Machine Learning for econometrics

Statistical learning and regularized linear models

Matthieu Doutreligne

January 10, 2025

A lot of today's content is taken from the excellent sklearn mooc (Estève et al., 2022)

About me 👋

Matthieu Doutreligne

- 2018: Master degree in statistical learning and artificial intelligence (Ensae/MVA)
- 2018-2020: Data scientist at the French Ministry of Health (Drees)
- 2020-2023: PhD in statistics and informatics (SODA / scikit-learn inria team):

Causal inference with machine learning applied to clinical data

- Same time: Statistician since 4 years at Haute Autorité de santé (HAS)
- First course at ENSAE

More from the machine learning than economics culture

Objectives

Important concepts and methods of machine learning…

Useful for empirical work in economics.

Introduction of the course

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Important concepts and methods of machine learning…

Useful for empirical work in economics.

Philosophy

- More Intutions than equations
- Basics and references for formal understanding
- Focus on practical skills: Coding 🤦‍♂️

Course syllabus

8 sessions, two teachers: Matthieu Doutreligne (MD), Bruno Crépon (BC)

Sessions

- Statistical learning and regularized linear models (MD)
- Double-lasso for statistical inference (BC)
- Flexible models for tabular data (MD)
- Reminders of potential outcomes and Directed Acyclic Graphs (MD)
- Event studies: Causal methods for pannel data (MD)
- Double machine learning: Neyman-orthogonality (BC)
- Heterogeneous treatment effect (BC)
- Oral presentations of the evaluation projects (MD + BC)

Evaluation of the course

Coding project

- Causal inference on a small dataset of your choice: several datasets provided.
- Objective: ask a sound causal question, discuss hypotheses and estimate a causal effect with a machine learning method, discuss the design and the results.

Details

- Handing over a notebook with code and comments on a github: (Python, R or stata)
- Presenting your work in a 20-30 minutes oral during the last session.
- Details and datasets: https://straymat.github.io/causal-ml-course/evaluation.html
- Inscription: email sent to every students.

Course ressources for my four sessions

Website

Detailed syllabus: https://straymat.github.io/causal-ml-course/syllabus.html

Slides: https://straymat.github.io/causal-ml-course/slides.html

Practical sessions: https://straymat.github.io/causal-ml-course/practical_sessions.html

Today's program

Predictive inference in high dimensions

- Statistical learning basics
- Regularized linear models for predictive inference
- Putting it into practice with scikit-learn

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Next two sessions

- Double-Lasso: using penalized linear models for causal inference (Bruno Crépon)
- Flexible models: Trees, Random Forests, Gradient Boosting and more scikit-learn (Me)

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Statistical learning framework

Statistical learning, ie. predictive inference

Goal

- Predict the value of an outcome based on one or more input variables.

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Setting

- Data: n pairs of (features, outcome), $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ identically and independently distributed (i.i.d.) from an unknown distribution P.
- Goal: find a function $\hat{f} : \mathcal{X} \to \mathcal{Y}$ that approximates the true value of y ie. for a new pair (x, y), we should have:

$$\hat{y} = \hat{f}(x) \approx y$$

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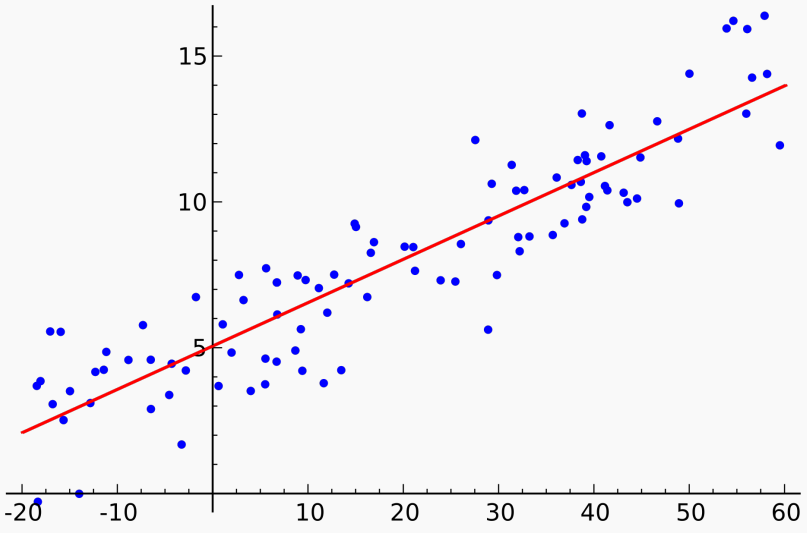
Vocabulary: Fitting the model

