Revisiting Model Complexity in the Wake of Overparameterized Learning

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Based on joint work with Ryan Tibshirani

Overparameterization in machine learning

Modern machine learning involves fitting a huge number of parameters. Such overparameterization seems to be useful for:

- Representation: allows rich, expressive models for diverse real data
- Optimization: simple, local optimization methods often find near-optimal solutions to empirical risk minimization on training data
- Generalization: despite overfitting, models generalize well in practice

This talk is broadly about the generalization aspect.

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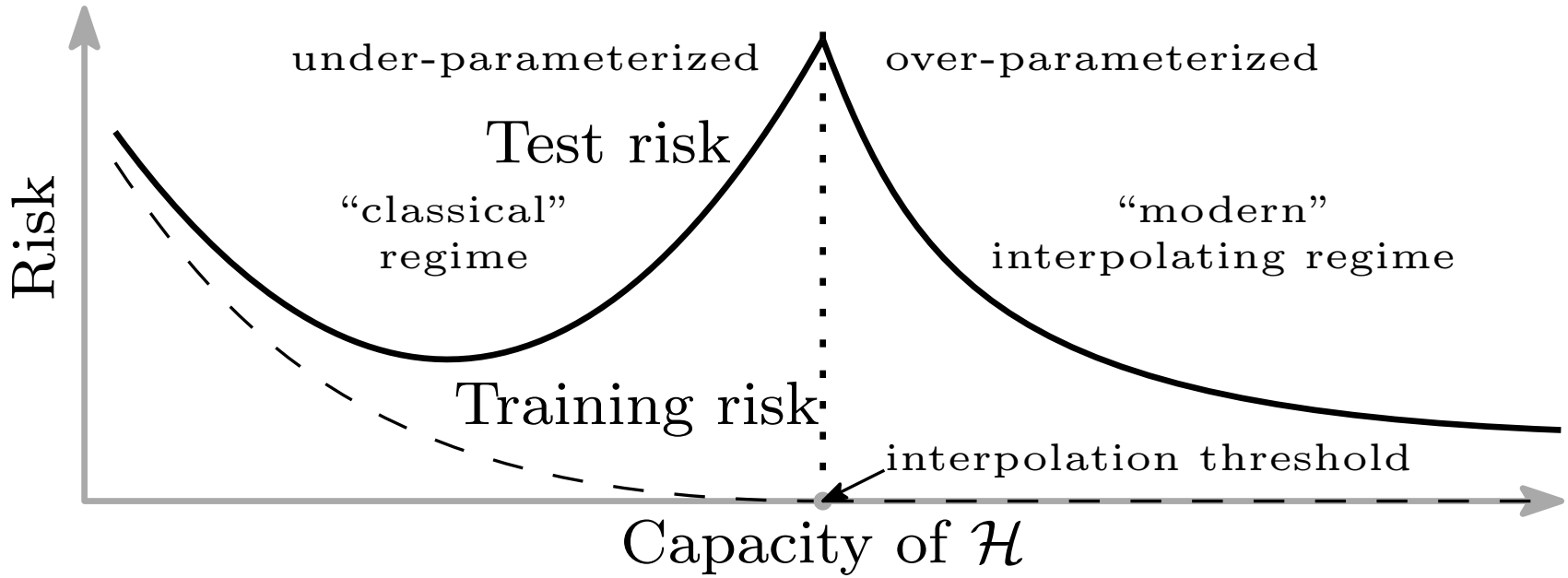

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Belkin, Hsu, Ma, Mandal, 2018

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- This trend holds for many model classes including linear regression, kernel regression, random forest, boosting, neural networks, etc.

Is there an equivalent "reparameterization" of "overparameterization"?

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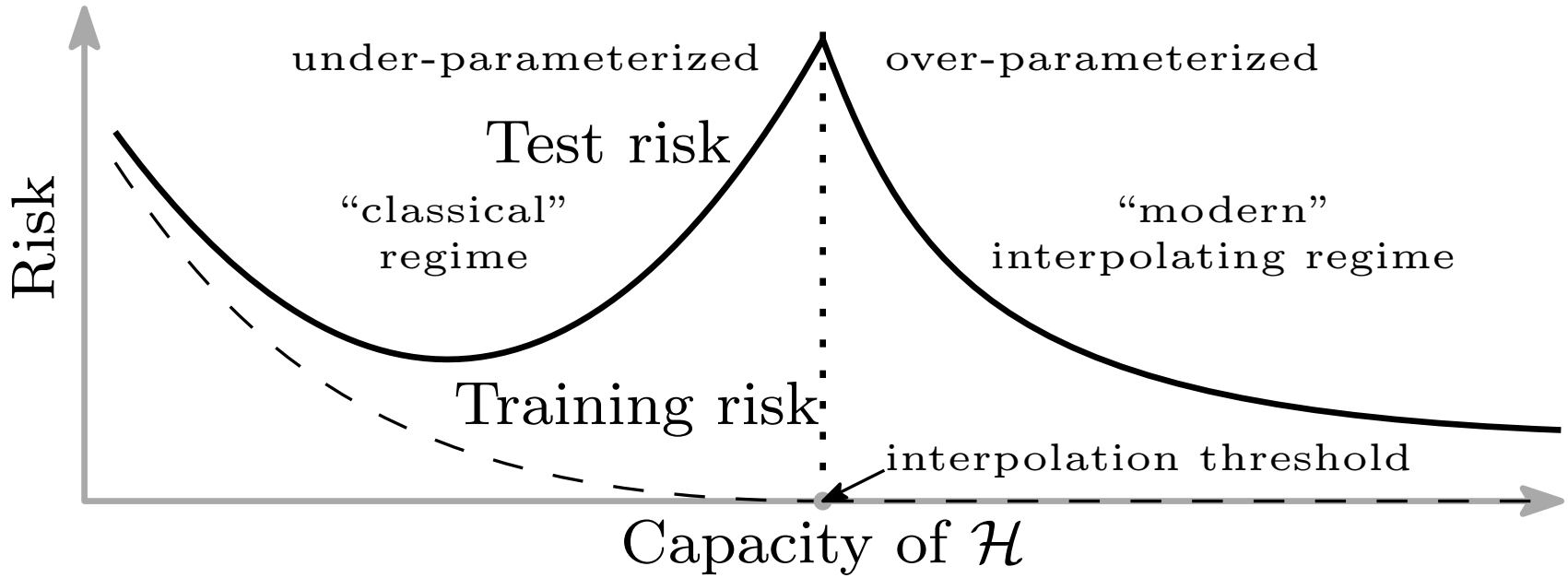

