

Machine Learning in Finance

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Embracing (Infinite Dimensional) Complexity

- ▶ We observe labelled data (y_t, X_t)

- ▶ We know

$$y_t = f_*(X_t) + \varepsilon_t \quad (1)$$

- ▶ How do we attack this problem?
- ▶ Scientific approach: Dimensionality reduction. Find a low-dimensional set of X_t and only then estimate
- ▶ (Non-parametric) Statistical Approach: Look for $f_*(x)$ in the space of **all functions?**
Really? How do we even start??
- ▶ This is what ML is about

Basic Setup i

- ▶ **Data** : A vector $x \in \mathbb{R}^d$.
- ▶ **A (Machine Learning) Model = family of functions**

$$\text{Function}(\text{Data}; \text{Parameters}) = f(x; \theta) \quad (2)$$

where

$$\text{Parameters} = (\text{Parameter}_1, \dots, \text{Parameter}_P) = \theta = (\theta_1, \dots, \theta_P) \in \mathbb{R}^P \quad (3)$$

- ▶ P = parametrization
- ▶ large P = rich parametrization

Optimizing a model = selecting a “good” parameter vector $\theta_* \in \mathbb{R}^P$

Parametric Families and Neural Networks i

Examples:

- ▶ Linear functions family: $x \in \mathbb{R}^1$, $\theta = (\theta_0, \theta_1) \in \mathbb{R}^2$:

$$\text{Function}(\text{Data}; \text{Parameters}) = f(x; \theta) = \theta_0 + \theta_1 x \quad (4)$$

- ▶ 2-dimensional linear functions family: $x = (x_1, x_2) \in \mathbb{R}^2$, $\theta = (\theta_0, \theta_1, \theta_2) \in \mathbb{R}^3$:

$$f(x; \theta) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 = \underbrace{(\theta_0, \theta_1, \theta_2)}_{\text{inner product}} \underbrace{\begin{pmatrix} 1 \\ x_1 \\ x_2 \end{pmatrix}}_{\text{matrix multiplication}} = \underbrace{\theta' \begin{pmatrix} 1 \\ x \end{pmatrix}}_{\text{matrix multiplication}}, \quad (5)$$

where we have used the notation

$$\theta = \underbrace{\begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{pmatrix}}_{\text{vertical vector}}, \quad \underbrace{\theta'}_{\text{transposition}} = \underbrace{(\theta_0, \theta_1, \theta_2)}_{\text{horizontal vector}} \quad (6)$$

Parametric Families and Neural Networks ii

- ▶ when $x = (x_1, \dots, x_d)$ is d -dimensional, linear family always has **parametrization**
 $P = d + 1$: **linear families have few(er) parameters**
- ▶ Simplest **non-linear** family: Pick a function $h(x)$ and create

$$f(x; \theta) = h(\theta'x) \quad (7)$$

This function family is *non-linear*. E.g., a popular choice is

$$\text{ReLu}(x) = \max(x, 0) = \begin{cases} x, & x > 0 \\ 0, & x \leq 0 \end{cases}$$

- ▶ We can now take **linear combinations** of such functions. E.g.,

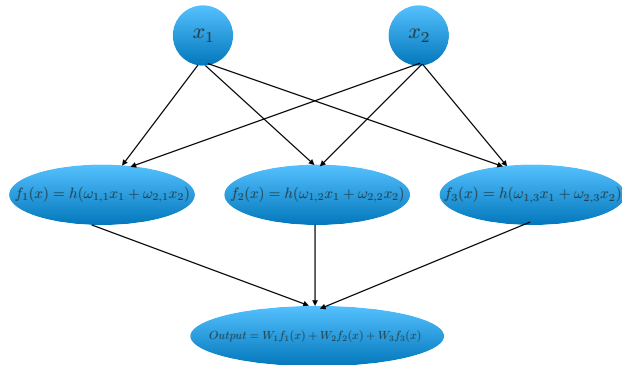
$$\begin{aligned} f_1(x) &= h(\omega_{1,1}x_1 + \omega_{2,1}x_2) \\ f_2(x) &= h(\omega_{1,2}x_1 + \omega_{2,2}x_2) \\ f_3(x) &= h(\omega_{1,3}x_1 + \omega_{2,3}x_2) \\ f(x; \theta) &= W_1 f_1(x) + W_2 f_2(x) + W_3 f_3(x) \\ \theta &= (W_1, W_2, W_3, \omega_{1,1}, \omega_{2,1}, \omega_{1,2}, \omega_{2,2}, \omega_{1,3}, \omega_{2,3}) \end{aligned} \quad (8)$$

Parametric Families and Neural Networks iii

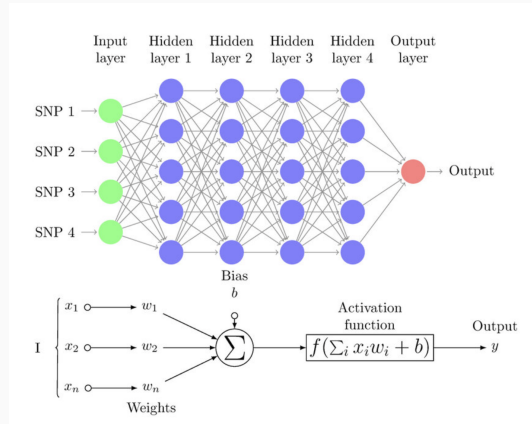
$$\underbrace{P = 9}_{\text{parametrization}} > \underbrace{d}_{\text{data dimension}} + 1 = 3$$

- **Observation: Non-linear Models = Rich parametrization**
- **Note: Human Beings Always construct recursive functions.** Perhaps this is how our brains function. In the example above:

$$\text{Linear Combinations} \rightarrow \text{Non-linearity } h(x) \rightarrow \text{Linear Combinations} \quad (9)$$



