# Revisiting Model Complexity in the Wake of Overparameterized Machine Learning

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*Based on joint work with Jin-Hong Du and Ryan Tibshirani*

`https://pratikpatil.io/papers/model-complexity.pdf`

# Overparametrization in machine learning

Modern machine learning models typically fit 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 problem
- Generalization: despite overfitting, models generalize well in practice

This talk is about generalization aspect in overparameterized learning.

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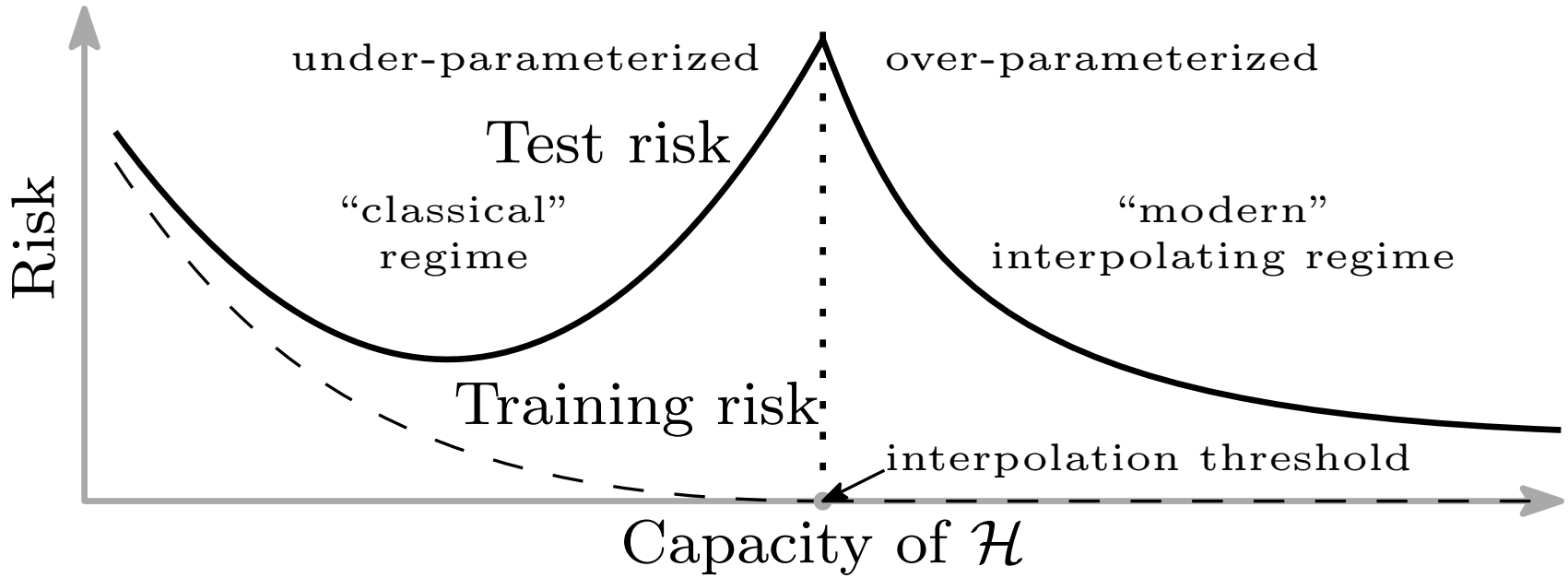
# The double/multiple descent phenomenon




"Reconciling modern machine learning practice and the bias variance tradeoff"
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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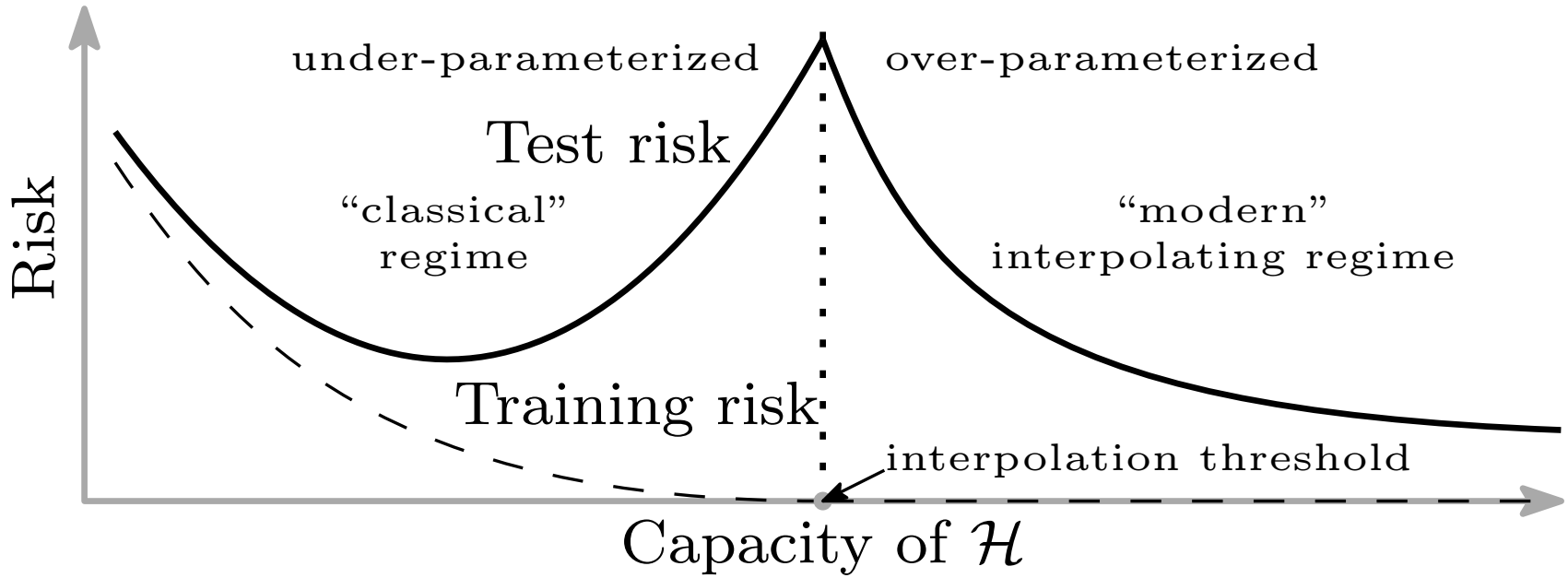


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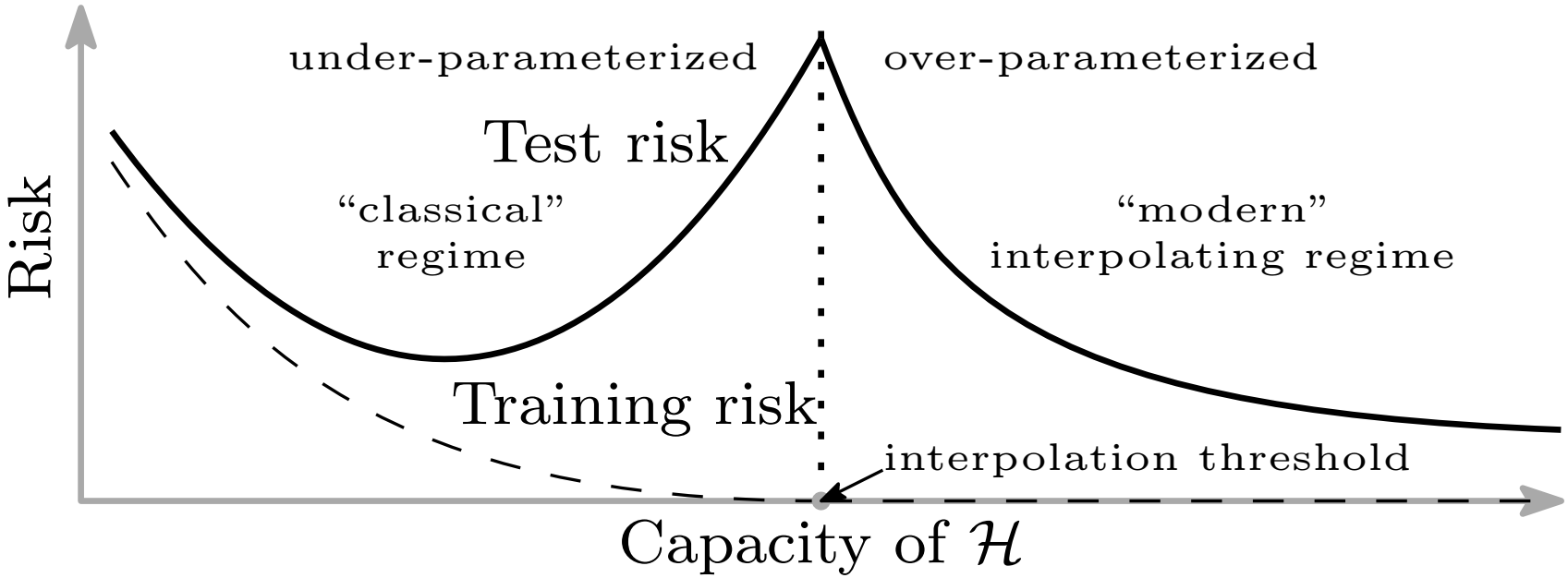