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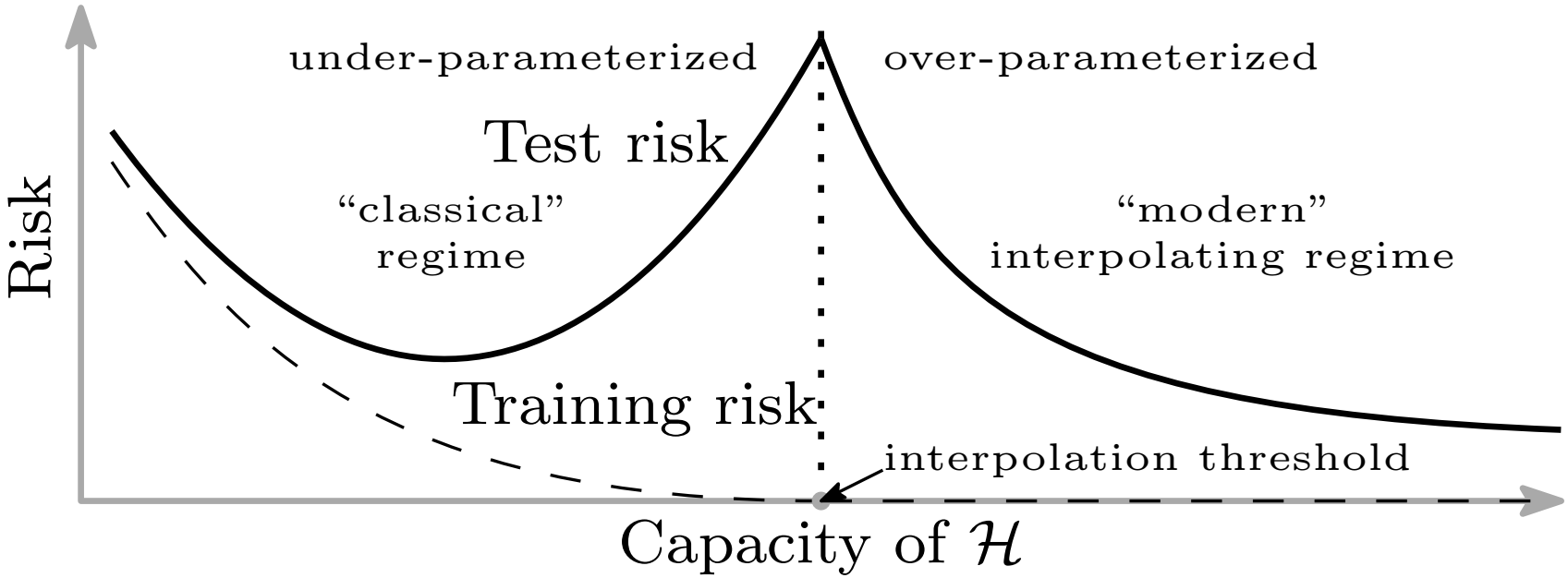

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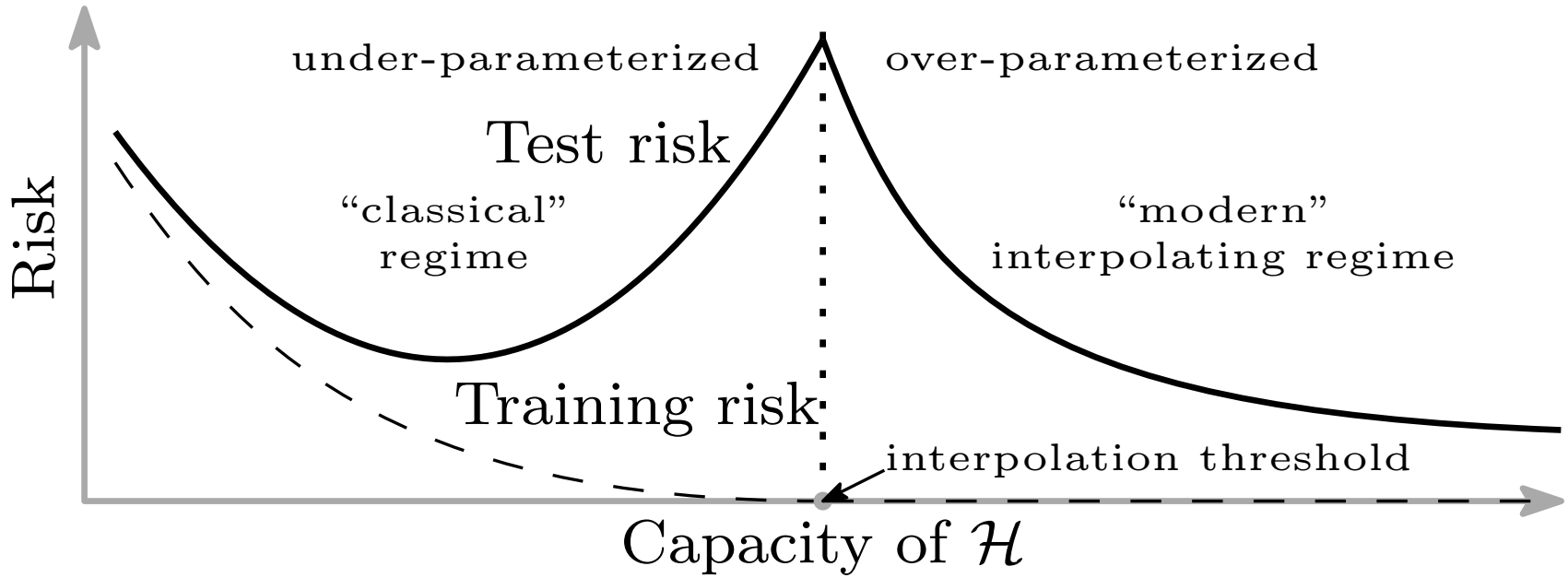

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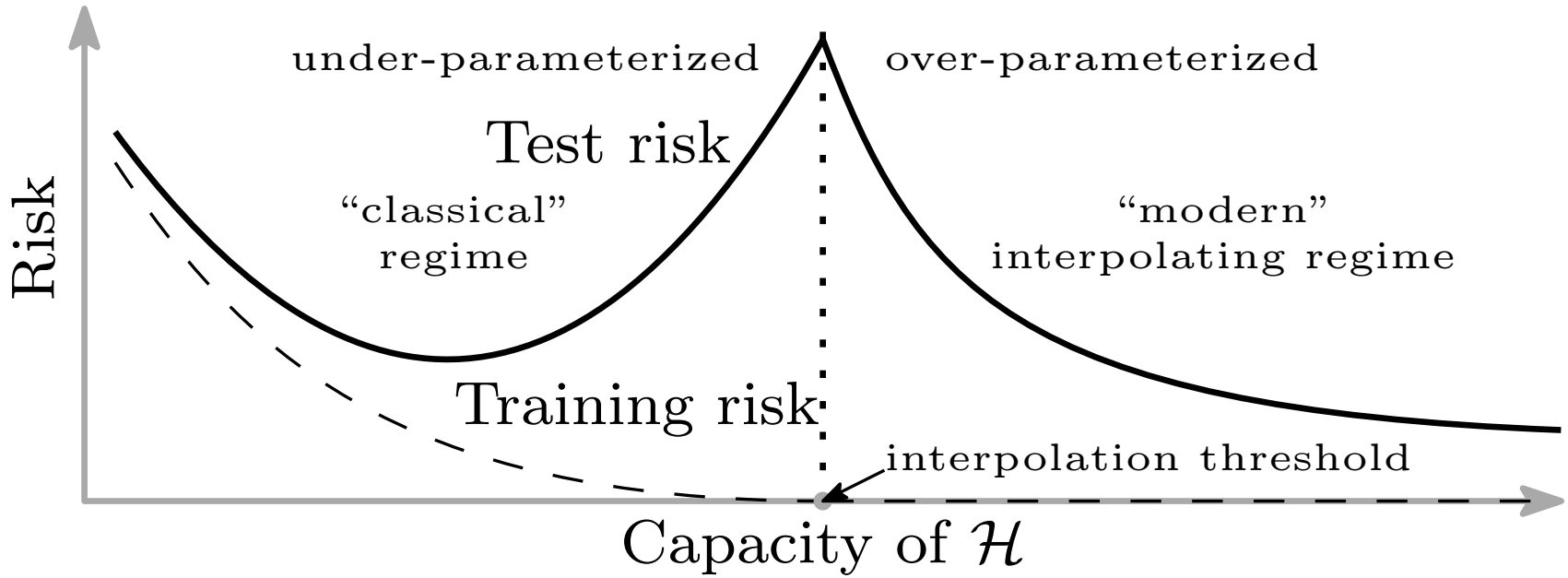