Deep Neural Networks: Huge P



So, What is Machine Learning? i



Figure: Linear family $f(x; \alpha, \beta) = \alpha + \tan(\beta)x$. **Error** = $y - f(x; \alpha, \beta)$

So, What is Machine Learning? ii

Ingredients:

- **A (Machine Learning) Model = family of functions**

$$\text{Function}(\text{Data}; \text{Parameters}) = f(x; \theta)$$

- Stuff to be modelled/Explained = **labels** = y
- **Training Data**: T observations on which the model learns (=In-Sample Data); and
Testing Data: observations on which the model is tested Out-Of-Sample

$$\text{Training Data} = (\text{label}(t), \text{Data}(t))_{t=1, \dots, T} = \left(\underbrace{y(t), x(t)}_{\text{observation number } t} \right)_{t=1}^T \quad (10)$$

- **Errors**

$$\text{Error}(\text{label}, \text{Data}, \text{Parameters}) = \text{label} - \text{Function}(\text{Data}; \text{Parameters}) \quad (11)$$

So, What is Machine Learning? iii

- **Objective function.** E.g., distance between labels and decisions: and

$$\begin{aligned} \text{Objective}(\theta; \text{Training Data}) &= \text{Mean Squared Error} \\ &= \frac{1}{T} \text{Sum}_{\text{Data}(t) \in \text{Training Data}} (\text{Error}(\text{label}(t), \text{Data}(t), \text{Parameters}))^2 \\ &= \frac{1}{T} \sum_{t=1}^T \underbrace{(y(t) - f(x(t); \theta))^2}_{\text{Error on } t\text{-th observation}} \end{aligned} \tag{12}$$

- But in finance (asset pricing), there are **other, more natural objectives** (more on this later)
- A **learning algorithm** tries to solve

$$\theta_* = \arg \min_{\theta} \text{Objective}(\theta; \text{Training Data}) \tag{13}$$

So, What is Machine Learning? iv

- But what we really care about is the **out-of-sample performance of the model**: We want the model to work for $\tau > T$ so that

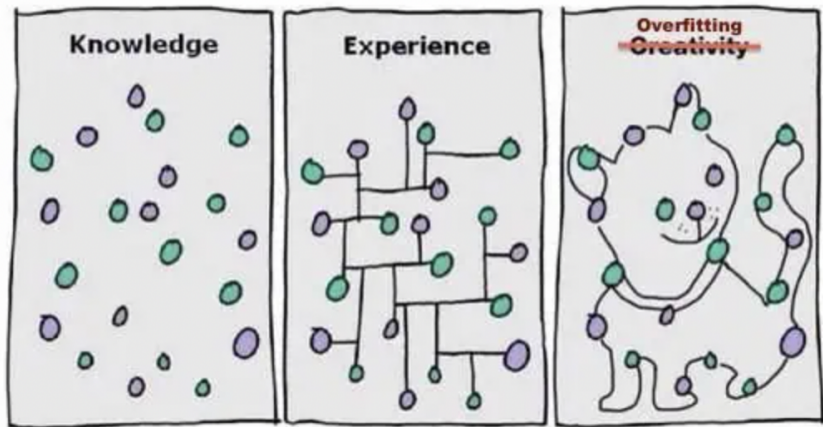
$$\begin{aligned} \text{Test Error} &= \text{Average}((\text{Error}(\text{Testing label}, \text{Testing Data}, \text{Parameters}))^2) \\ &= \frac{1}{T_{\text{test}}} \sum_{\tau=T+1}^{T+T_{\text{test}}} \left(\underbrace{y_{\tau}}_{\text{out-of-sample label}} - \underbrace{f(x_{\tau}, \theta_*)}_{\text{out-of-sample predictions}} \right)^2 \end{aligned} \quad (14)$$

to be **small**.

The Billion Dollar Question: Which Model (Parametrization) To Choose? i

- ▶ Conventional wisdom if we have n observations, we should have $P \ll n$.
- ▶ **Intuition: To avoid Overfit**
- ▶ P parameters can be used to **perfectly fit** P observations (one parameter per observation).

The Billion Dollar Question: Which Model (Parametrization) To Choose? ii



The Billion Dollar Question: Which Model (Parametrization) To Choose? iii

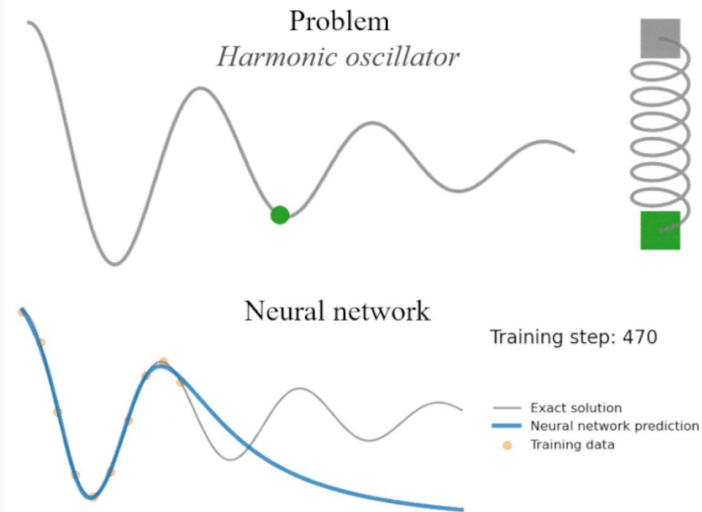
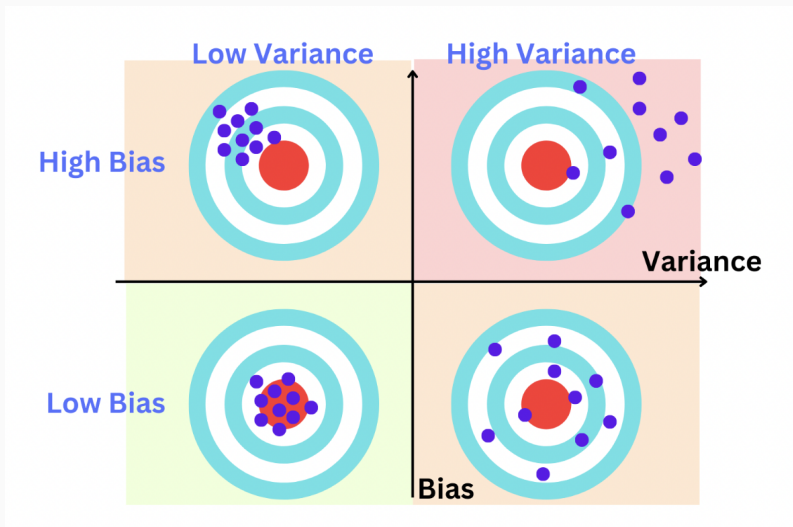