Finding the appropriate model $\hat{f}$ is called learning, training or fitting the model.

Statistical learning, two classes of problems

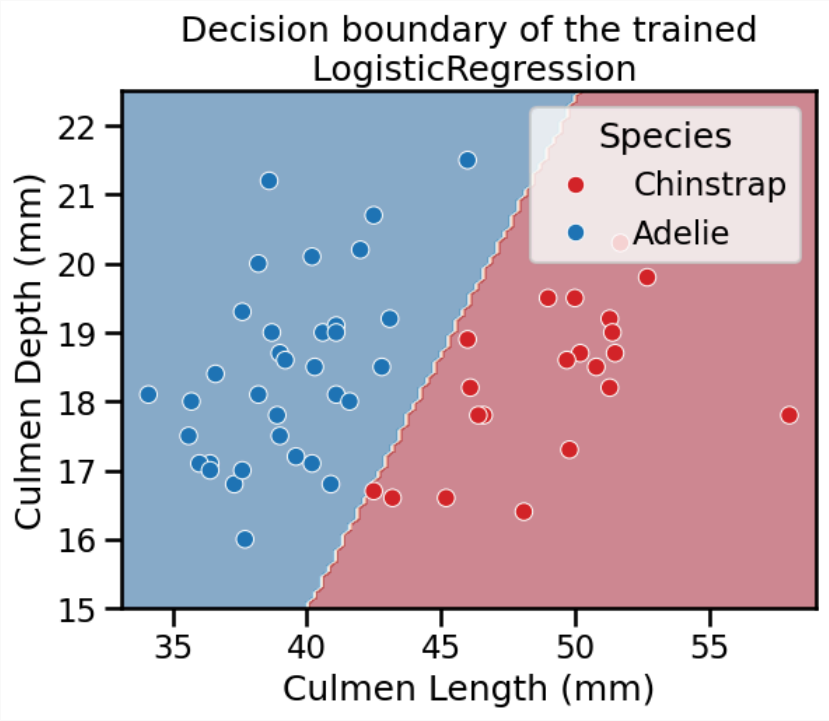


Regression

- The outcome is continuous: eg. wage prediction
- The error is often measured by the mean squared error (MSE):

$$\mathrm{MSE} = \mathbb{E}\left[\left(Y - \hat{f}(X)\right)^2\right]$$

Statistical learning, two classes of problems



Classification

- Outcome is categorical: eg. diagnosis, loan default, ...
- Error is often measured with accuracy:

$$\text{Misclassification rate} = \mathbb{E}\left[\mathbb{1}\left(Y \neq \hat{f}(X)\right)\right]$$

with $\hat{f} \in \{0, 1\}$ for binary classification

Motivation: why prediction?

Why do we need prediction for ?

Predictive inference

- Some problems in economics requires accurate prediction without a causal interpretation (Kleinberg et al., 2015), only knowledge of y (eg. stratifying on a risk score for loan, preventive care, ...)
- Reconstruct missing data: eg. imputation of missing values between two waves of a survey (eg. house prices, production of cultivation plots,...)