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Conceptual and theoretical challenges

Current machine learning practice suggests:

- we should design models to be highly overparametrized
- train until nearly zero training error (i.e., interpolate training data)
- the trained models still can generalize well and have good test error

Main statistical challenges for us:

- benign overfitting conceptually breaks classical bias-variance tradeoff
- trained models fall outside the realm of uniform convergence
- one of core questions is how to correctly measure model complexity

This work attempts to answer the following questions:

- Is there a good measure of model complexity for predictive models?
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Takaway points

- Propose measures of model complexity that are:
  - algorithm-specific and applies for any prediction algorithm
  - produce a number between 0 and n (the number of observations)
- Two variants of model complexities are:
  - emergent model complexity that depends on the prediction algorithm as well as underlying the regression function
  - intrinsic model complexity that depends on the prediction algorithm only and its adaptability to pure noise
- Results when applied to some illustrative examples:
  - min ℓ_2/ℓ_1-norm interpolators: the complexity measures maximized when $n \approx p$ and typically decreases as p increases beyond n
  - we can reparameterize every overparameterized model into an equivalent underparameterized model in terms of risk behavior

Based on extension of ideas from optimism theory and degrees of freedom.

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Outline

Degrees of freedom at large

Degrees of freedom means different things in different fields, but they're more or less similar. There is a core concept behind it.

It essentially has to do with the dimension or effective number of parameters of "something".

- In mechanics, that something = mechanical system.
- In physics and chemistry, something = physical system.
- In statistics, something = prediction procedure.

A nice commonality is that we can usually guess the degrees of freedom based on intuition, at least qualitatively.

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Degrees of freedom in statistics

Degrees of freedom in statistics is defined, intuitively, as the effective number of parameters used by a prediction procedure.

While this seems vague, it has a precise definition for a broad class of estimation problems. We will define this shortly.

Why is this an important concept? Why you would ever go to the trouble of describing degrees of freedom?

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Definition under squared error loss

Consider data $(x_i, y_i) \in \mathbb{R}^p \times \mathbb{R}$, $i = 1, \ldots, n$ such that $y_i = f(x_i) + \varepsilon_i$ where $f : \mathbb{R}^p \to \mathbb{R}$ is regression function, ε_i has mean 0 and variance σ^2.

Let $\mathcal{A}$ be any fitting algorithm that maps $\{(x_i, y_i)\}_{i=1}^n \overset{\mathcal{A}}{\mapsto} \widehat{f}$.
The degrees of freedom of predictor $\widehat{f}$ is defined as

$$\mathrm{dfF}(\widehat{f}) = \sum_{i=1}^{n} \mathrm{Cov}(y_i, \widehat{f}(x_i))/\sigma^2 = \mathrm{tr}\left[\mathrm{Cov}(y, \widehat{f}(X))\right]/\sigma^2,$$

where y: response vector, X: feature matrix, $\widehat{f}(X)$: predicted response

Where does squared error loss come into play?

$$\underbrace{\mathbb{E}\Big[\sum_{i=1}^{n}(\tilde{y}_i - \widehat{f}(x_i))^2\Big]}_{\text{fixed-X prediction error} =: \mathrm{ErrF}(\widehat{f})} - \underbrace{\mathbb{E}\Big[\sum_{i=1}^{n}(y_i - \widehat{f}(x_i))^2\Big]}_{\text{expected training error} =: \mathrm{ErrT}(\widehat{f})} = 2\sigma^2 \mathrm{dfF}(\widehat{f})$$

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Degrees of freedom in linear regression

- Suppose $p \leq n$ and X has full (column) rank, and we take $\widehat{f}$ to be ordinarly least squares predictor $\widehat{f}(X) = X\widehat{\beta}$, where

$$\widehat{\beta} = \underset{\beta \in \mathbb{R}^p}{\arg\min} \, \|y - X\beta\|_2^2 = (X^T X)^{-1} X^T y.$$

$$\mathrm{dfF}(\widehat{f}) = \mathrm{tr}[\mathrm{Cov}(y, X\widehat{\beta})]/\sigma^2 = \mathrm{tr}[\sigma^2 X(X^T X)^{-1} X^T]/\sigma^2 = p.$$

- Suppose $p \geq n$ and X has full (row) rank, and we take $\widehat{f}$ to be min ℓ_2-norm least squares predictor $\widehat{f}(X) = X\widehat{\beta}$, where

$$\widehat{\beta} = \underset{\beta \in \mathbb{R}^p}{\arg\min} \{\|\beta\|_2 : X\beta = y\} = (X^\top X)^\dagger X^\top y.$$

$$\mathrm{dfF}(\widehat{f}) = \mathrm{tr}[\mathrm{Cov}(y, X\widehat{\beta})]/\sigma^2 = \mathrm{tr}[\sigma^2 X^\top (XX^\top)^{-1} X]/\sigma^2 = n.$$

Thus, $\mathrm{dfF}(\widehat{f})$ is p for $p \leq n$, but is always n for $p \geq n$ (not meaningful).

This is fixed-X degrees of freedom. How to extend for random-X setting?

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This is fixed-X degrees of freedom. How to extend for random-X setting?

Degrees of freedom in linear regression

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Outline

Re-interpreting fixed-X degrees of freedom

Fixed-X degrees of freedom is a standard algorithm specific measure of complexity, but no notion of random-X degrees of freedom we know of.

We cast fixed-X degrees of freedom from a different perspective.