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So, How do We Choose a Model: Bias-Variance Tradeoff i

So, How do We Choose a Model: Bias-Variance Tradeoff ii



- ▶ $P =$ **model complexity**
- ▶ Large $P \rightarrow$ **low bias** because a complex model can approximate **any ground truth**.
Always true!
- ▶ Large $P \rightarrow$ **high variance**: **Used to be true in 20th century**. Intuition:

$$\text{Variance} = \text{Var}[\theta_{\text{feature1}}] + \cdots + \text{Var}[\theta_{\text{feature}P}] \quad (15)$$

Bias-Variance Tradeoff, Complexity, Train Error, and Test Error

- As we increase complexity,

$$\text{Train Error} \rightarrow 0$$

$$\text{Test Error} \not\rightarrow 0$$

(16)

- So why even care about train error?

Statistical Wisdom and Overfitting

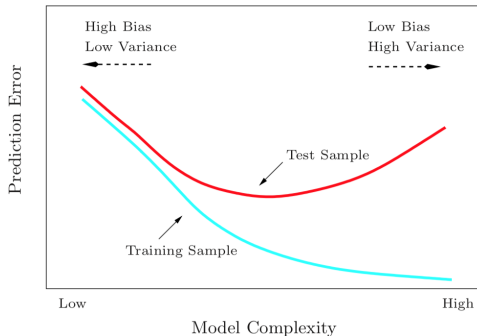
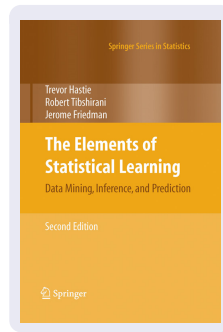


FIGURE 2.11. *Test and training error as a function of model complexity.*

Figure 2.11 shows the typical behavior of the test and training error, as model complexity is varied. The training error tends to decrease whenever we increase the model complexity, that is, whenever we fit the data harder. However with too much fitting, the model adapts itself too closely to the training data, and will not generalize well (i.e., have large test error). In



Statistical Wisdom and Overfitting

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2. How to Construct Nonparametric Regression Estimates?

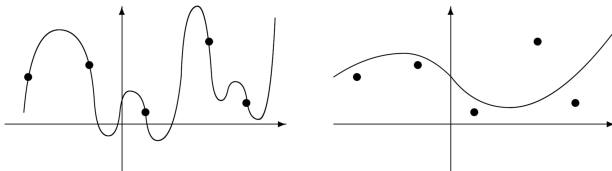
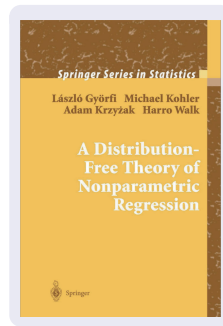
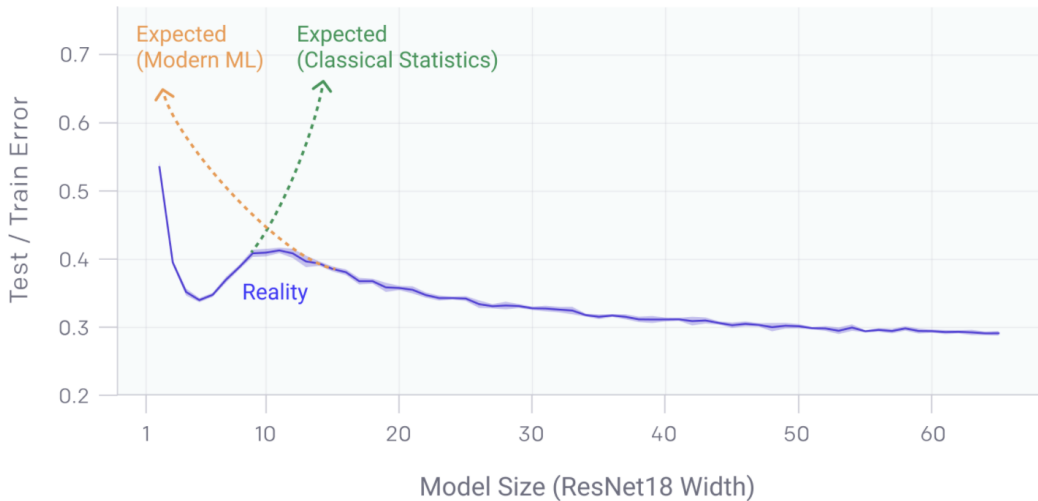
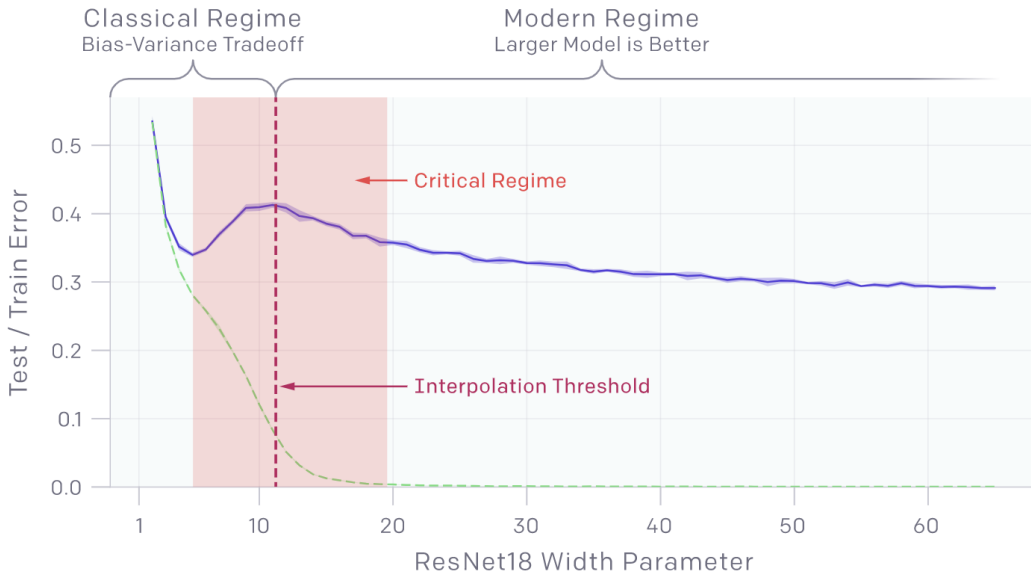