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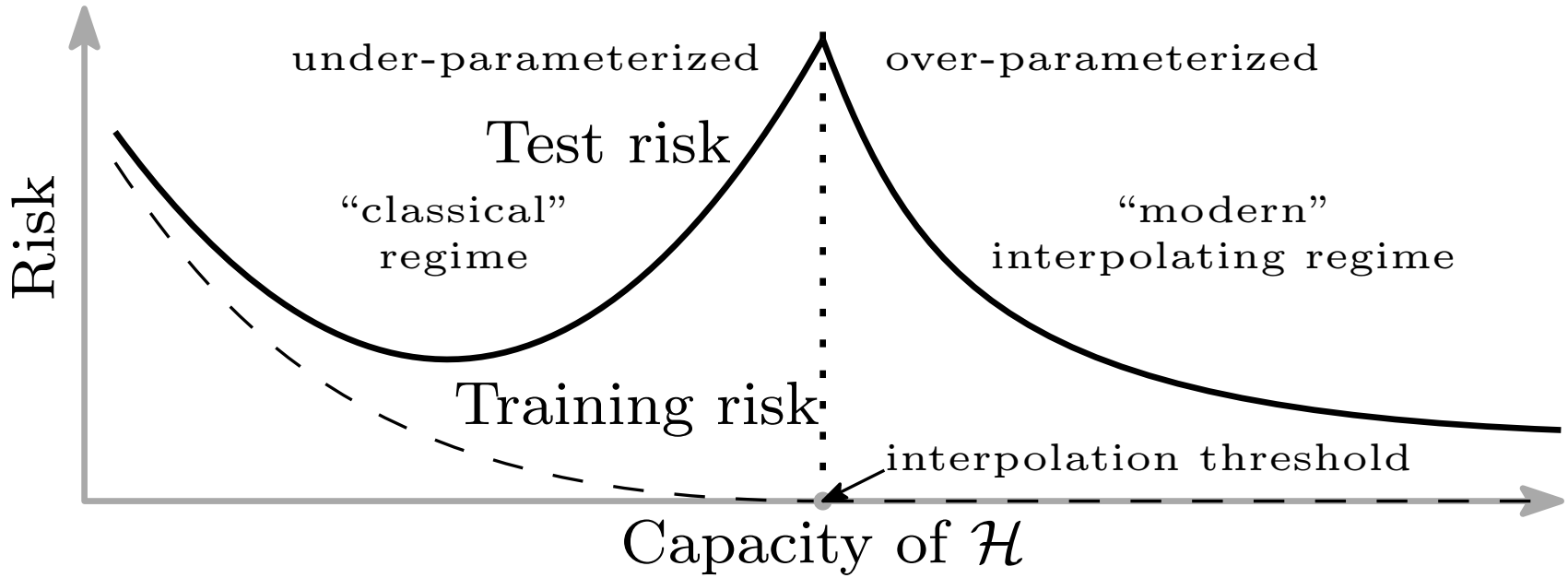


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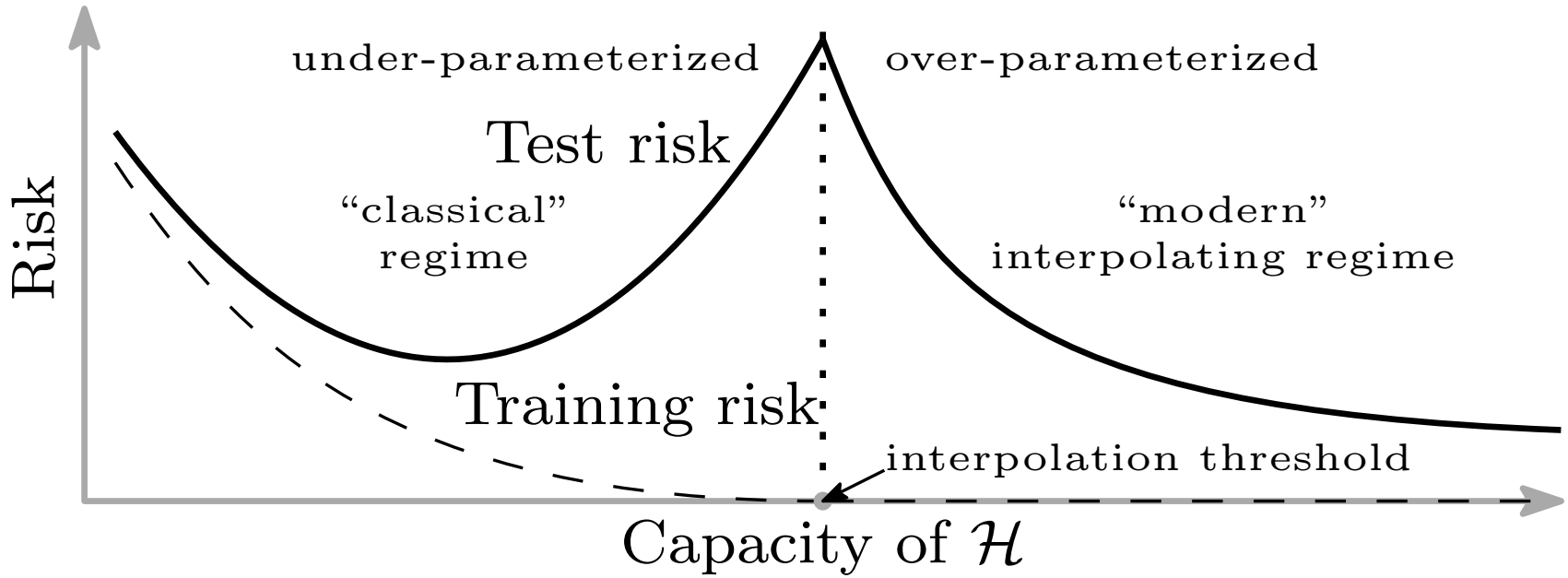


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# Recent theoretical developments

Understanding generalization of interpolators in simpler settings:

- Linear regression
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  - Mei, Montanari, 2019
- Kernel regression
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# What do we currently understand?

- In nearly all applications, current practice suggests we should design models to be massively overparametrized
- Once trained (typically by SGD), these models interpolate the training data (achieve zero training error)
- Still they are capable of having (often do have) good test error

Current understanding of this? In full theoretical rigor, not great.

However, the story is fairly well-understood for linear models, kernel models, and random feature models. See, e.g., nice monographs:

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# Goals of this work

This work attempts to answer the following questions:

- Is there a good measure of model complexity for predictive models?
- How to compare model complexity of different (near) interpolators?

# 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 $\ell_2/\ell_1$-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

# Interlude 1: why interpolators?

Perfectly reasonable question: *Why should we care about interpol- ating least squares?*

Because in certain high-dimensional problems, the optimal amount of regularization can actually be none!

Insight: limit of vanishing regularization is still implicitly regularized. For example, in ridge regression:

$$\lim_{\lambda \to 0^+} (X^\top X + \lambda I)^{-1} X^\top Y = (X^\top X)^+ X^\top Y$$

which is the minimum $\ell_2$ norm or "ridgeless" least squares estimator. Surprisingly, $\lambda = 0^+$ (ridgeless) can actually be the optimal level of regularization in high dimensions!

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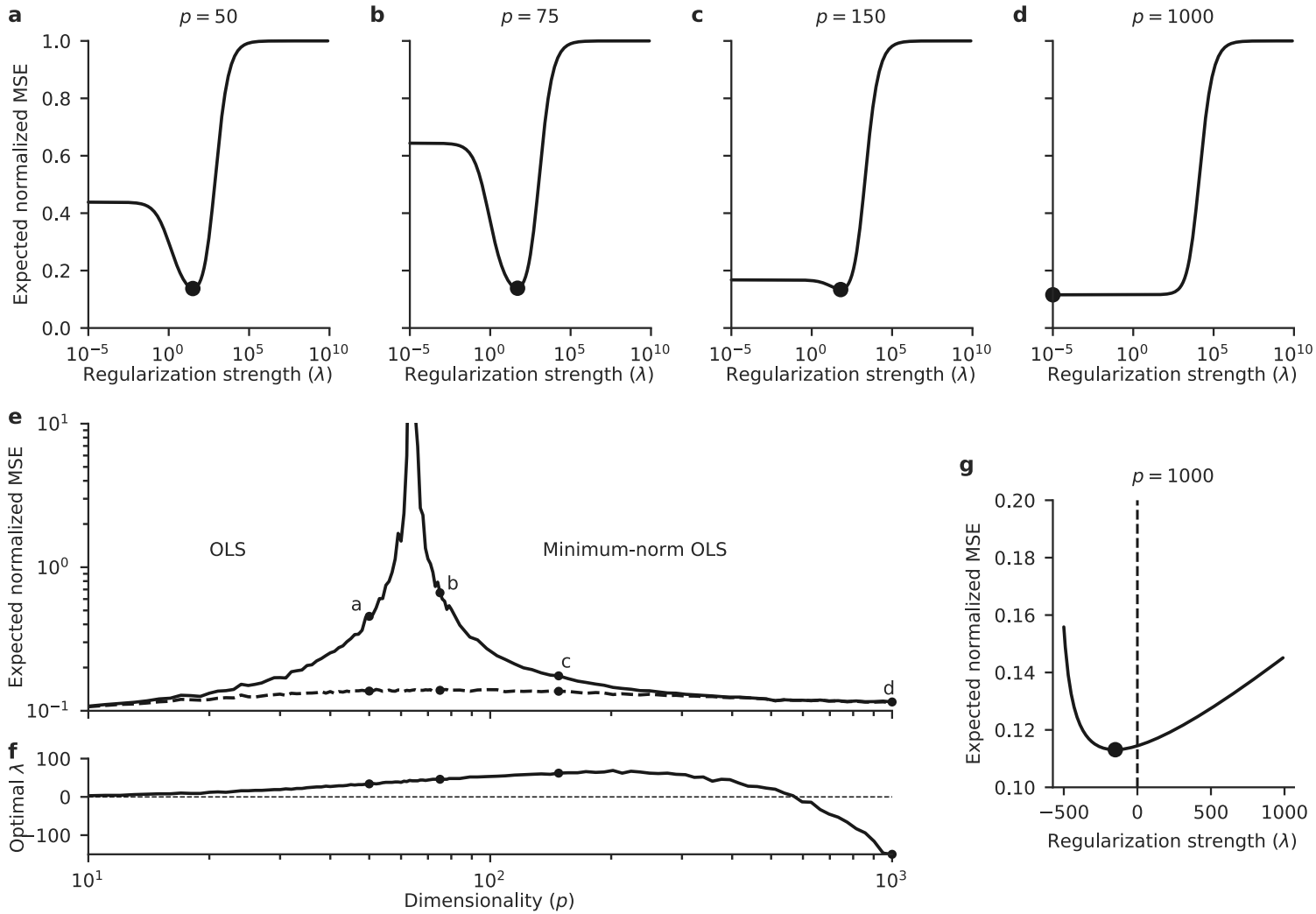
# Example: ridgeless optimality