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Statistical/causal inference

- Infer the effect of an intervention with a causal interpretation
- Powerful predictive models are used to regress "away" the relationship between the treatment/outcome and the confounders

  -> More on this in sessions on Double machine learning and Directed Acyclic Graphs.

Do we need more than linear models?

Let:

- p is the number of features
- n is the number of observations

Maybe no

- Low-dimensional data: $n \gg p$
- No non-linearities, no or few interactions between features

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Maybe yes

- High-dimensional data: ie. $p \gg n$
- Non-linearities, many interactions between features

What high-dimension means: Is p >> n common in economics?

⚠️ **p can be greater than the number of columns in the dataset**

Characteristics leading to high-dimensionality

- Categorical variables with high cardinality, eg. job title, diagnoses...
- Text data: eg. job description, medical reports...
- Technical regressors to handle non-linearities, eg. polynomials, splines, log, ...

What high-dimension means, concrete example

- Population referencing individual files (INSEE): $n = 19,735,576$; $n_{\text{cols}} = 88$ 🤞
- But many variables with cardinality: more than 555 pairs of (variable, category).
- Adding interaction of degree 2: $\binom{p}{2} = \binom{555}{2} = \frac{555*554}{2} = 153735$ features 😓
- Adding interactions of any degree: $2^p - p - 1 = 2^{555} - 554$ 🤯

Is this common? Yes

- Categorical with high cardinality or text data are increasingly common.
- Image data is high-dimensional by nature.
- Automation of data collection and storage leads to more datasets and more variables.

Some problems where high dimensional data is common

Some examples

- The US Current Population Survey (CPS) dataset has hundreds of variables, many of which are categorical
- The Système National des Données de Santé (SNDS) in France = healthcare claims : many hundreds of variables, many of which are categorical.

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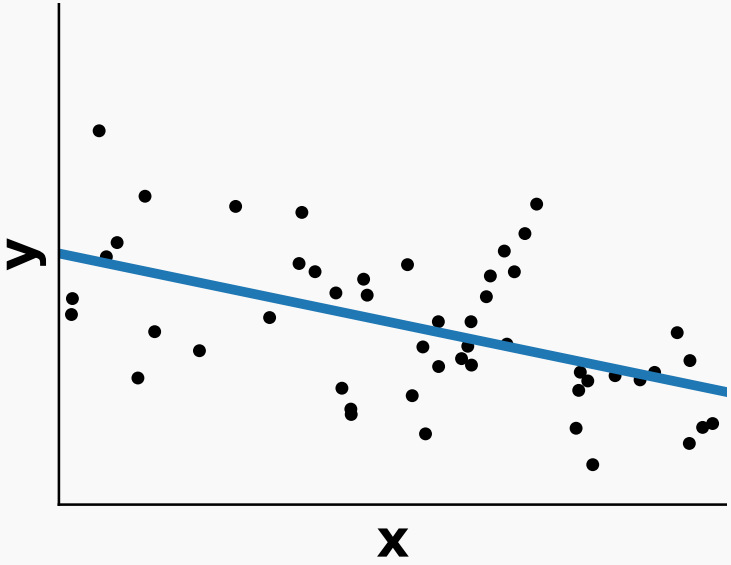
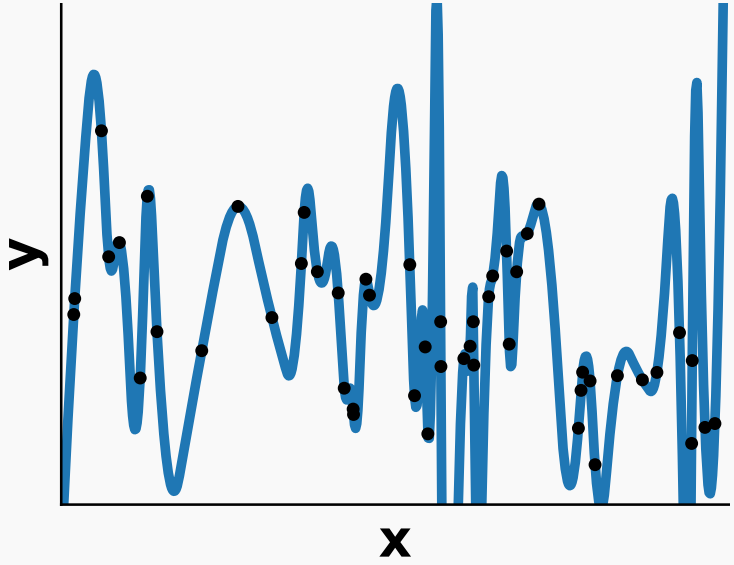
Other area