Figure 2.3. The estimate on the right seems to be more reasonable than the estimate on the left, which interpolates the data.

over $\mathcal{F}_n$. Least squares estimates are defined by minimizing the empirical L_2 risk over a general set of functions $\mathcal{F}_n$ (instead of (2.7)). Observe that it doesn't make sense to minimize (2.9) over all (measurable) functions f , because this may lead to a function which interpolates the data and hence is







DEEP DOUBLE DESCENT: WHERE BIGGER MODELS AND MORE DATA HURT

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ABSTRACT

We show that a variety of modern deep learning tasks exhibit a “double-descent” phenomenon where, as we increase model size, performance first gets *worse* and then gets better. Moreover, we show that double descent occurs not just as a function of model size, but also as a function of the number of training epochs. We unify the above phenomena by defining a new complexity measure we call the *effective model complexity* and conjecture a generalized double descent with respect to this measure. Furthermore, our notion of model complexity allows us to



Scaling Laws for Neural Language Models

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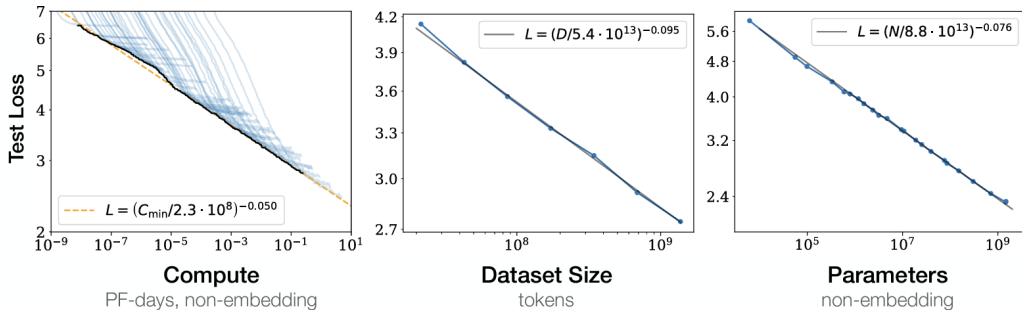
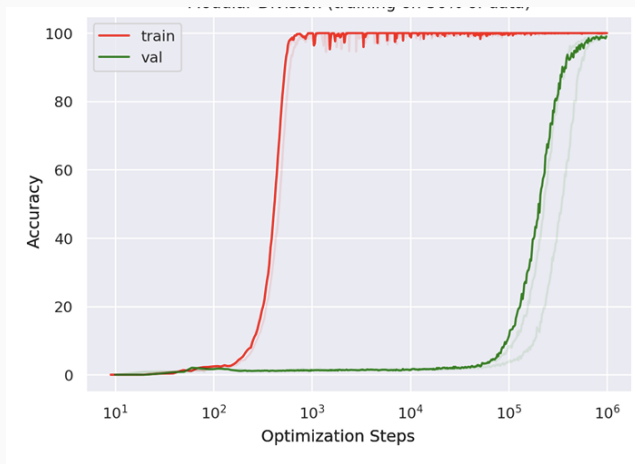


Figure 1 Language modeling performance improves smoothly as we increase the model size, dataset size, and amount of compute² used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

Grokking: Keep (and never stop) Training!



Grokking

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Virtue of Complexity for the SR

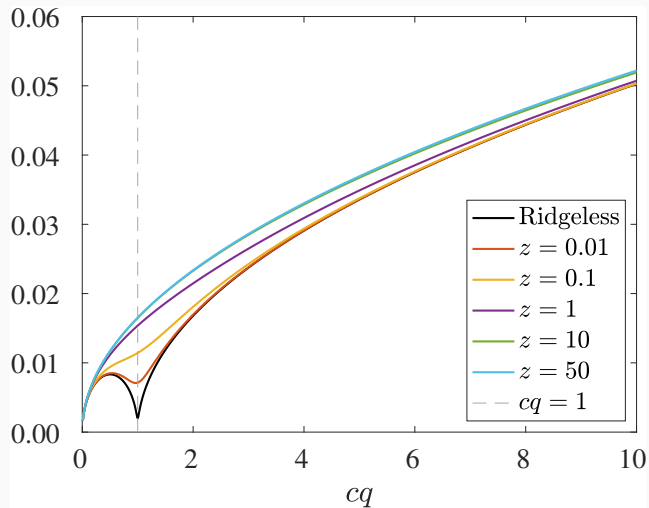


Figure: Expected Out-of-sample Timing Strategy Sharpe Ratio

Conditional Expectations

$$Objective = \frac{1}{T} \sum_t (R_{t+1} - f(X_t; \theta))^2 \quad (17)$$

Why is this the right objective?