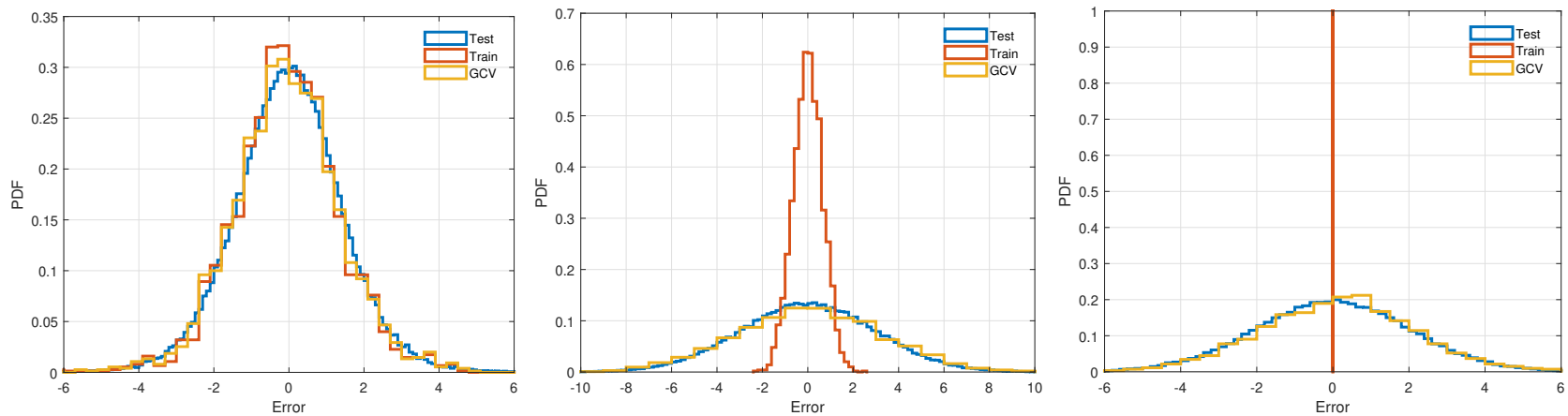

Kobak, Lomond, and Sanchez (2020)

# Interlude 2: cross-validation

A natural follow-up: *Does cross-validation (CV) still "work" in the overparametrized regime, when optimal $\lambda$ can be zero?*

For ridge, answer is yes: Patil, Rinaldo, Wei, and T. (2021), Patil, Rinaldo, and T. (2022) prove CV is uniformly consistent for ridge risk under a proportional asymptotics model, weak assumptions

Empirical verification: $n = 2500$, $p = 100/2000/5000$, and $\lambda = 0^+$:



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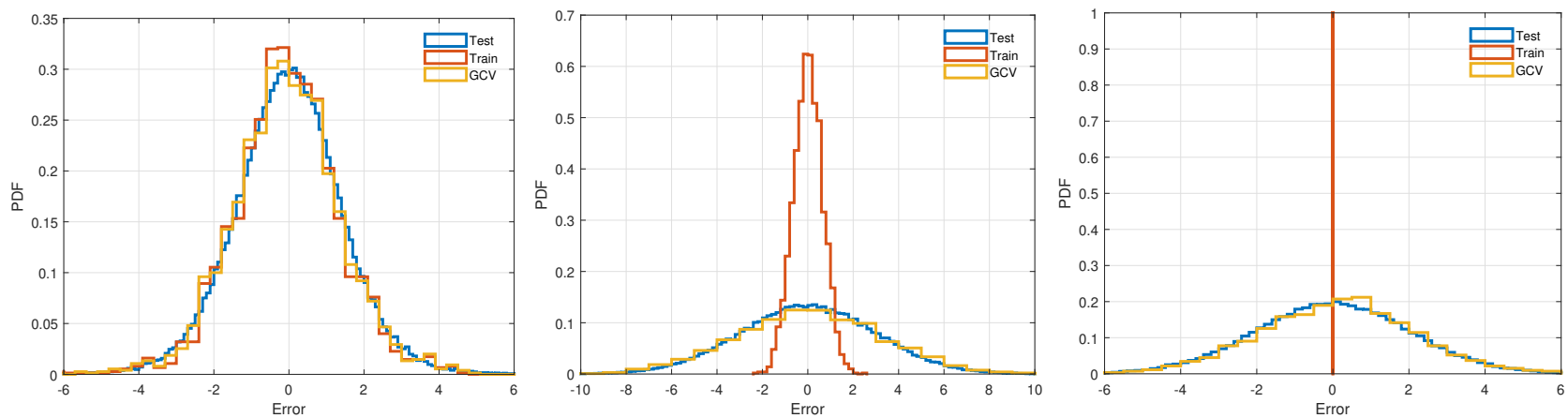

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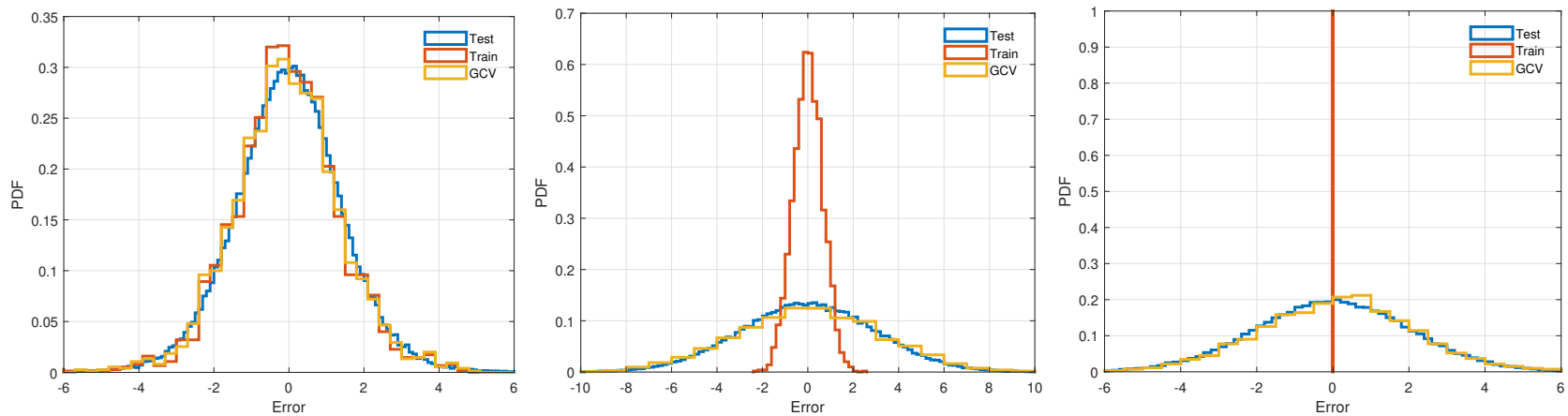

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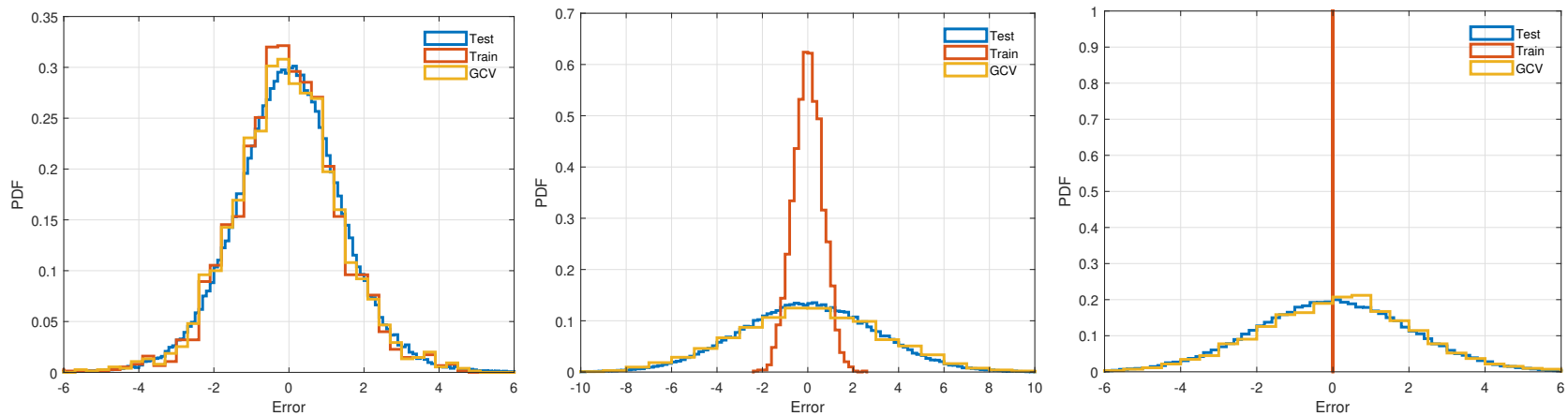