- Country characteristics in cross-country wealth analysis,
- Housing characteristics in house pricing/appraisal analysis,
- Product characteristics at the point of purchase in demand analysis.

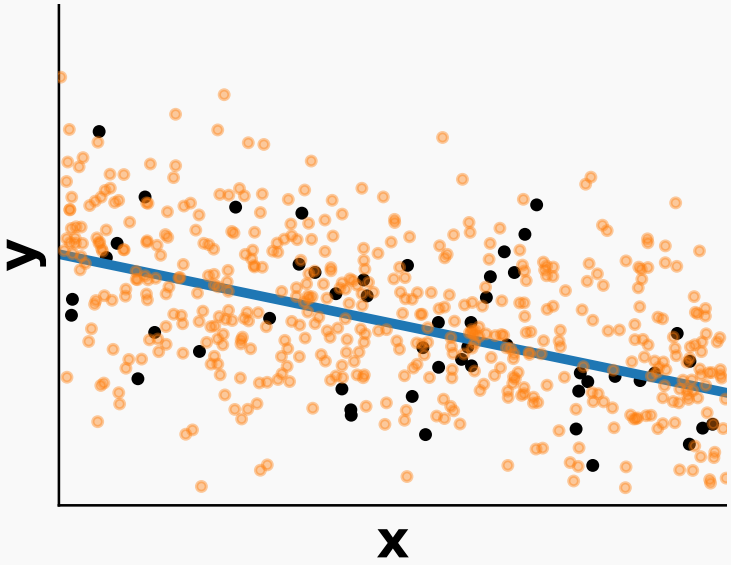
Statistical learning theory and intuitions

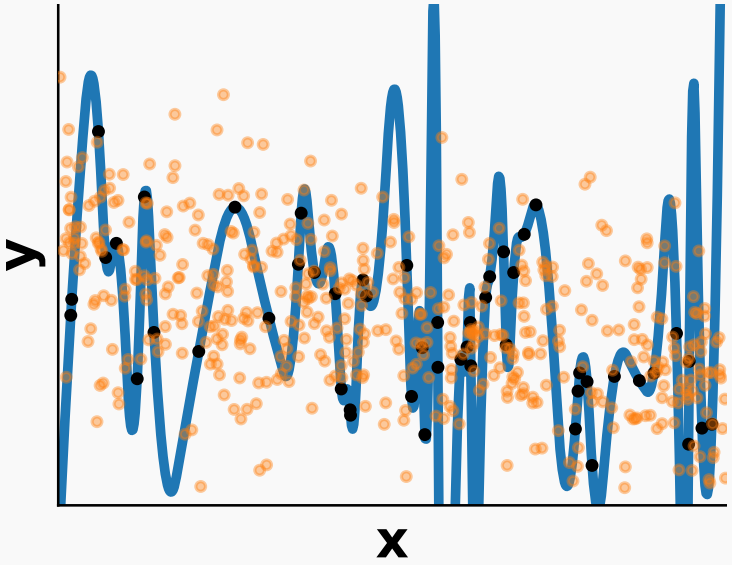
Which data fit do you prefer?