Incorporating Conditional Information: The conditional expectation i

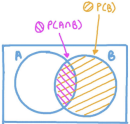
- We would like to incorporate conditional information. But how?

Nagwa

< > ⋮ ×

My love for you is UNCONDITIONAL ... probably!

CONDITIONAL PROBABILITY



$P(A|B) = \frac{P(A \cap B)}{P(B)}$

$P(A|B) = \frac{P(A \cap B)}{P(B)}$

If $P(A|B) = P(A)$, and $P(B|A) = P(B)$, then events A and B are INDEPENDENT

Incorporating Conditional Information: The conditional expectation ii

- Conditional expectation

$$E_t[X] = \sum x \underbrace{P(X = x | \text{Information at time } t)}_{\text{conditional probability}}$$

- Practitioners often use **rolling window estimates**

$$\text{Practitioner } E_t[R_{t+1}] = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau}, \quad T = \text{Rolling Window}$$

- But this is a very naive approach. What if some other signals are informative about stock returns?
- Here, we will need the notion of conditional expectation. Formally,

$$\underbrace{E_t[X_{t+1}]}_{\text{conditional expectation}} = \text{best prediction of } \mathbf{X}_{t+1} \text{ given time } - t \text{ information} \quad (18)$$

Incorporating Conditional Information: The conditional expectation iii

- Formally, if $S_t \in \mathbb{R}^P$ for some huge $P!$ is all our relevant information set at time t ,

$$\underbrace{E_t[X_{t+1}]}_{\text{conditional expectation}} = F_*(S_t) = \text{best non-linear function of } S_t \text{ that predicts } X_{t+1} \quad (19)$$

- Even more formally,

$$F_* = \arg \min_F E[\|X_{t+1} - F(S_t)\|^2] \quad (20)$$

- The reality is that we still cannot compute $E[\cdot]$ because we do not have enough data (see the picture curse of dimensionality)
- So, we will still be doing

$$\hat{F}_* = \arg \min_F \frac{1}{T} \sum_t |X_{t+1} - F(S_t)|^2 \quad (21)$$

Understanding Conditional Expectation (Good to Understand it Even we Cannot Estimate It) i

Theorem

If $F(S_t)$ is the true conditional expectation, then

$$X_{t+1} = F(S_t) + \varepsilon_{t+1} = \underbrace{E_t[X_{t+1}]}_{\text{predictable part}} + \underbrace{\varepsilon_{t+1}}_{\text{unpredictable noise}} \quad (22)$$

and we have the variance decomposition

$$\underbrace{\text{Var}[X_{t+1}]}_{\text{total variation}} = \underbrace{\text{Var}[E_t[X_{t+1}]]}_{\text{predictable variation}} + \underbrace{\text{Var}[\varepsilon_{t+1}]}_{\text{unpredictable variation}} \quad (23)$$

Proof:

$$E[\varepsilon_{t+1}] = 0, E[\varepsilon_{t+1}E_t[X_{t+1}]] = 0, \text{Cov}[E_t[X_{t+1}], \varepsilon_{t+1}] = 0 \quad (24)$$

Understanding Conditional Expectation (Good to Understand it Even we Cannot Estimate It) ii

and hence

$$\text{Var}[X_{t+1}] = \text{Var}[E_t[X_{t+1}] + \varepsilon_{t+1}] = \text{Var}[E_t[X_{t+1}]] + \text{Var}[\varepsilon_{t+1}] + \underbrace{2\text{Cov}[E_t[X_{t+1}], \varepsilon_{t+1}]}_{=0} \quad (25)$$

Why is this important?

- We would like to find the true amount of predictability:

$$R^2 = \frac{\text{Var}[E_t[X_{t+1}]]}{\text{Var}[X_{t+1}]} = 1 - \frac{E[\varepsilon_{t+1}^2]}{\text{Var}[X_{t+1}]} \quad (26)$$

and the true residuals

$$\varepsilon_{t+1} = X_{t+1} - F(S_t). \quad (27)$$

Examples: True Expectations

- ARMA process:

$$R_{t+1} = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau} + \varepsilon_{t+1}, \quad E_t[R_{t+1}] = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau} \quad (28)$$

Here,

$$S_t = (R_{\tau})_{\tau=t-T}^t, \quad F(S_t) = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau} \quad (29)$$

- Linear prediction:

$$R_{t+1} = \sum_{j=1}^P \beta_j S_{j,t} + \varepsilon_{t+1}, \quad E_t[R_{t+1}] = \sum_{j=1}^P \beta_j S_{j,t} \quad (30)$$

Here,

$$F(S_t) = \sum_{j=1}^P \beta_j S_{j,t} \quad (31)$$

is linear

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Learning Is Impossible Without Some Kind of Bias

The ugly duckling theorem. Classification is not really possible without some sort of bias.

*"Suppose that one is to list the attributes that plums and lawnmowers have in common in order to judge their similarity. It is easy to see that the list could be infinite: Both weigh less than 10,000 kg (and less than 10,001 kg), both did not exist 10,000,000 years ago (and 10,000,001 years ago), both cannot hear well, both can be dropped, both take-up space and so on. Likewise, the list of differences could be infinite. . . any two entities can be arbitrarily similar or dissimilar by **changing the criterion of what counts as a relevant attribute.**"*

Inductive Biases

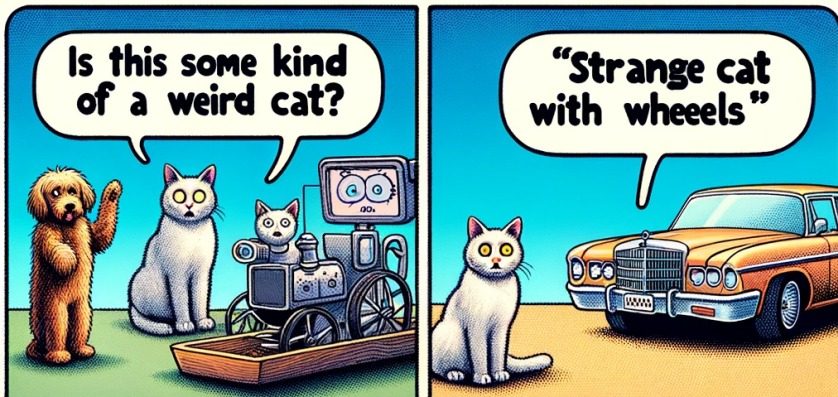
So how do we decide which attributes (features; characteristics) matter?