# Interlude on the interlude: LOO at $\lambda = 0$?

Recall, leave-one-out (LOO) CV for ridge:

$$\mathrm{loo}(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - x_i^\top \widehat{\beta}_\lambda^{-i}\right)^2 = \underbrace{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - x_i^\top \widehat{\beta}_\lambda}{1 - [S_\lambda]_{ii}}\right)^2}_{\text{"shortcut formula"}}$$

where $S_\lambda = X(X^\top X + \lambda I)^{-1}X^\top$ is the ridge smoother matrix

For $\lambda = 0$ in overparametrized regime, all summands are $0/0$ ... but there is a fix! Hastie, Montanari, Rosset, and T. (2022) propose:

$$\mathrm{loo}(0) = \lim_{\lambda \to 0^+} \mathrm{loo}(\lambda) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{[(XX^\top)^+ Y]_i}{[(XX^\top)^+]_{ii}}\right)^2$$

(Continuation at $\lambda = 0$ works for GCV as well, as does consistency)

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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.
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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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Given an estimator $\widehat{f}$ of the regression function (i.e., $\widehat{f}(x)$ estimates $\mathbb{E}[y|x]$), trained on $(x_i, y_i)$, $i = 1, \ldots, n$, we define

$$\mathrm{df}(\widehat{f}) = \frac{1}{\sigma^2} \sum_{i=1}^{n} \mathrm{Cov}(y_i, \widehat{f}(x_i))$$

where $\sigma^2 = \mathrm{Var}(y|x)$, and each $x_i$ is treated as fixed

Key fact. For $\widehat{f}$ the least squares estimator of response $Y \in \mathbb{R}^n$ on feature matrix $X \in \mathbb{R}^{n \times p}$, with $p$ linearly independent columns,

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# Connection to fixed-X error

This definition is intrinsically connected to fixed-X test error:

$$\underbrace{\mathbb{E}_{Y,Y^*}\left[\frac{1}{n}\sum_{i=1}^{n}(y_i^* - \widehat{f}(x_i))^2\right]}_{\mathrm{ErrF}(\widehat{f})} = \underbrace{\mathbb{E}_{Y}\left[\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{f}(x_i))^2\right]}_{\mathrm{train_F}(\widehat{f})} + \frac{2\sigma^2}{n}\mathrm{df}(\widehat{f})$$

The difference between test and training error is called optimism:

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Also points to a big shortcoming ... fixed-X error is not as relevant to modern stat/ML practice which is driven by random-X error

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Classically—for smooth functions, in low dimensions—we can tie fixed-X and random-X errors together (e.g., by empirical process theory)

But beyond this—nonsmooth functions, or high dimensions—they can be very different.
Epitomized by generalizing interpolators:

- $\mathrm{ErrR}(\widehat{f}) \to 0$, but
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Similarly, for any interpolator $\widehat{f}$:

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- $\mathrm{ErrF}(\widehat{f}) = \mathbb{E}[n^{-1} \sum_{i=1}^{n} (y_i^* - y_i)^2] = 2\sigma^2$

Similarly, for any interpolator $\widehat{f}$:

$$\mathrm{df}(\widehat{f}) = \frac{1}{\sigma^2} \sum_{i=1}^{n} \mathrm{Cov}(y_i, y_i) = n$$

which is useless!

# Example: 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

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

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

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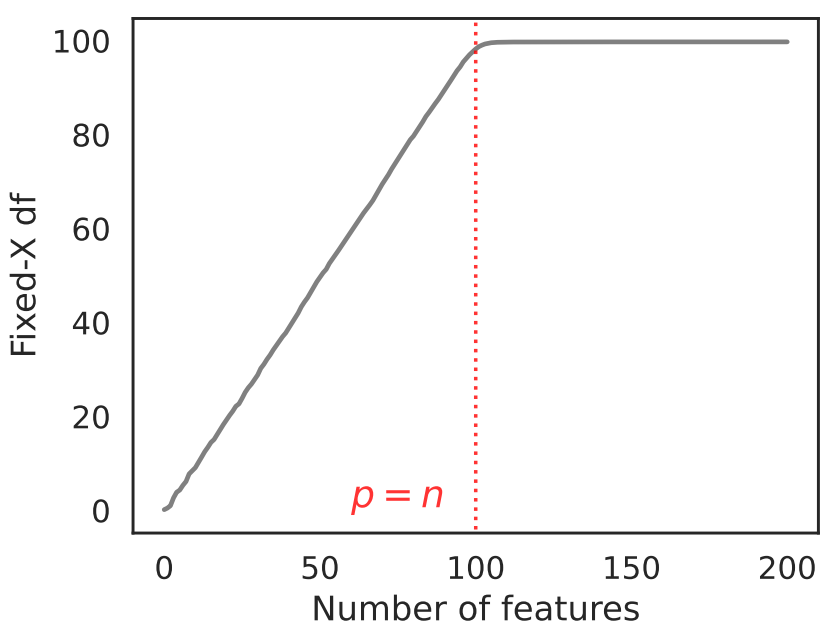
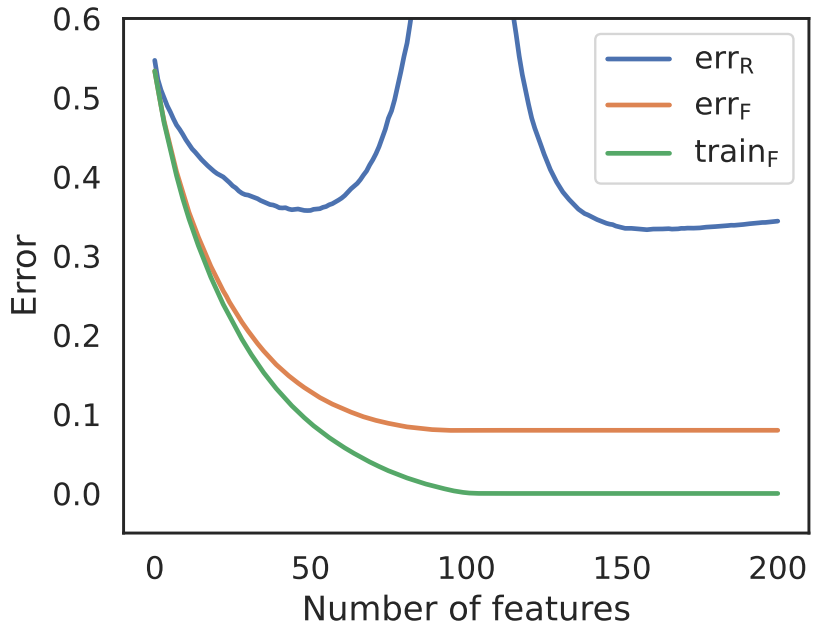
# Example: ridgeless least squares df

Classical, fixed-X df for ridgeless least squares, with $n = 100$:



# Can we generalize df to random-X, and beyond?

Goals:

- Generalize df so that it connects to random-X error, and gives meaningful answers for any estimator (even interpolators)
- Allow for decomposition of df according to some user-specified components

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# Outline

# What is complexity?

What makes up a measure of complexity? Two things:

- a metric
- a reference model

That is, the metric assigns a number to the given model $\widehat{f}$, and the reference model $\widehat{f}^{\text{ref}}$ provides units, so we can interpret the metric

A bit more detail:

- Metric should be "negatively oriented" for complexity—smaller values mean less complex
- Reference model should be something whose parameters we are "happy to count"

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# Re-interpreting degrees of freedom

We can actually re-interpret the classical definition of df in this light, with: metric $= \mathrm{OptF}$, and $\widehat{f}^{\mathrm{ref}} =$ least squares

That is, *we will define* $\mathrm{df}(\widehat{f}) = k$, for the number $k \geq 0$ such that

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where $\widehat{f}_k^{\mathrm{ls}}$ is the least squares estimator of the given $Y \in \mathbb{R}^n$ on a feature matrix $X \in \mathbb{R}^{n \times k}$ with $k$ linearly independent columns

Think about it this way: $\mathrm{df}(\widehat{f}) = 5.3$ means $\widehat{f}$ has the same fixed-X optimism as least squares with 5.3 parameters

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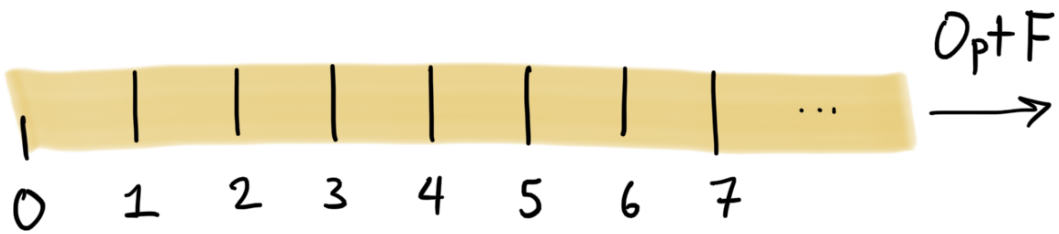

# Lifting this idea to random-X

Naturally we can lift this to the random-X setting. We define

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We will again use $\widehat{f}_k^{\mathrm{ls}}$ for reference class: least squares on $k$ features. However, in the random-X setting, it matters:

- what these features are (law of $x_i$)
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(Recall, none of this mattered in the fixed-X setting ...)