Which data fit do you prefer? (new data incoming)



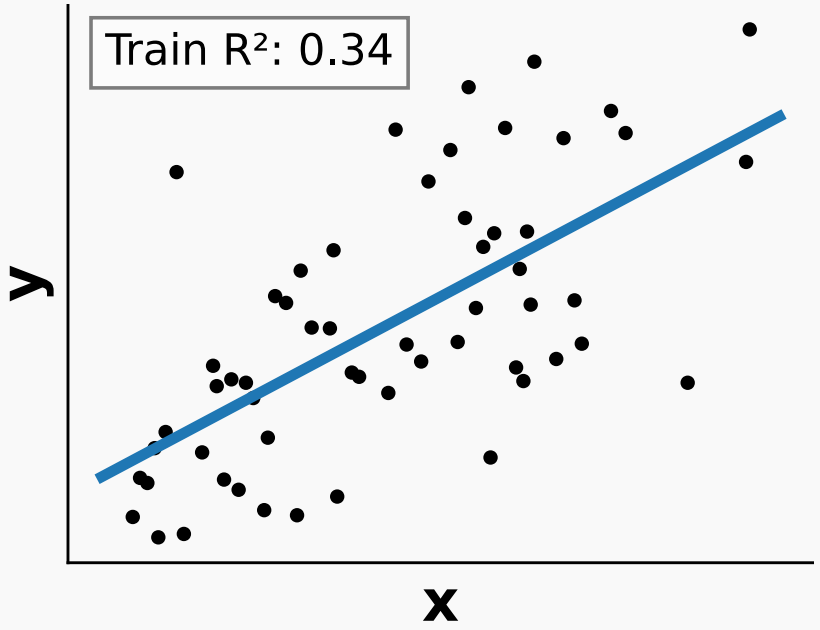


- Answering this question might be hard.
- Goal: create models that generalize.
- The good way of framing the question is: how will the model perform on new data?

Train vs test error: simple models

Measure the errors on the training data

=> fitting



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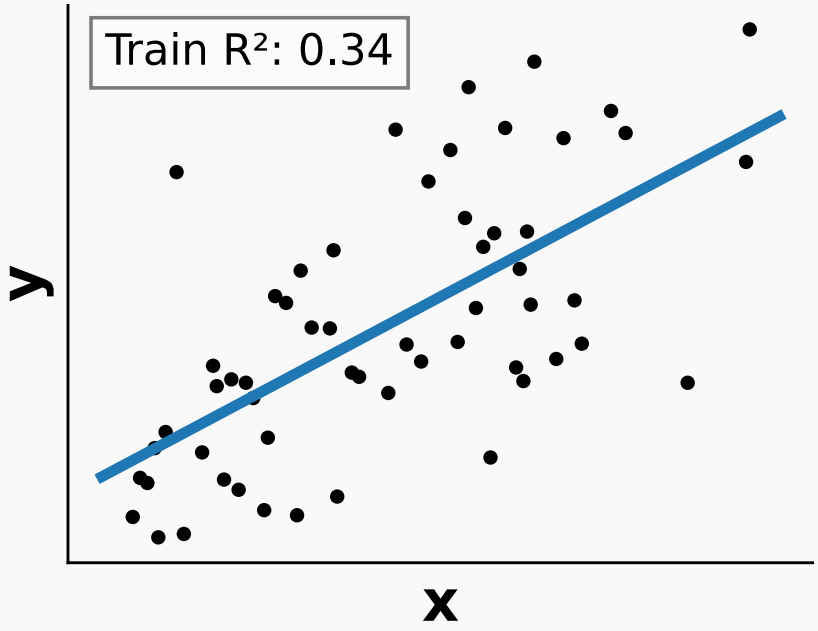