We use **Inductive Biases!**

Definition. *Inductive bias is the set of assumptions a learning algorithm makes to generalize beyond the training data. In other words, it's what allows the algorithm to "induce" a hypothesis from a limited amount of data, guiding it on how to predict unseen examples. For instance, a linear regression model assumes that the underlying relationship is approximately linear—even if the true relationship is more complex—so it is biased towards linear solutions. This bias is essential: without it, an algorithm would have no basis for generalization and might simply memorize the training data without making any useful predictions on new data.*

The Cat-astrophe Bias

Imagine a photo recognition AI trained exclusively on images of cats. Its inductive bias is that all important entities in the world are cats. Show it a picture of a dog, and it's perplexed. "Is this some kind of weird cat?" it wonders. A car? "Strange cat with wheels!" A tree? "Clearly, a tall, wooden cat!"



An Analyst with Extrapolative Expectations

- I believe past returns predict future returns and I will use

$$E_t[R_{t+1}] = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau}$$

- Fantastic bias if

$$R_{t+1} = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau} + \varepsilon_{t+1}, \quad E_t[R_{t+1}] = \frac{1}{T} \sum_{\tau=t-T}^t R_{\tau} \quad (34)$$

- OK bias if

$$R_{t+1} = R_t + \varepsilon_{t+1}, \quad E_t[R_{t+1}] = R_t \quad (35)$$

will be positively related to the analyst's guess

- Horrible bias if returns are mean-reverting:

$$R_{t+1} = -R_t + \varepsilon_{t+1}, \quad E_t[R_{t+1}] = -R_t \quad (36)$$

An Economist Who Believes in Linearity

- I believe that

$$E_t[R_{t+1}] = \sum_{j=1}^P \beta_j S_{j,t}$$

- Fantastic bias if

$$R_{t+1} = \sum_{j=1}^P \beta_j S_{j,t} + \varepsilon_{t+1} \quad (37)$$

- OK bias if

$$R_{t+1} = \underbrace{S_{1,t} + 5S_{17,t}}_{\text{sparse: only 1 and 17 matter}} + \varepsilon_{t+1}, \quad E_t[R_{t+1}] = R_t \quad (38)$$

- Horrible bias if non-linear:

$$R_{t+1} = S_{15,t}^2 + \varepsilon_{t+1} \quad (39)$$

More Complex Biases

- We believe

$$E_t[X_{t+1}] = \theta' S_t$$

but $\|\theta\|$ is small (small $\|\theta\|$ inductive bias). Implementation: ridge penalty

$$\min_{\theta} \|R - \theta' S\|^2 + \underbrace{\lambda}_{\text{ridge penalty}} \|\theta\|^2, \|\theta\|^2 = \sum_i |\theta_i|^2$$

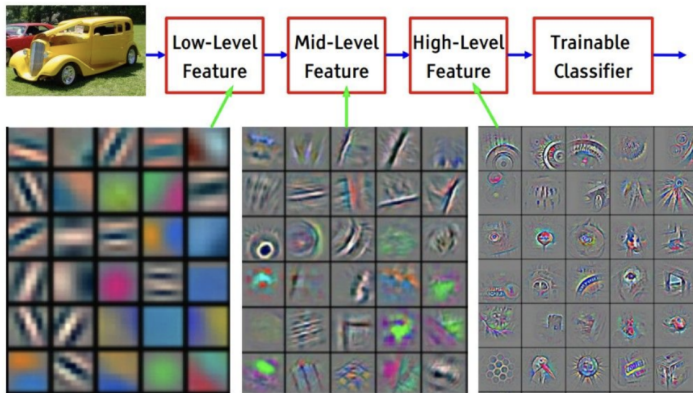
- We believe θ is sparse: only a few coordinates are non-zero. The sparsity bias.
Implementation: **LASSO**

$$\min_{\theta} \|R - \theta' S\|^2 + \underbrace{\lambda}_{\text{ridge penalty}} \|\theta\|_1, \|\theta\|_1 = \sum_i |\theta_i|$$

Deep Learning Trained by Gradient Descent: The Most Powerful Inductive Bias Human Beings Have Discovered So Far i

- ▶ **Inductive Bias of DNNs:** The world has a smooth, hierarchical structure

Deep Learning Trained by Gradient Descent: The Most Powerful Inductive Bias Human Beings Have Discovered So Far ii



Learning Hierarchical Concepts

LLM concepts by combining nonlinear predictors over multiple layers

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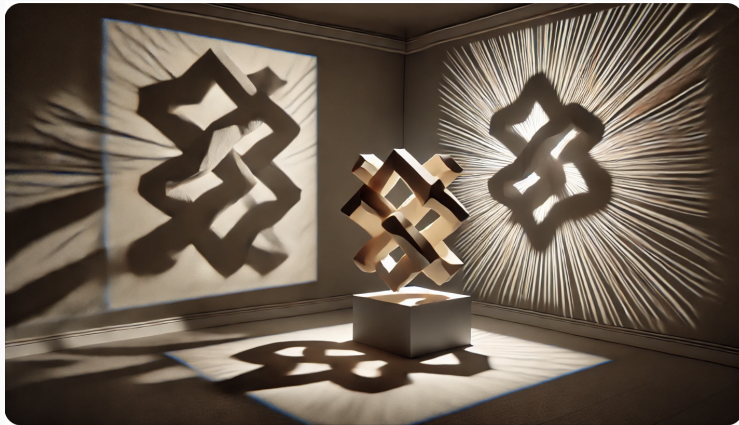
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The Birth of a New Inductive Bias?