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So what data generating distribution should we use for our reference model in the random-X setting?

# Universal asymptotics

Consider i.i.d. samples $(x_i, y_i)$, $i = 0, \ldots, n+1$, from the following standard random matrix theory (RMT) model:

- $x_i = \Sigma^{1/2} z_i$, where $\Sigma \in \mathbb{R}^{p \times p}$ is deterministic with eigenvalues bounded away from 0 and $\infty$; and $z_i \in \mathbb{R}^p$ has i.i.d. coordinates with zero mean, unit variance, and finite 4th moment
- $y_i = x_i^\top \beta + \epsilon_i$, where $\epsilon_i$ has zero mean, unit variance, and is independent of $x_i$

Theorem. Under the standard RMT model above, as $n, p \to \infty$ with $p/n \to \gamma < 1$, the random-X optimism least squares satisfies:[1]

$$\mathrm{OptR}(\widehat{f}_p^{\mathrm{ls}}) - \sigma^2 \left( \frac{n}{n-p} - \frac{n-p}{n} \right) \to 0$$

[1] Convergence is actually almost sure wrt training features $X \in \mathbb{R}^{n \times p}$; need uniform integrability to get convergence in expectation.

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# Emergent random-X df

Using this we can define a quantity we call emergent random-X df: $\mathrm{df}^{\mathrm{e}}(\widehat{f}) = k$, for the number $k \geq 0$ such that

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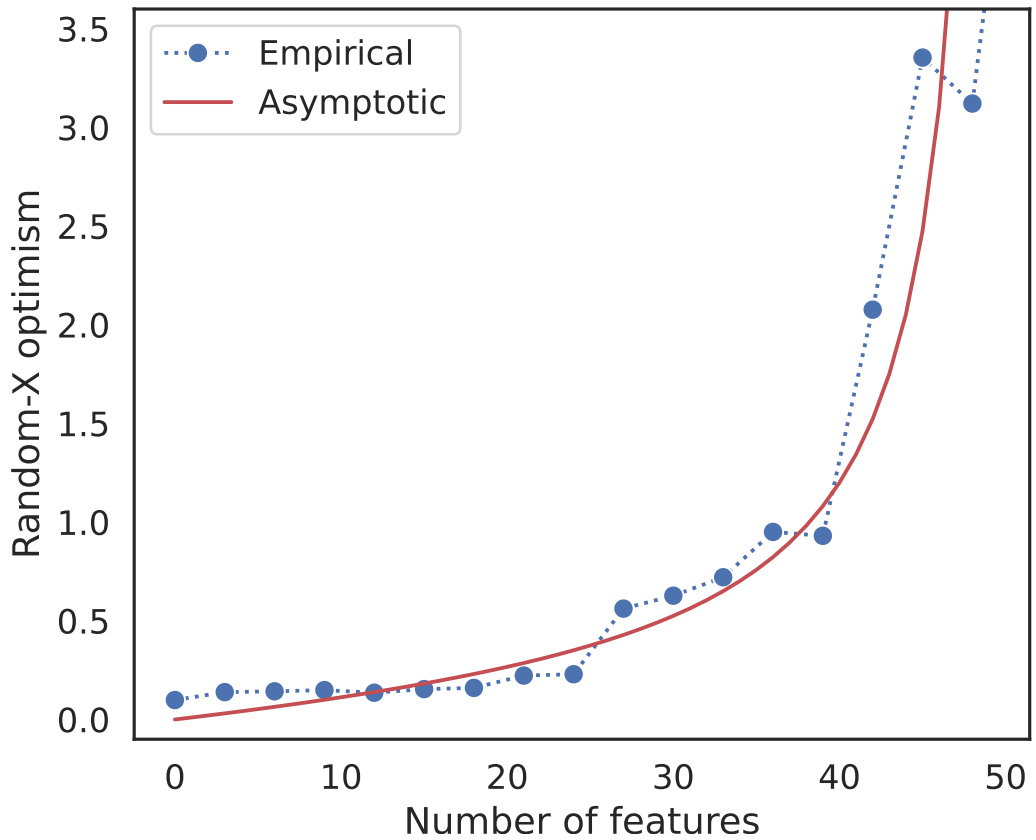
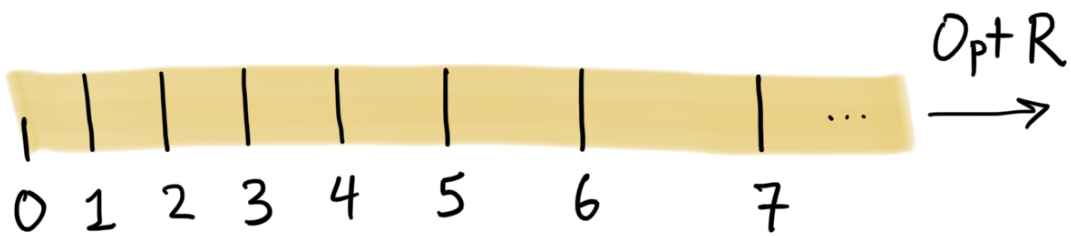
# Illustration: least squares as reference

Random-X optimism for least squares, with $n = 50$:



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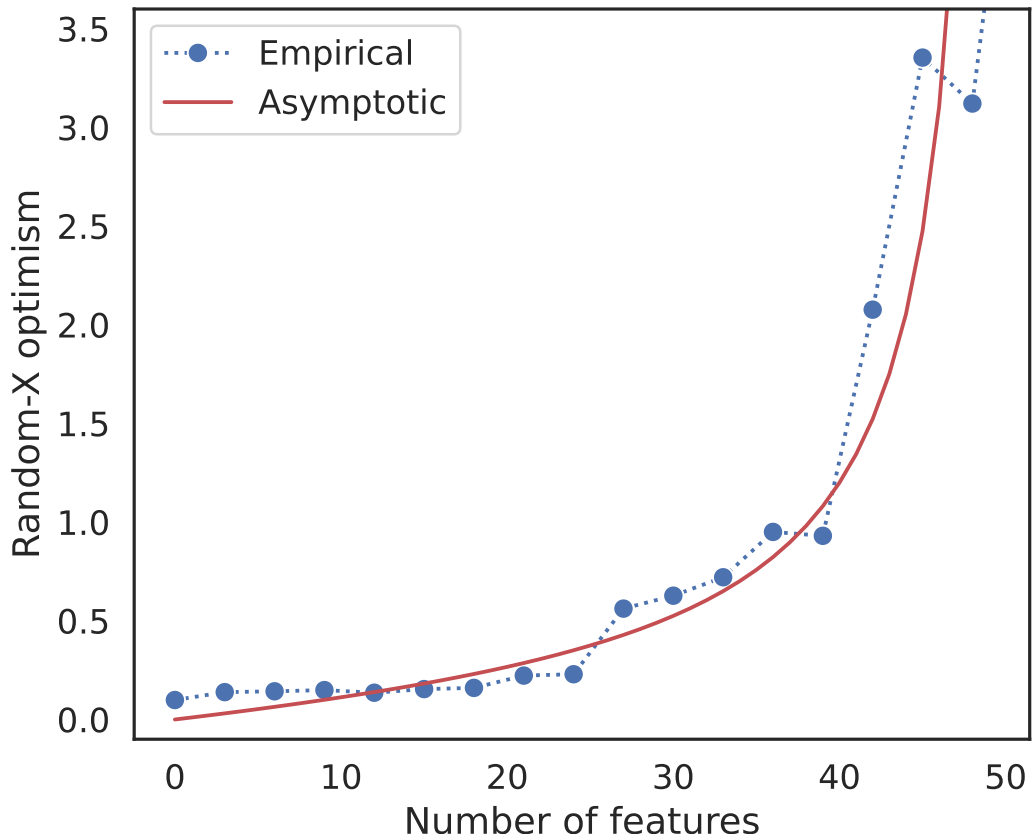
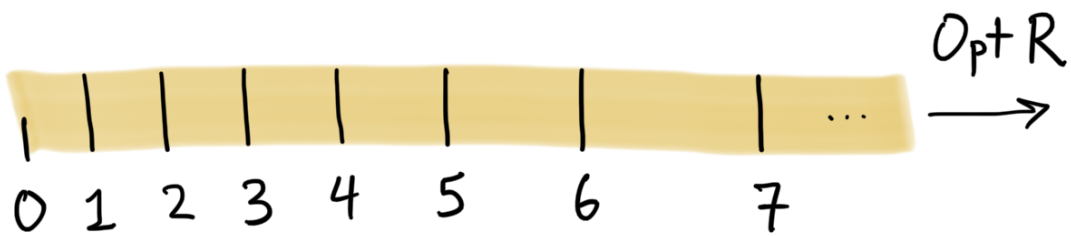
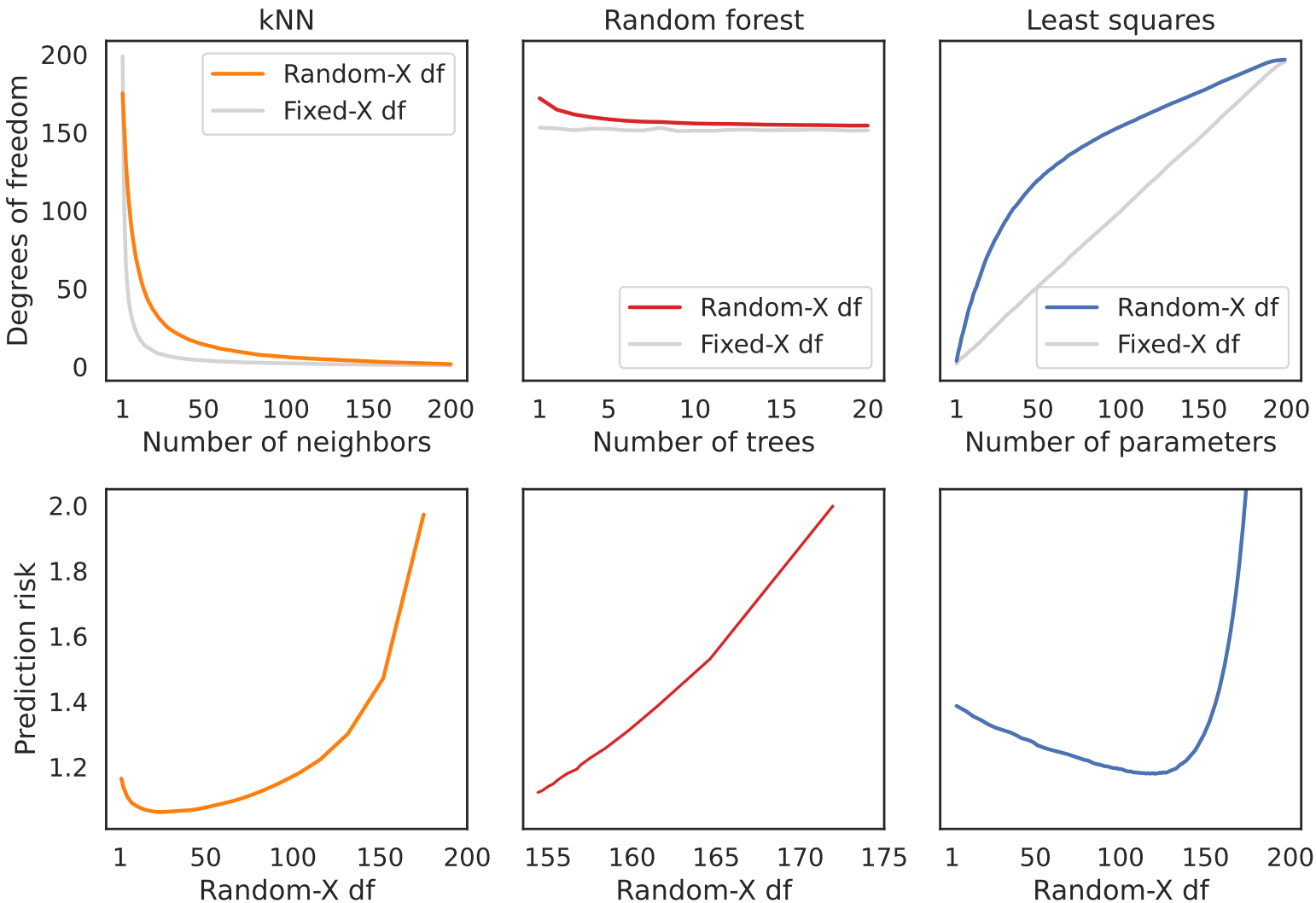