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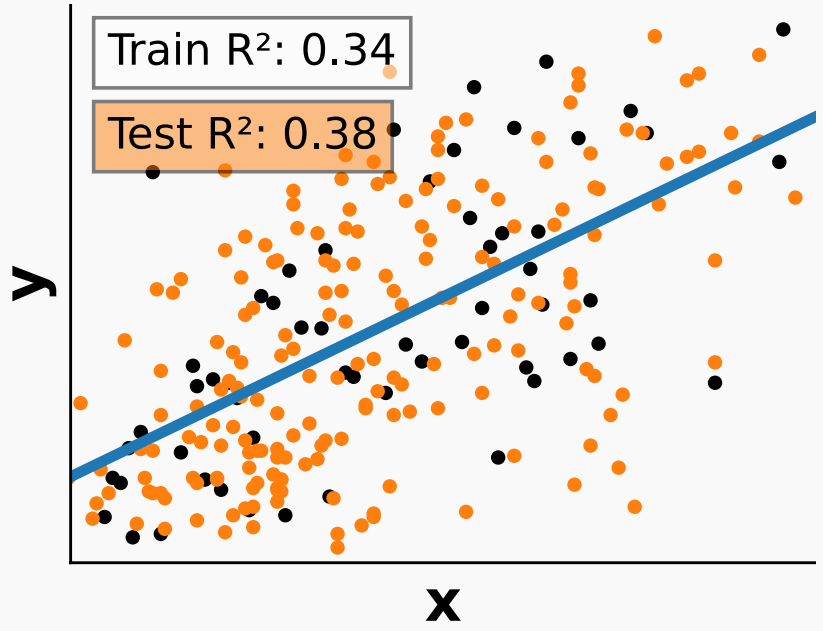

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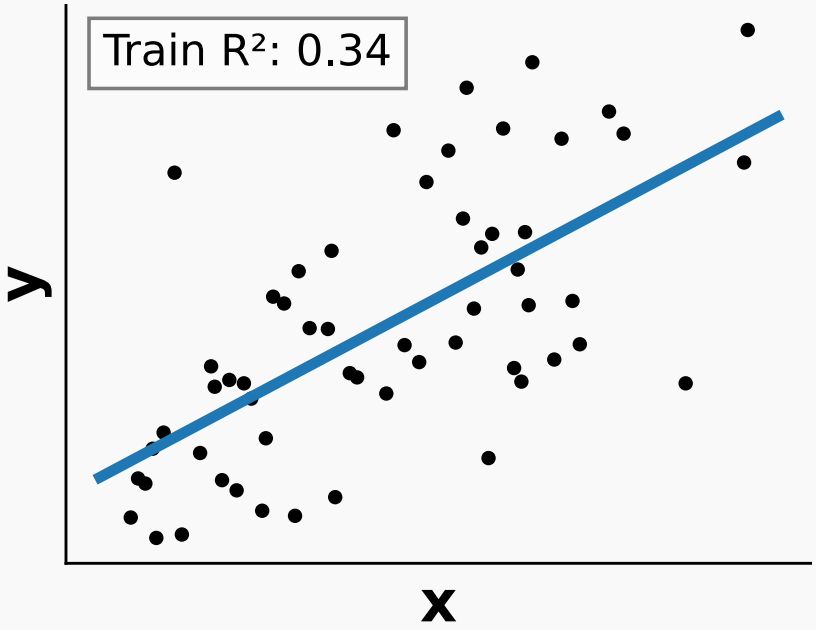