- ▶ Learning is about **inductive biases**: sets of assumptions a learning algorithm uses to make predictions or generalize beyond the given training data.
- ▶ The above findings suggest that we should reconsider the **Inductive Bias** known as the principle of parsimony
- ▶ The new Inductive Bias is:
Complex (with more parameters than observations) Statistical Models Seem to Explain Stock Market Data Better
- ▶ Thus, we need to understand:
 - What do complex statistical models learn?
 - Why do they work so well?
 - What happens in equilibrium if agents use complex models?

What do complex statistical models learn? Plato's Cave

- ▶ When learn $P > T$ parameters, you project data on T dimensions (but, in fact, much less than T)



Why do they work so well? Alignment

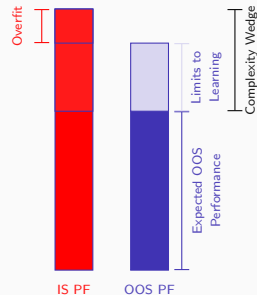
- ▶ The manifold hidden inside the big NNs is mysteriously aligned with the true nature of the data

Alignment and the Complexity Wedge

1. “Complexity wedge” = IS Performance – Expected OOS Performance

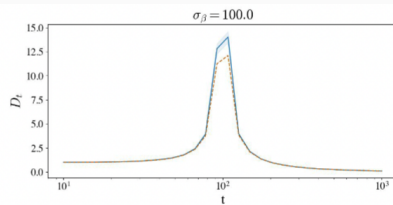
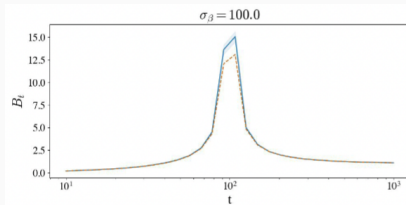
$$\text{“Complexity wedge”} = \underbrace{\text{IS} - \text{True}}_{\text{“Overfit”}} + \underbrace{\text{True} - \text{OOS}}_{\text{“Limits to Learning”}}$$

- Quantifiable based on training data
- Can infer performance of true PF and how far you are from it, but cannot recover it.

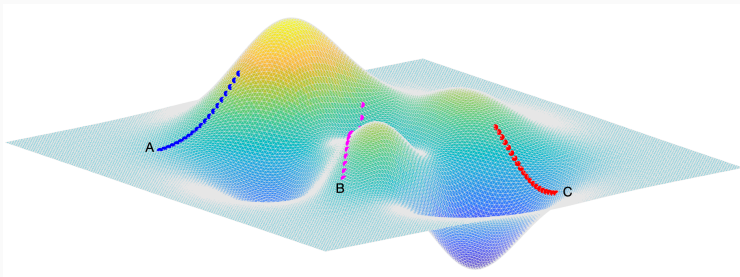


2. Show how to infer optimal shrinkage, z^* , from training data
3. There is no low-rank rotation of complex factors that preserves model performance (cf. Kozak, Nagel, and Santosh, 2020)

What happens in equilibrium if agents use complex models? The Beliefs Divergence Principle



(Almost) Every Inductive Bias has a Place to Be: The Multiplicity of Models



Understanding The Virtue of Complexity

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OLS i

- ▶ Predictors' vector $S_t \in \mathbb{R}^P$
- ▶ We organize them like an excel spreadsheet, $S = (S_t)_{t=1}^T \in \mathbb{R}^{T \times P}$.
- ▶ OLS (linear regression, Carl Friedrich Gauss):

$$\hat{\beta}_{OLS} = \arg \min_{\beta} \left\| \underbrace{R}_{T \times 1} - \underbrace{S}_{T \times P} \underbrace{\beta}_{P \times 1} \right\|^2 = \arg \min_{\beta} \sum_t \left(R_{t+1} - \sum_j S_{j,t} \beta_j \right)^2$$

and

$$\hat{\beta}_{OLS} = \underbrace{\hat{\Psi}_T^{-1}}_{P \times P} T^{-1} \sum_t \underbrace{S_t}_{P \times 1} \underbrace{R_{t+1}}_{1 \times 1} \in \mathbb{R}^P$$

►

$$\hat{\Psi}_T = T^{-1} \sum_t S_t S_t' = \underbrace{T^{-1} S' S}_{(P \times T) \times (T \times P)} \in \mathbb{R}^{P \times P} \quad (40)$$

is the **sample covariance matrix**

► Defining $R = (R_t)_{t=1}^T \in \mathbb{R}^T$, we can rewrite

$$\hat{\beta}_{OLS} = (T^{-1} S' S)^{-1} T^{-1} S' R. \quad (41)$$

How to Run Regression when $P > T$? Ridge Regression i

$$\hat{\beta} = \arg \min_{\beta} (T^{-1} \|R - S\beta\|^2 + z\|\beta\|^2)$$

gives

$$\hat{\beta}(z) = \left(zI + T^{-1} \sum_t S_t S_t' \right)^{-1} T^{-1} \sum_t S_t R_{t+1} = (zI + T^{-1} S' S)^{-1} T^{-1} S' R.$$

Ridgeless Limit and the Moore-Penrose Quasi-Inverse

When P moves beyond T , there are more parameters than observations, and the least squares problem has multiple solutions. A particularly interesting solution invokes the Moore-Penrose pseudo-inverse, which can be computed as follows:

$$A = U \text{diag}(D)U' \Rightarrow A^+ = U \text{diag}((D^{-1} \text{ if } D > 0 \text{ else } 0))U' \quad (42)$$

As we show below, as the shrinkage parameter approaches zero, we converge to the **Ridgeless Estimator**:

$$\hat{\beta}(0^+) = \lim_{z \rightarrow 0^+} \hat{\beta}(z) = \left(T^{-1} \sum_t S_t S_t' \right)^+ \frac{1}{T} \sum_t S_t R_{t+1}.$$

Proving this is non-trivial and requires a bit of algebra.