- Define fixed-X optimism of $\widehat{f}$ by $\mathrm{OptF}(\widehat{f}) = \mathrm{ErrF}(\widehat{f}) - \mathrm{ErrT}(\widehat{f})$.
- Consider the following family of "reference" models:
  - $\mathcal{A}^{\mathrm{ref}}$ is the least squares reference algorithm,
  - (U_k, v) is random design with k features, and noise with level σ^2.
- Recall that $\mathrm{dfF}(\mathcal{A}^{\mathrm{ref}}(U_k, v)) = k$ so long as $\mathrm{rank}(U_k) = k$.
- Thus, for a fitting procedure $\widehat{f} = \mathcal{A}(X, y)$, $\mathrm{dfF}(\widehat{f})$ is also equal to the value of k that satisfy the following relation:

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Emergent random-X degrees of freedom

"Matching optimism" interpretation can be extended to random-X setting and leads to the definition of random-X degrees of freedom.

- Define random-X optimism of $\widehat{f}$ by $\mathrm{OptR}(\widehat{f}) = \mathrm{ErrR}(\widehat{f}) - \mathrm{ErrT}(\widehat{f})$, where $\mathrm{ErrR}(\widehat{f}) = \mathbb{E}[(y_0 - \widehat{f}(x_0))^2]$ is the random-X prediction error.
- We thus define the random-X degrees of freedom, $\mathrm{dfR}(\widehat{f})$, of any predictor $\widehat{f} = \mathcal{A}(X, y)$, as the value of k for which the following relation holds:

$$\mathrm{OptR}(\mathcal{A}(X, y)) = \mathrm{OptR}(\mathcal{A}^{\mathrm{ref}}(U_k, v)) \qquad \text{(dfR, emergent)}$$

Recall here:

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Intrisic random-X degrees of freedom

- The emergent random-X degrees of freedom, $\mathrm{dfR}(\widehat{f})$, depends of both the the predictor $\widehat{f}$ and the underlying regression function f.
- When matching optimisms, the observed random-X optimism of $\widehat{f}$ consists of bias, which may inflate the degrees of freedom.
- We thus also define intrinsic random-X degrees of freedom, denoted by dfR^i, as the k for which the following relation holds:

$$\mathrm{OptR}(\mathcal{A}(X, v)) = \mathrm{OptR}(\mathcal{A}^{\mathrm{ref}}(U_k, v)) \qquad \text{(dfR, intrinsic)}$$

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Computing random-X degrees of freedom

We have defining equations for random-X degrees of freedom, but how do we actually compute the solution in practice?

We need three numbers:

- $\mathrm{OptR}(\mathcal{A}(X, y))$: emergent random-X optimism
  Either supplied by user or via cross or held-out validation
- $\mathrm{OptR}(\mathcal{A}(X, v))$: intrinstic random-X optimism
  Simulate at noise level if known, otherwise average
- $\mathrm{OptR}(\mathcal{A}^{\mathrm{ref}}(X, v))$: reference optimism
  Either simulate or use invariant asymptotic limit that holds under quite generic conditions on the random design matrix and noise:

$$\frac{\mathrm{OptR}(\mathcal{A}^{\mathrm{ref}}(U_k, v))}{\sigma^2} \to \frac{1-(1-\xi)^2}{1-\xi} \text{ as } n, p \to \infty \text{ and } p/n \to \xi \in (0, 1),$$

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Under the asymptotic limit, solving for the random-X degrees of freedom by matching optimisms leads:

$$\mathrm{dfR}(\widehat{f})/n \to 1 + \frac{\psi}{2} - \sqrt{1 + \frac{\psi^2}{4}}.$$

where ψ is the normalized random-X optimism of the given predictor.

Remarks:

- There is a unique number in $[0, n]$ satisfying the desired relations.
- This is an interpretable range for random-X degrees of freedom:
  - The least complex predictor has dfR of 0,
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- There is a unique number in $[0, n]$ satisfying the desired relations.
- This is an interpretable range for random-X degrees of freedom:
  - The least complex predictor has dfR of 0,
  - The most complex predictor has dfR of n, as if saturated model.

Outline

Ordinary, min ℓ_2-norm and min ℓ_1-norm least squares

Given (X, y), consider predictors of the form $\widehat{f}(x) = x^\top \widehat{\beta}$, where

- Ordinary least squares

$$\widehat{\beta} = \underset{\beta \in \mathbb{R}^p}{\arg\min} \|y - X\beta\|_2^2$$

- Min ℓ_2-norm least squares (mn2ls)

$$\widehat{\beta} = \underset{\beta \in \mathbb{R}^p}{\arg\min} \{\|\beta\|_2 : y = X\beta\}$$

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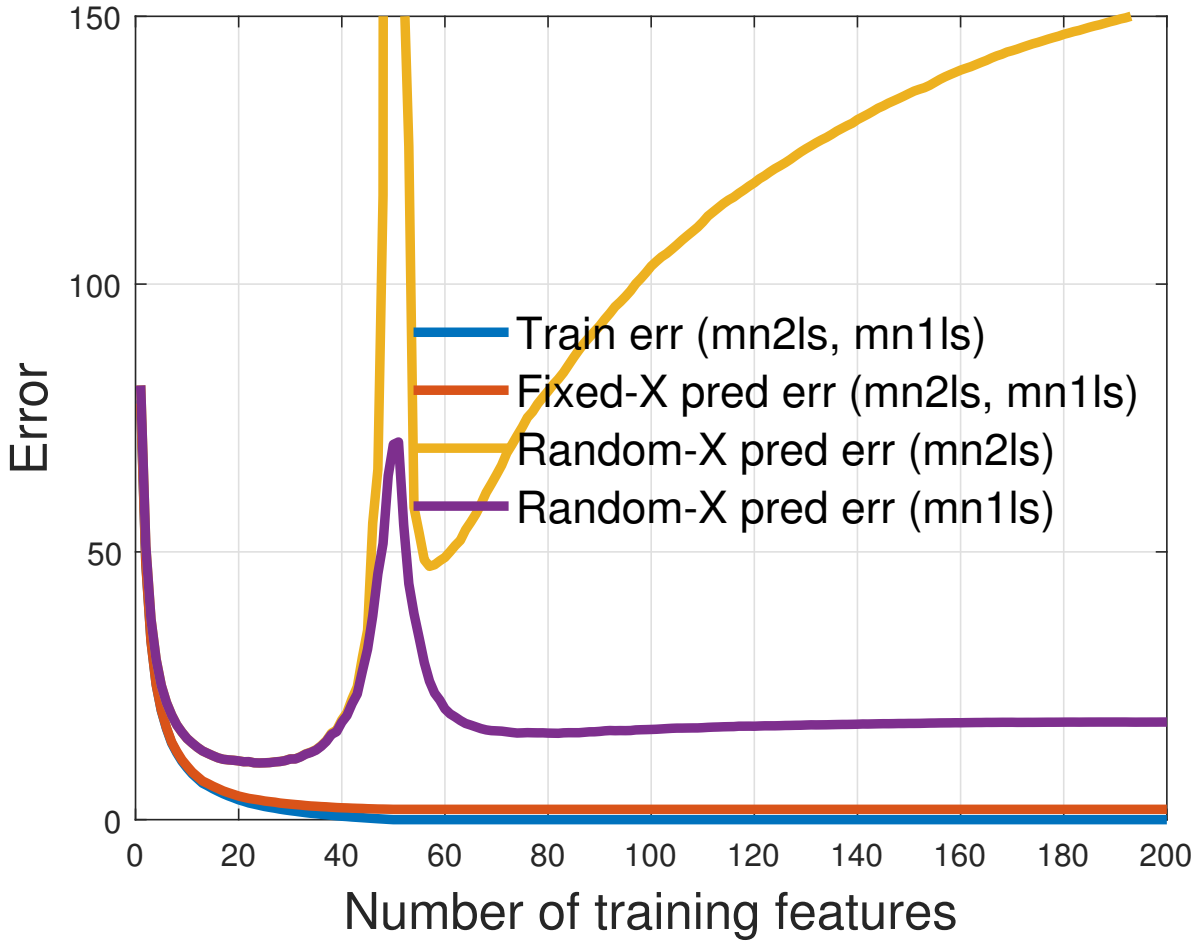
Errors (train, fixed-X, random-X) versus model size