# Example: emergent random-X df

Ex with $n = 200$ samples, $d = 300$ features, $\mathbb{E}[y|x]$ nonlinear in $x$:



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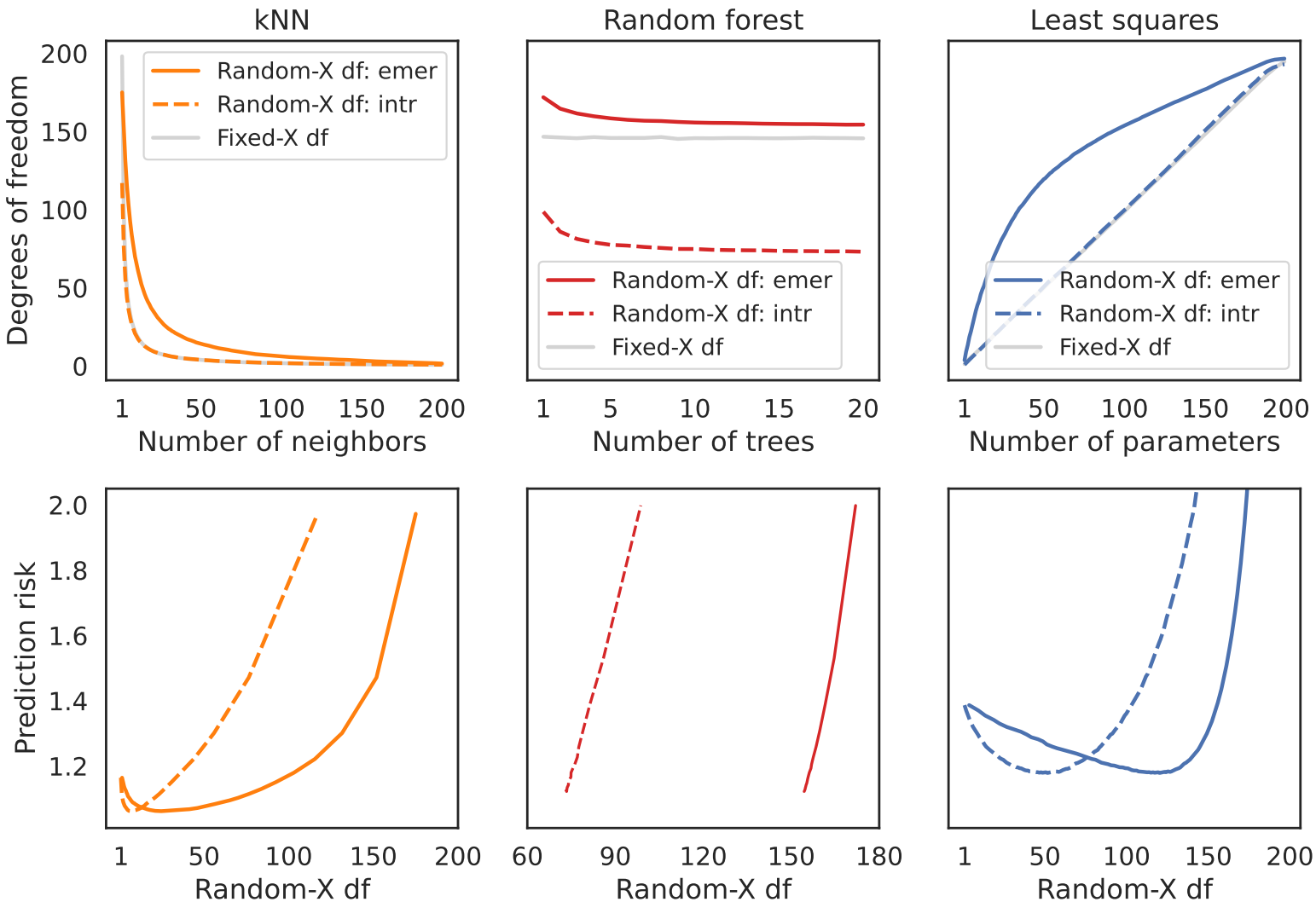

# Computing random-X degrees of freedom

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 $\psi$ 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 $\mathrm{dfR}$ of 0,
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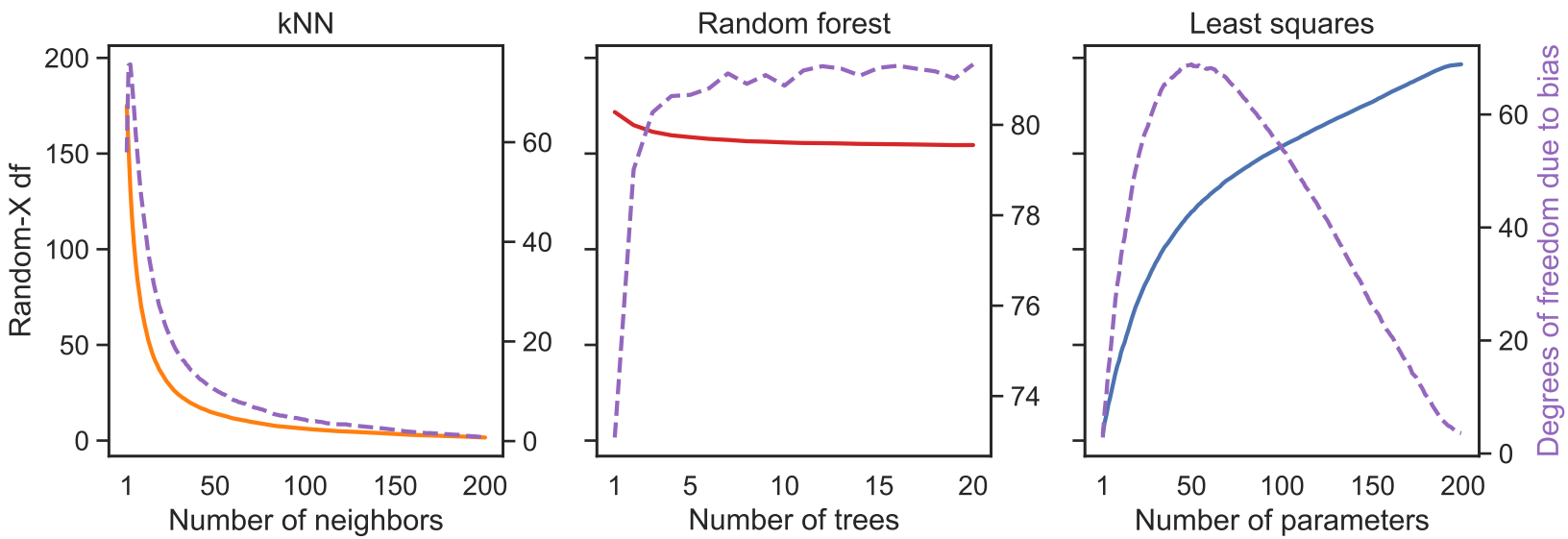
By subtracting emergent and intrinsic degrees of freedom, we are left with the df due to bias:

$$\mathrm{df}^{\mathsf{bias}}(\widehat{f}) = \mathrm{df}^{\mathsf{e}}(\widehat{f}) - \mathrm{df}^{\mathsf{i}}(\widehat{f})$$