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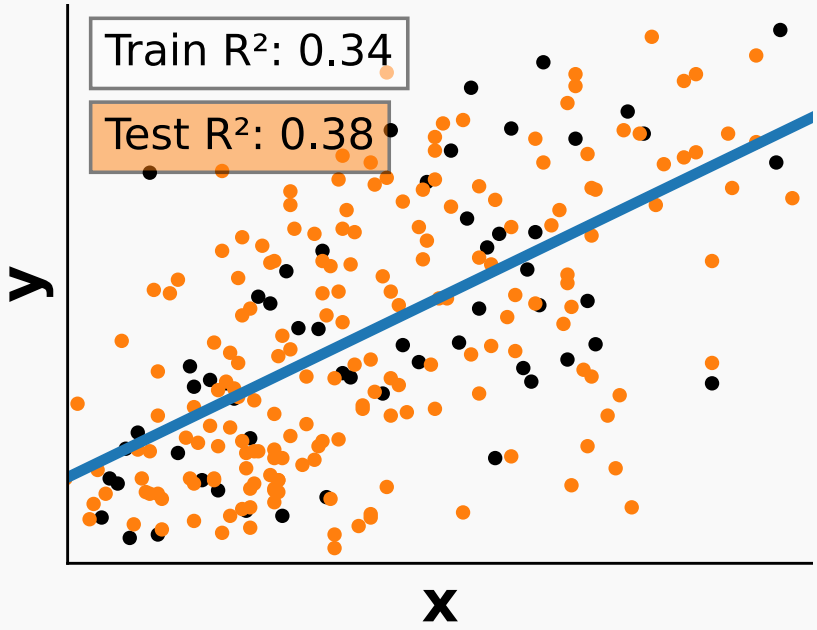
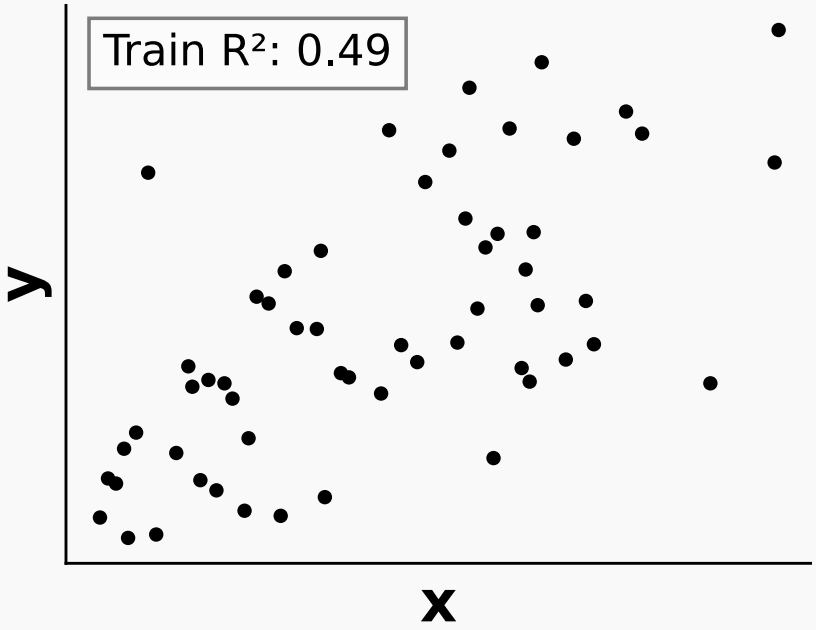


🎉 Here, no problem of overfitting: train vs test error are similar.