- Fixed data with $n = 50$ and response non-linear in $p = 200$ features
- Model class: estimators fitted on nested subsets of 1 to 200 features
- Train, fixed-X: descent then constant; random-X: double descent

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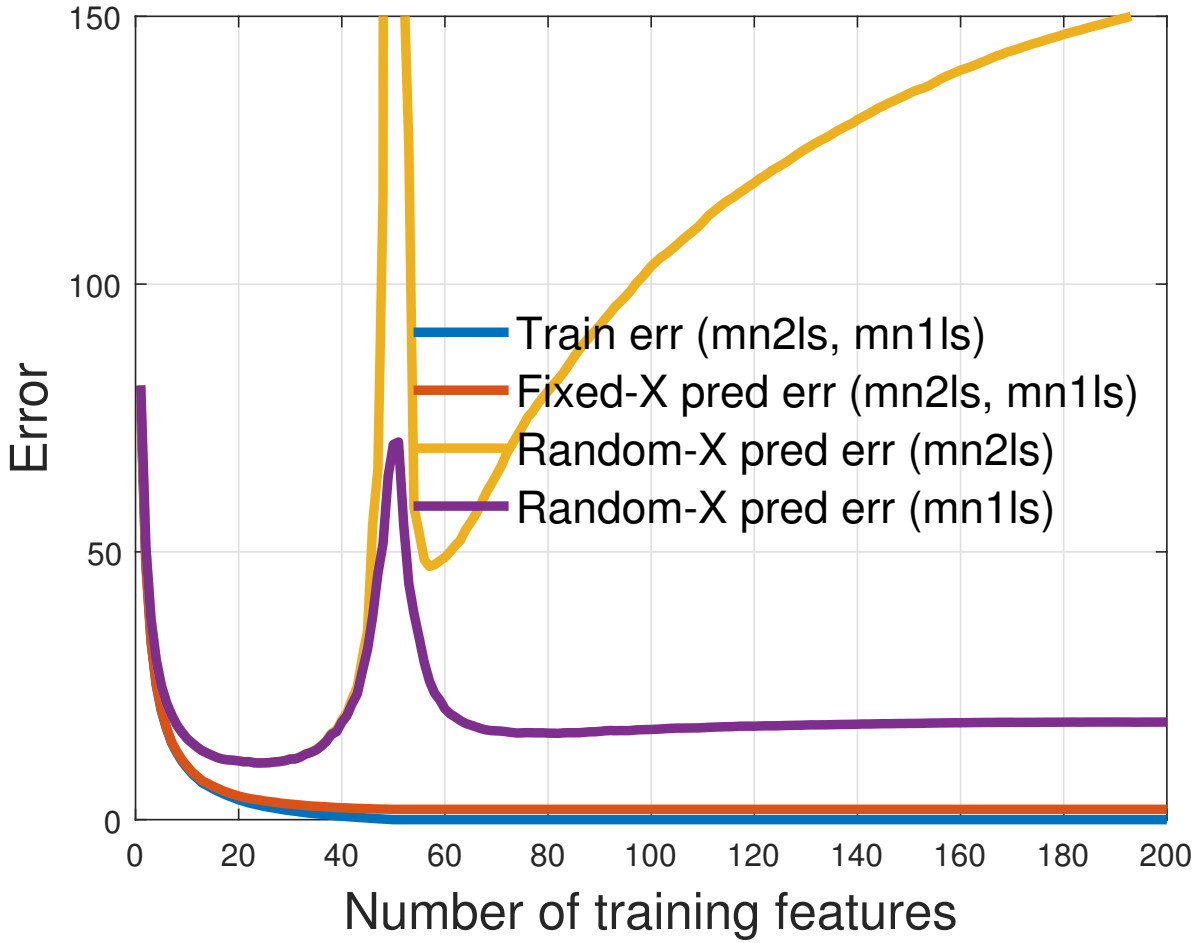

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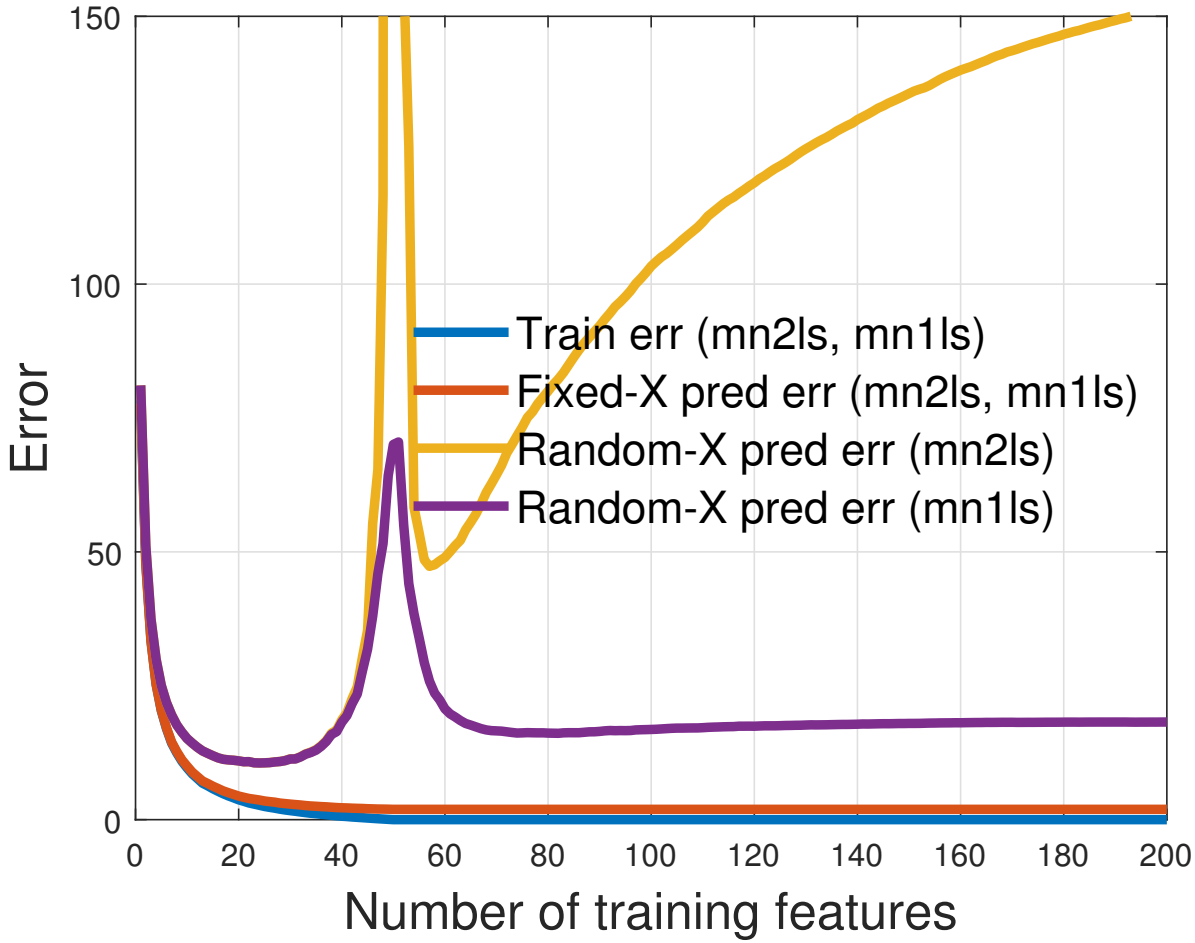