Back to our example:



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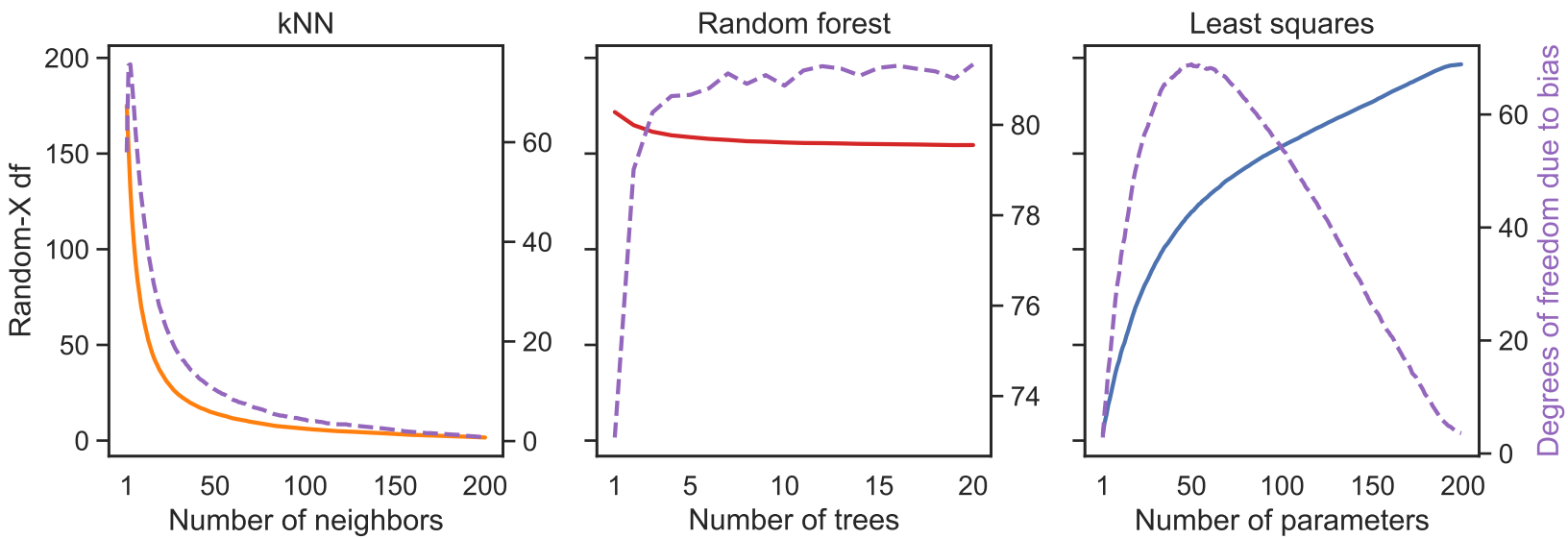

# General decomposition

Generic decompositions are possible. Let $e_1, \ldots, e_m$ be any list of user-chosen error components. E.g., $e_1 =$ bias, $e_2 =$ covariate shift, and so on

For any subset $S \subseteq \{e_1, \ldots, e_m\}$, let $\mathrm{df}^S(\widehat{f}) = k$, for the number $k \geq 0$ such that

$$\mathrm{OptR}(\widehat{f}; \{\text{data subject to } S\}) = \mathrm{OptR}(\widehat{f}_k^{\mathrm{ls}}; \{\text{RMT data}\})$$

We can then attribute $d_i$ df to each error component $e_i$, as follows:

$$d_i = \sum_{S \subseteq \{e_1, \ldots, e_m\} \setminus \{e_i\}} \frac{|S|!(m - |S| - 1)!}{m!} (\mathrm{df}^{S \cup \{e_i\}}(\widehat{f}) - \mathrm{df}^S(\widehat{f}))$$

This is an instance of a Shapley value. Therefore it obeys all of the Shapley axioms; in particular, efficiency: $\sum_{i=1}^m d_i = \mathrm{df}^{\mathrm{e}}(\widehat{f})$

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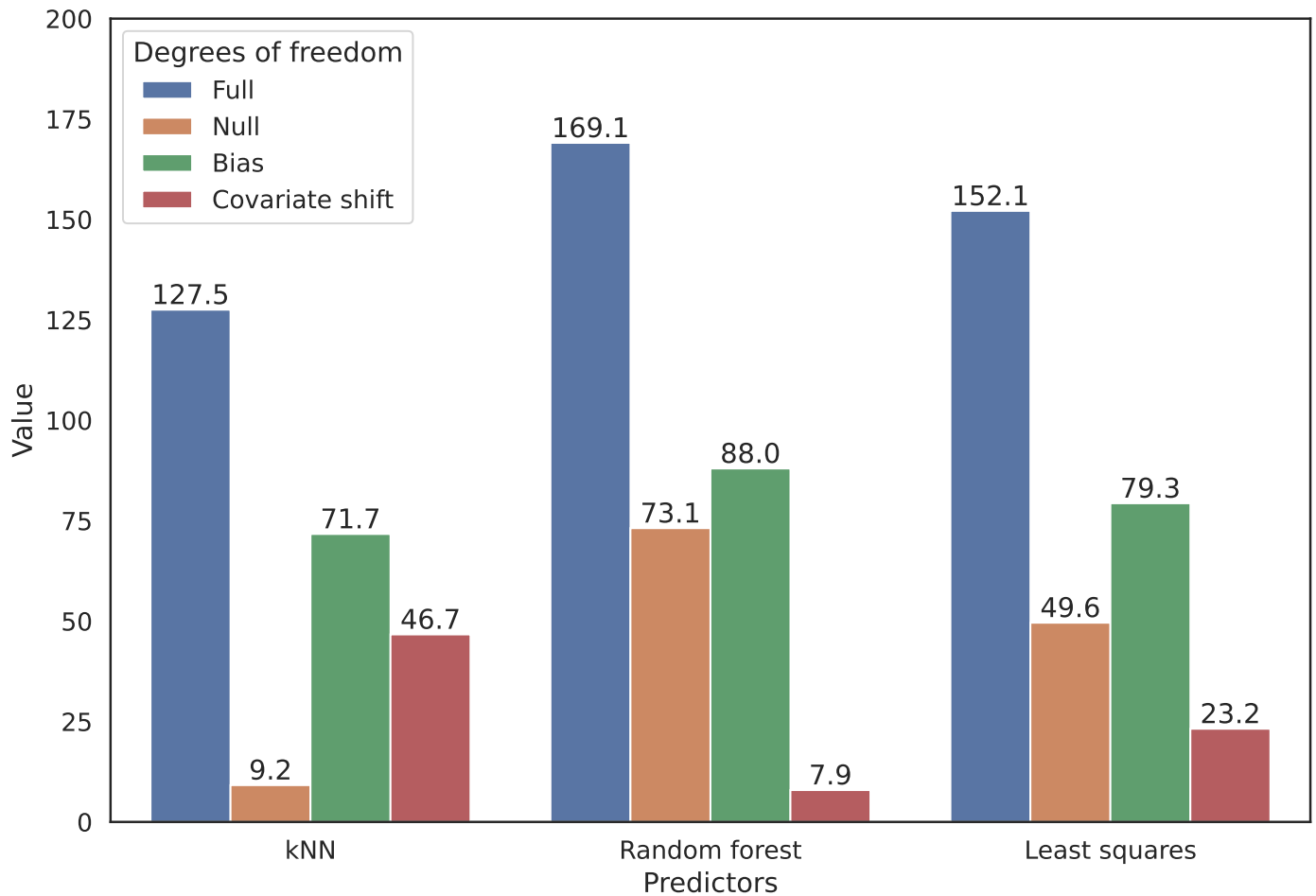
# Example: bias and covariate shift

Ex with $n = 200$ samples, $d = 300$ features, $\mathbb{E}[y|x]$ nonlinear in $x$, and covariate shift ($\Sigma \to \tilde{\Sigma}$):



# Double descent, revisited

We can use random-X df (any flavor) to reparametrize error curve for models with double descent. The df map is not monotone, but it shows that in the overparametrized regime, the effective number of parameters can actually be small

