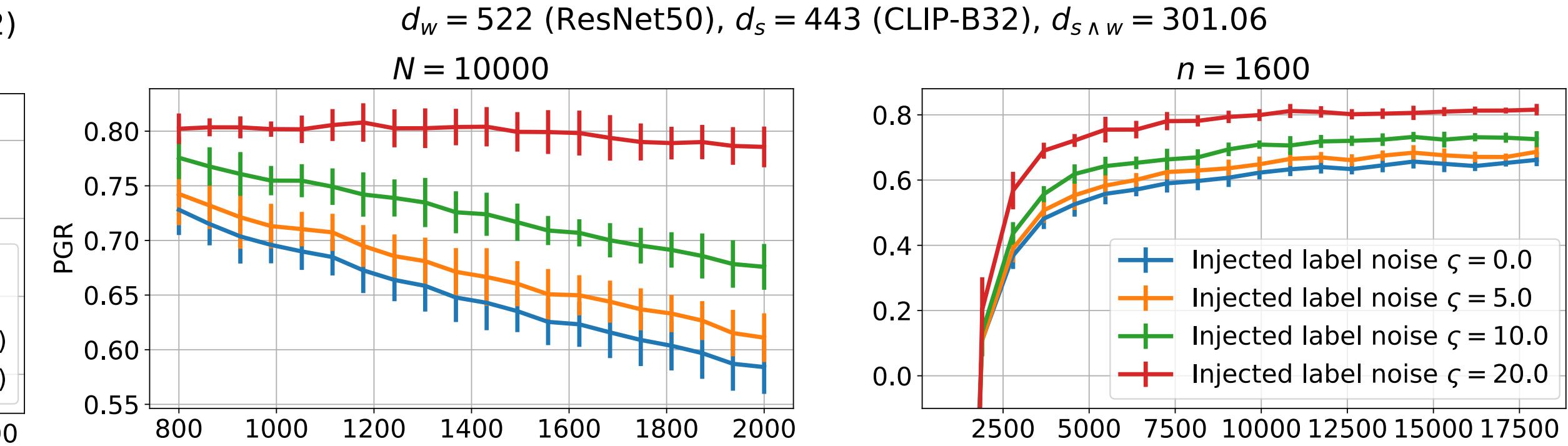
- Our bounds provide reasonably tight characterization for the generalization error, PGR, and OPR.
- W2S is more beneficial with limited label data n — PGR and OPR decrease as n increases!

UTKFace regression

Lower $d_{s \wedge w}/d_w \rightarrow$ better W2S



Larger variance \rightarrow more pronounced W2S



- UTKFace: age prediction (0-116) based on images, i.e., image regression.
- Lower $d_{s \wedge w}/d_w$ (larger discrepancy between ϕ_w, ϕ_s) brings higher PGR and OPR.
- Benefit of W2S is more pronounced on problems with larger variance.

Takeaway: teacher-student discrepancy → better W2S

How does W2S happen on easy tasks where weak and strong models both have low approximation errors?

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Through lens of low intrinsic dimension:

- Representation **efficiency**: $\text{rank}(\Sigma_s) = d_s, \text{rank}(\Sigma_w) = d_w \ll d$
- Representation **similarity**: correlation dimension $d_{s \wedge w} = \|V_s^\top V_w\|_F^2 \in [0, \min\{d_s, d_w\}]$

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With negligible FT approximation error, when $n \gtrsim d_w$ and $N \gtrsim d_s(d_w/d_{s \wedge w} - 1)$,

$$\text{PGR} \geq 1 - O(d_{s \wedge w}/d_w) \quad \text{and} \quad \text{OPR} \geq \Omega(d_s/d_{s \wedge w})$$

Thank you! Happy to take any questions



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