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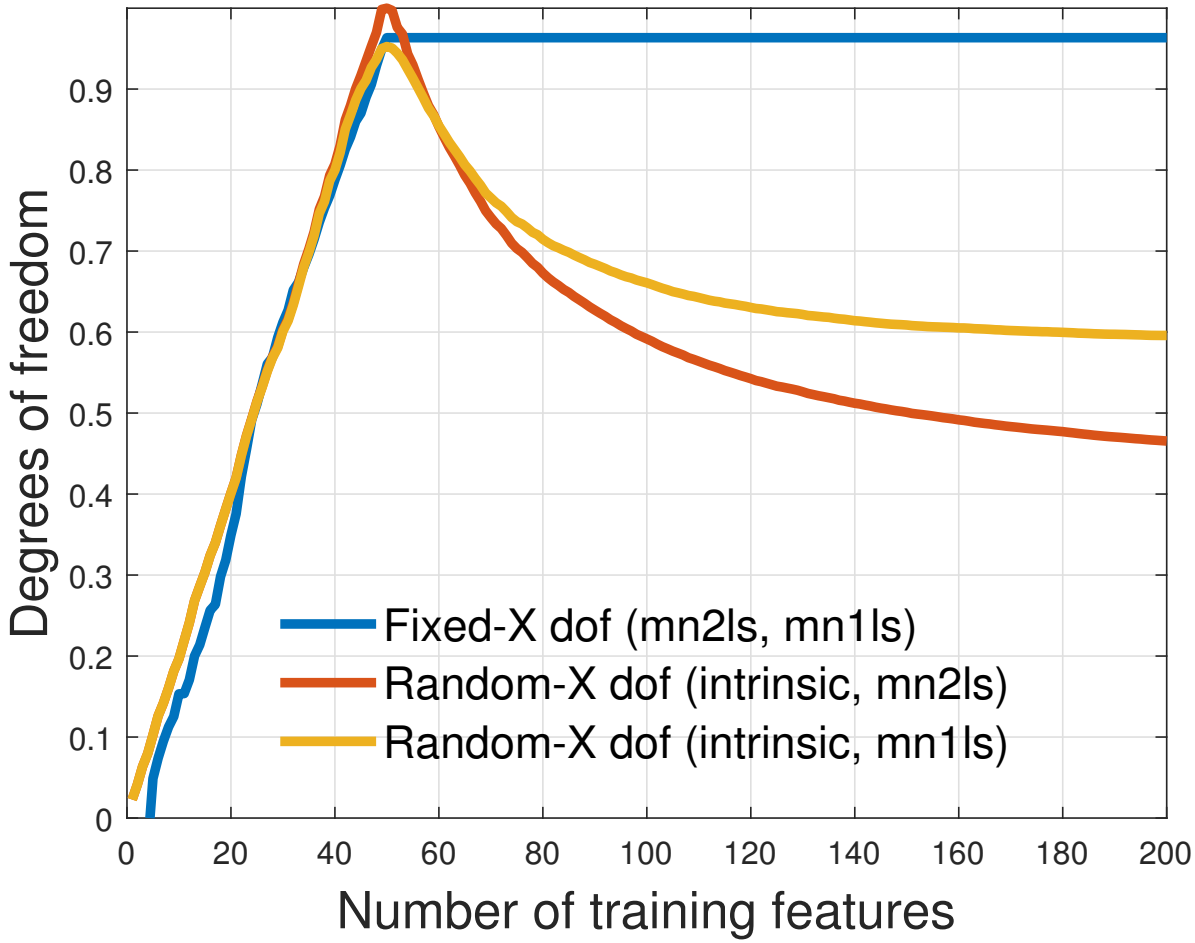
Degrees of freedom (fixed-X, random-X) versus model size