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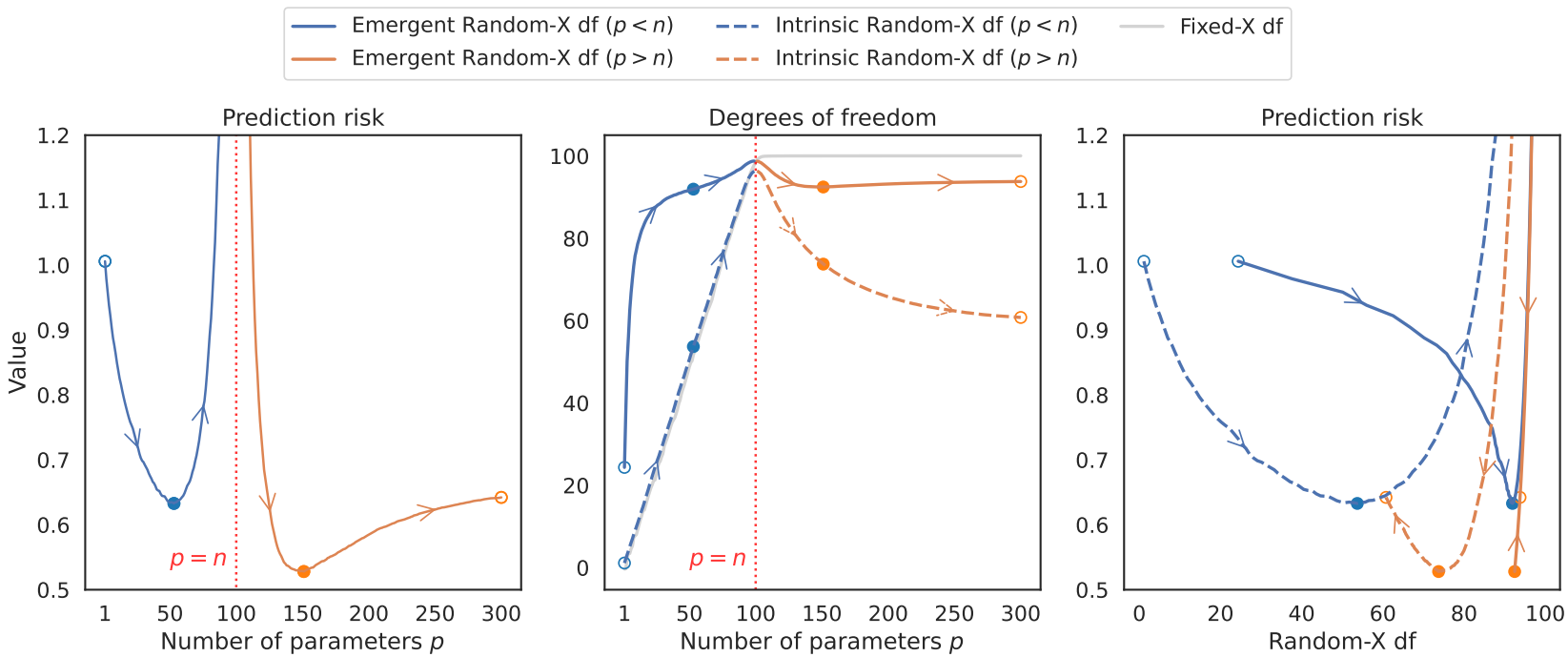

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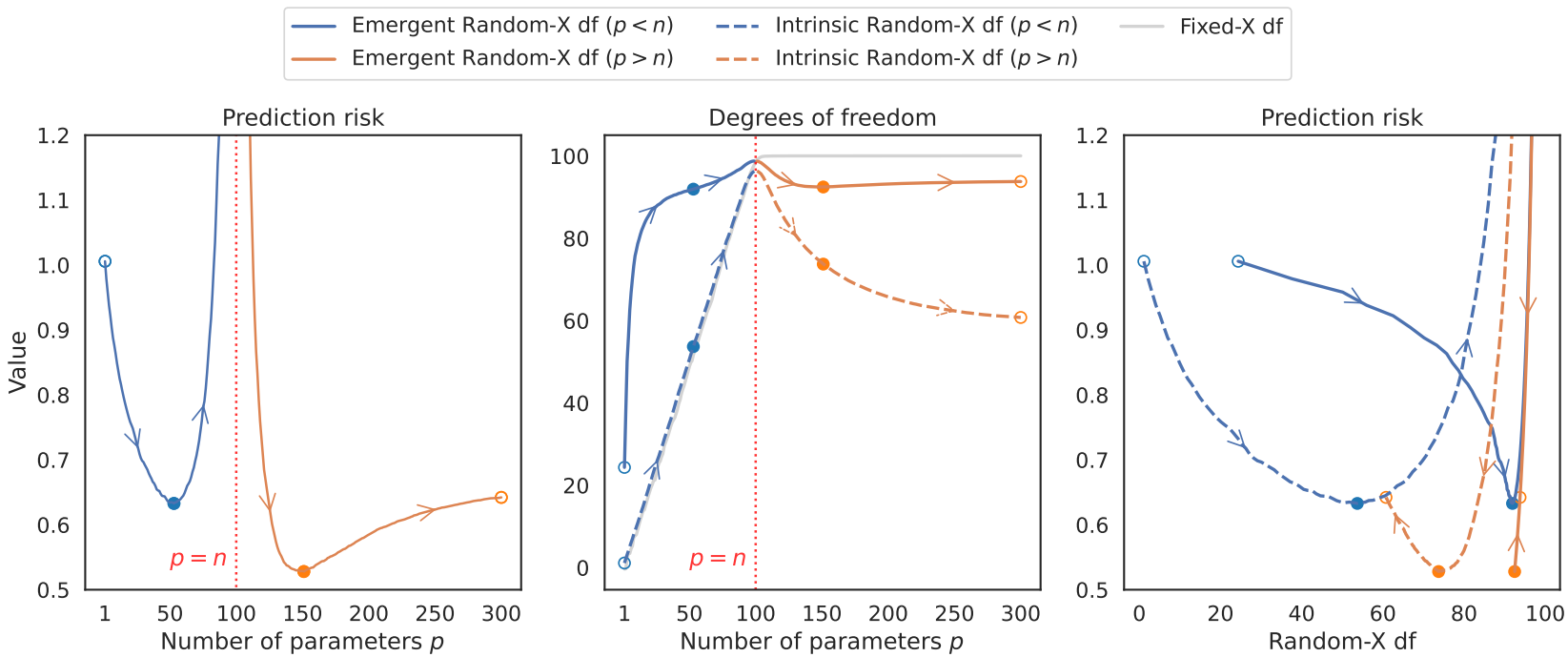

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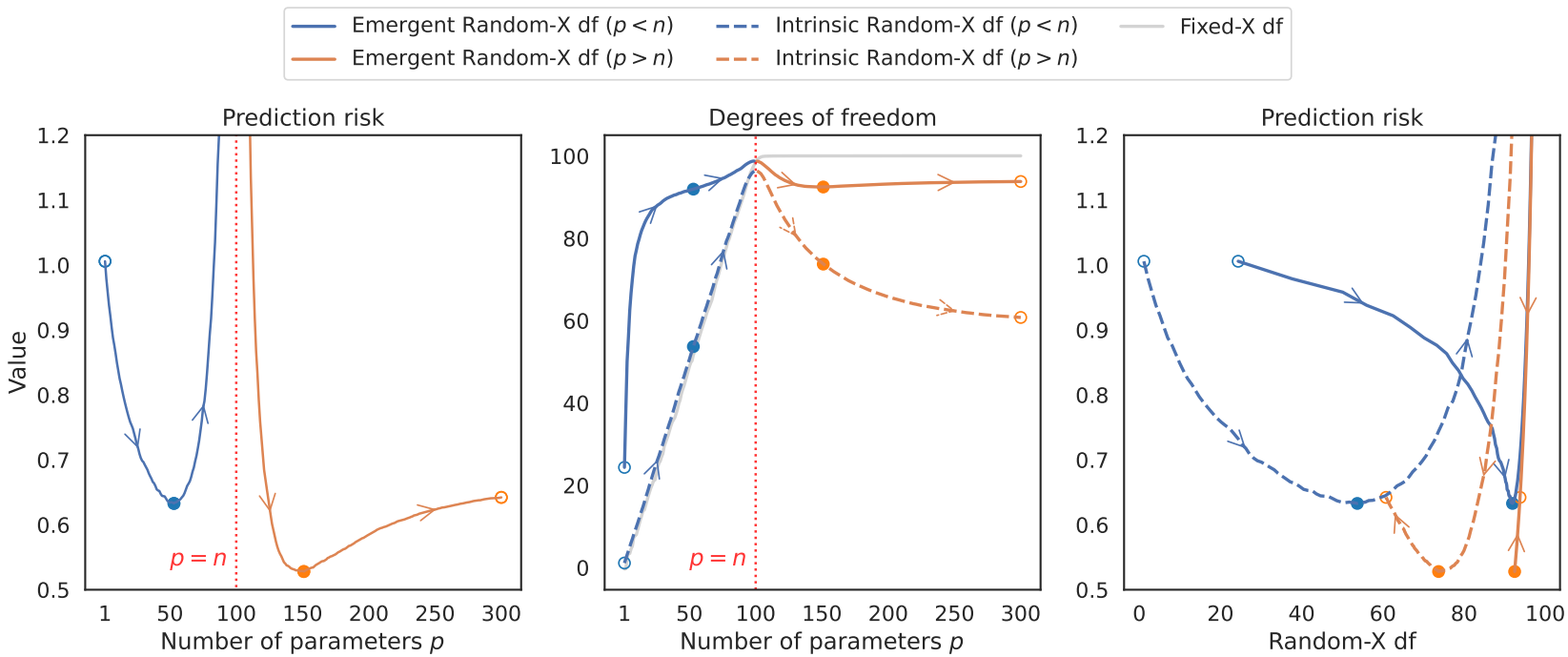

# Outline

# 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 . . .

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- Unsupervised setting?

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Thanks for listening!

Questions/comments/thoughts?