The Magic of Ridge: Playing with Dimension i

Lemma (Swapping Dimension)

Let $S \in \mathbb{R}^{T \times P}$. Then,

$$\underbrace{(zI + \underbrace{S'S}_{P \times P})^{-1} S'}_{\text{impossible to compute for } P \gg T} = S' (zI + \underbrace{SS'}_{T \times T})^{-1} \quad (43)$$

Proof.

We have

$$\begin{aligned} (zI + S'S)^{-1} S' &= S' (zI + SS')^{-1} \Leftrightarrow \\ S' (zI + SS') &= (zI + S'S) S' \Leftrightarrow \\ S' z + S' SS' &= z S' + S' SS' \end{aligned} \quad (44)$$

■

The Magic of Ridge: Playing with Dimension ii

We use this in the Jupyter Notebook to get fast regression in very high dimensions

Corollary

$$\hat{\beta}(z) = \left(zI + T^{-1} \underbrace{S'S}_{P \times P} \right)^{-1} \frac{1}{T} S'R = S' \left(zI + T^{-1} \underbrace{SS'}_{T \times T} \right)^{-1} \frac{1}{T} R \quad (45)$$

and

$$\hat{\beta}(0+) = \underbrace{S'}_{P \times T} \left(\underbrace{SS'}_{T \times T} \right)^{-1} \underbrace{R}_{T \times 1} \quad (46)$$

Let us now prove that

$$\hat{\beta}(0+) = (S'S)^+ S'R. \quad (47)$$

Indeed,

$$\hat{\beta}(0+) = S'(SS')^{-1}R = (S'S)^+ S'R \quad (48)$$

The Magic of Ridge: Playing with Dimension iii

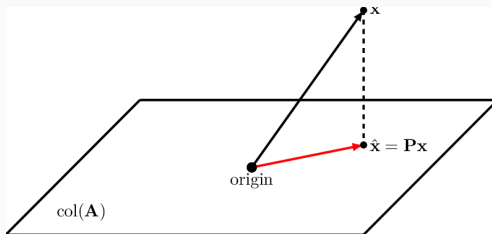
because $\text{Im}(S') \perp \ker(S) = \ker(S'S)$.

$\hat{\beta}(0+)$ is an interpolator:

$$S\hat{\beta}(0+) = SS'(SS')^{-1}R = R \quad (49)$$

Orthogonal Projection in Linear Algebra i

Given a vector x and a subspace S of $\mathbb{R}^n$, given by the span of columns of a matrix A (denoted by $\text{col}(A)$), the **orthogonal projection** P of x onto S , is the closest vector $\hat{x}$ in S to x .



Orthogonal Projection in Linear Algebra ii

Lemma

Let $\Pi = (AA')^+ AA'$. Then, Π is the orthogonal projection onto the $\text{col}(A)$.

Proof.

First, Π is symmetric and positive definite. Second, $AA' = U \text{diag}(D)U'$, and hence

$$(AA')^+ AA' = U(D(D^{-1}\mathbf{1}_{D>0}))U' = U \text{diag}(\mathbf{1}_{D>0})U' \quad (50)$$

and hence Π is the projection onto the image of AA' , while it kills the kernel of AA' . But $AA'x = 0$ means $x'AA'x = 0$ means $A'x = 0$ and we know

$$\ker A' = (\text{Im} A)^\perp. \quad (51)$$

■

What does the Ridgeless Regression Do? i

Any solution $\hat{\beta} \in \mathbb{R}^P$ to the system

$$\hat{\beta}' S_t = R_{t+1}, \quad t = 1, \dots, T \quad (52)$$

of T equations and P variables is called an **interpolator**.

Lemma

Suppose that $R \in \text{span}(S)$, so that (52) has a solution. Then, any solution β to (52) can be written down as

$$\beta = \underbrace{\hat{\beta}(0^+)}_{\in \text{span}(S)} + \underbrace{\beta^\perp}_{\text{orthogonal to } \text{span}(S)} \quad (53)$$

In particular, $\hat{\beta}(0^+)$ gives the **minimal norm interpolator**:

$$\hat{\beta}(0^+) = \arg \min \{ \|\beta\|^2 : \beta \text{ satisfies (52)} \} \quad (54)$$

What does the Ridgeless Regression Do? ii

Proof.

We have

$$\hat{\beta}(0^+) = (SS')^+ S'R \quad (55)$$

Let

$$S'\beta = R \quad (56)$$

be some other interpolator. Then,

$$SS'\beta = S'R \Rightarrow (SS')^+ SS'\beta = (SS')^+ S'R = \hat{\beta}(0^+). \quad (57)$$

Let $\Pi = (SS')^+ SS'$. Then, Π is the orthogonal projection onto the $\text{span}(S)$. Thus,

$$\Pi\beta = \hat{\beta}(0^+) \quad (58)$$

and the claim follows. ■

What does the Ridgeless Regression Do? iii

Summarizing, we can formulate the complexity principle.

Theorem (heuristic)

$\|\hat{\beta}(0+)\|$ is monotone decreasing in P . Thus, if the small norm of β is a good **inductive bias**, ridgeless regression generalizes better when P gets larger.

Generalizes better = has lower test (out-of-sample) error

Experiments with High Dimensional Regressions

Please click on the link:

Understanding High-Dimensional Regressions

Random Features for Goyal-Welch