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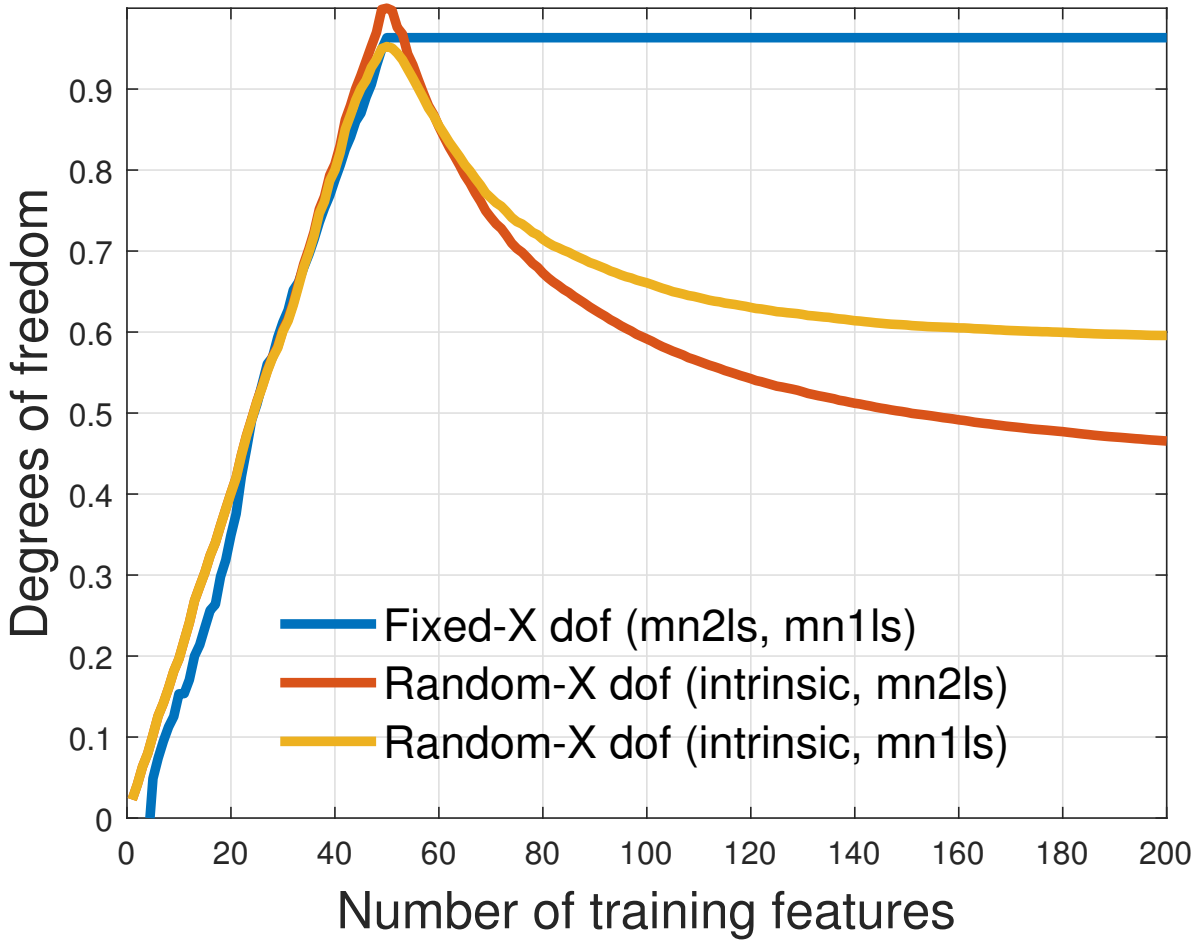

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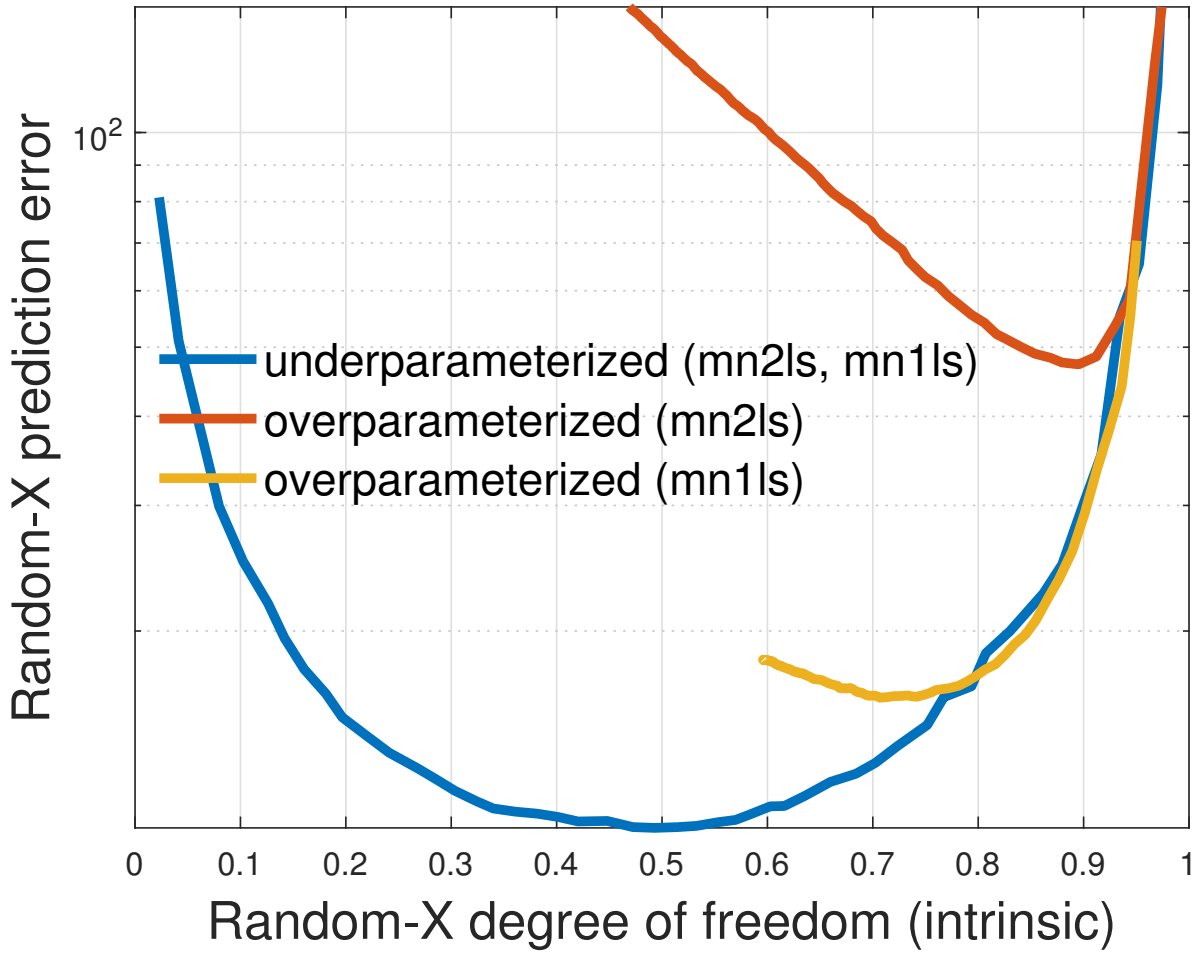
Prediction error (random-X) versus model size



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- Underparameterized: *U*-curve; overparameterized: also *U*-curve!
- Punchline: map from overparameterized to underparameterized

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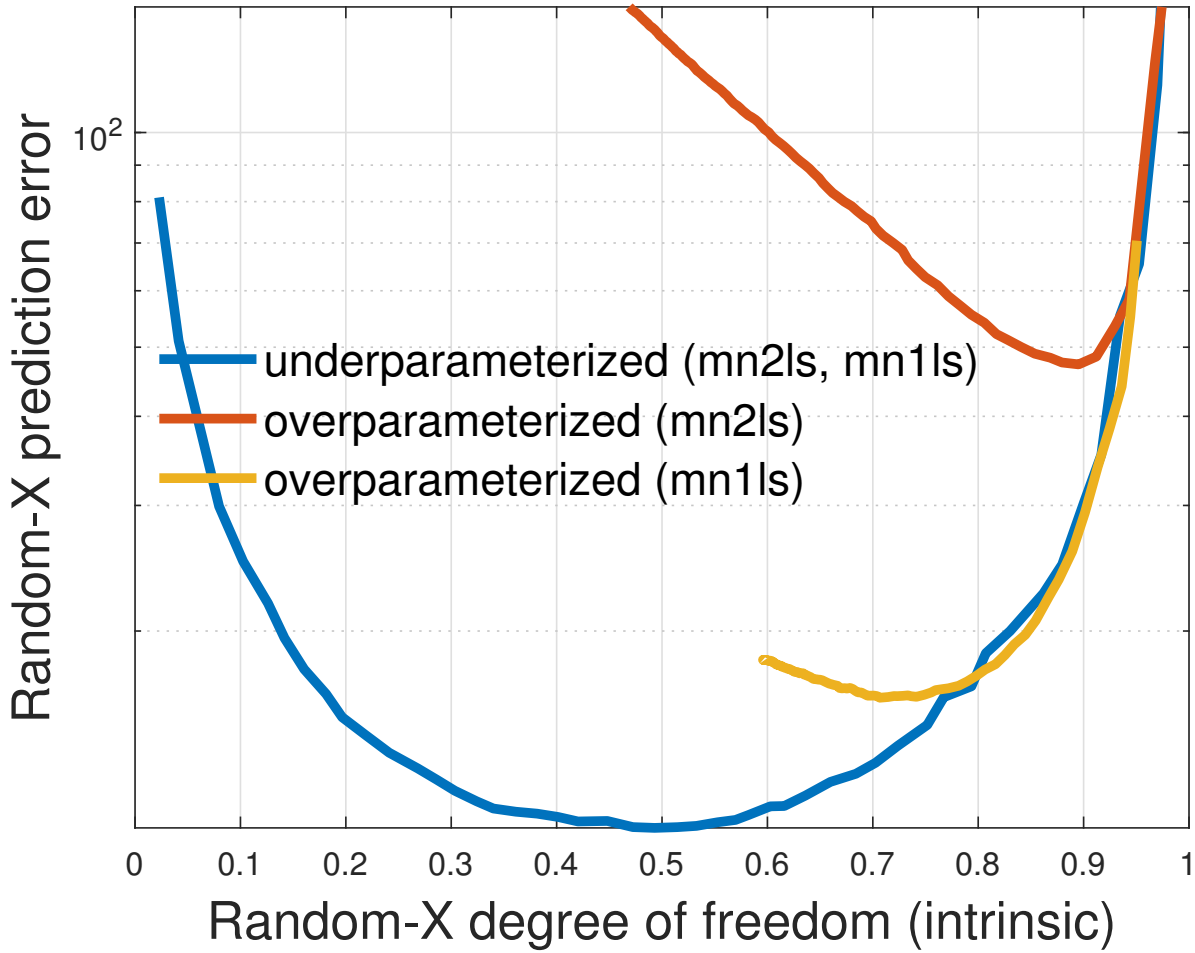

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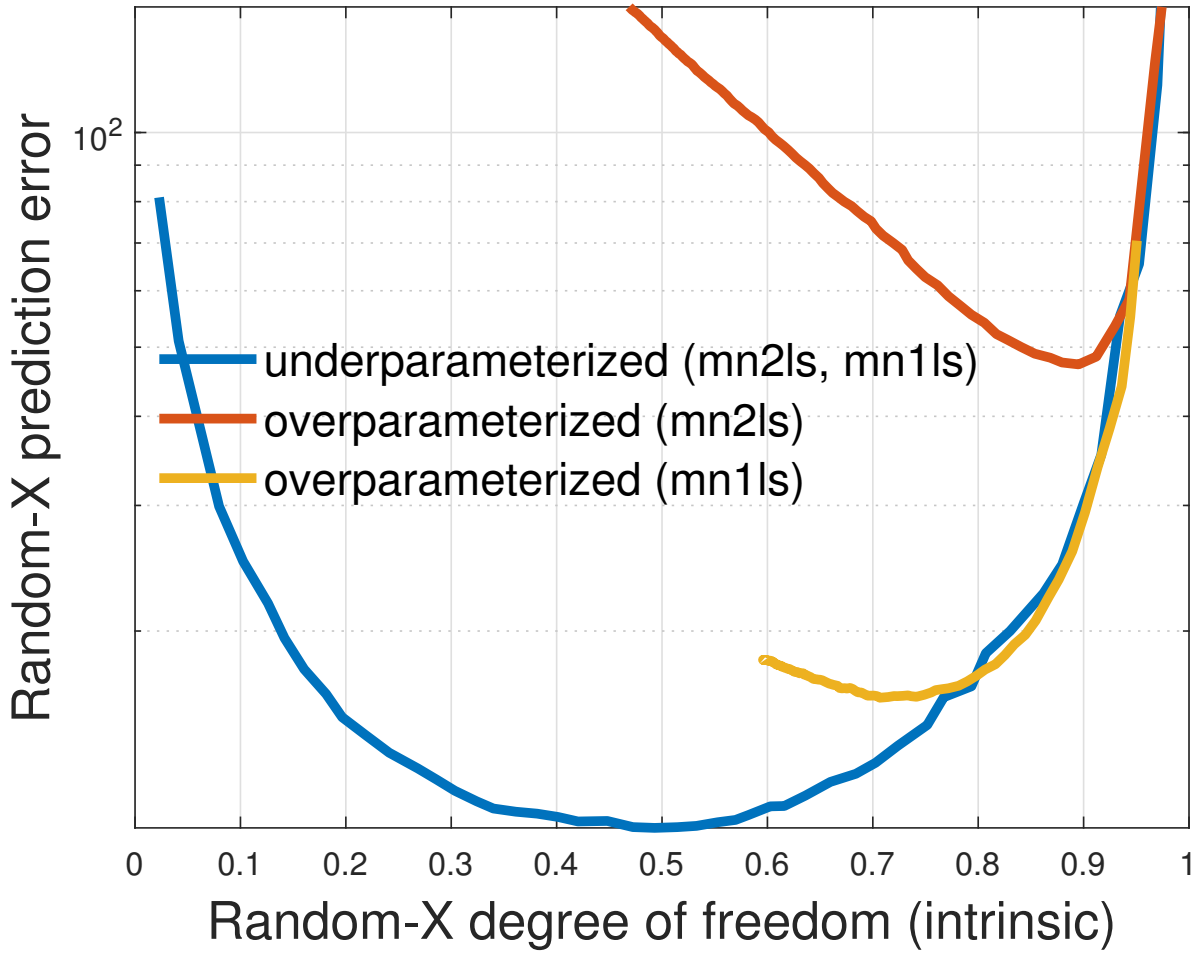

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Outline

Discussion and future directions

A high-level view of the work:

- Suppose we are given a family of models for which we want a complexity measure under a specific error metric.
- Construct a family of "reference" models spanning same optimisms.
- Find the model in the reference family that is closest to the observed optimism. Declare complexity as complexity of that reference model.

Key relation:

$$\mathrm{OptR}(\widehat{f}) = \mathrm{OptR}(\widehat{f}^{\mathrm{ref}})$$

Going beyond . . .

- Attribute total complexity to various components: bias, variance, covariate shift, etc.
- Other error metrics beyond squared error
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Thanks for listening!

Questions/comments/thoughts?