Train vs test error: flexible models

Measure the errors on the training data = fitting



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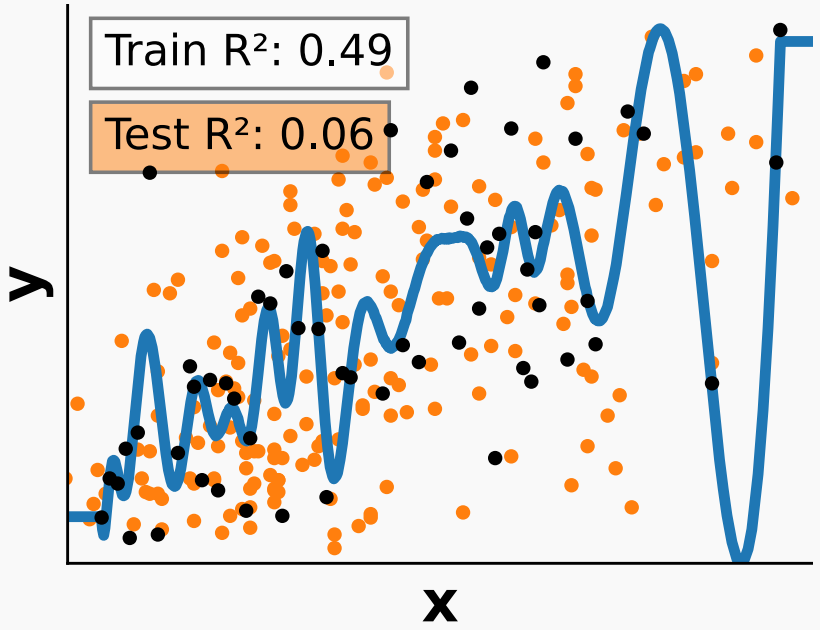
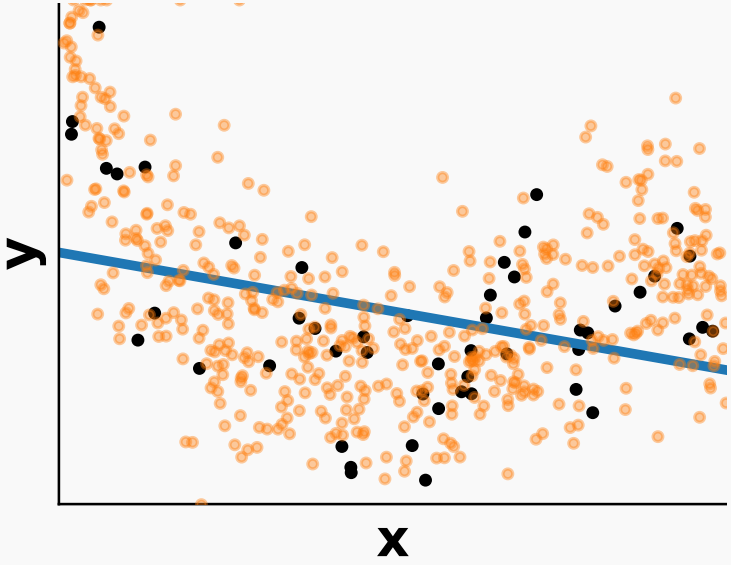
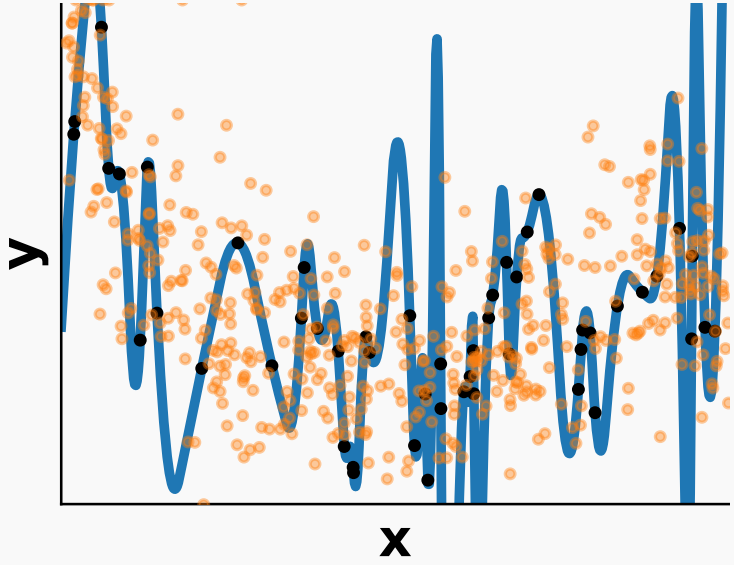


😫 Overfitting: the model is too complex and captures noise.

How to choose the complexity of the model?





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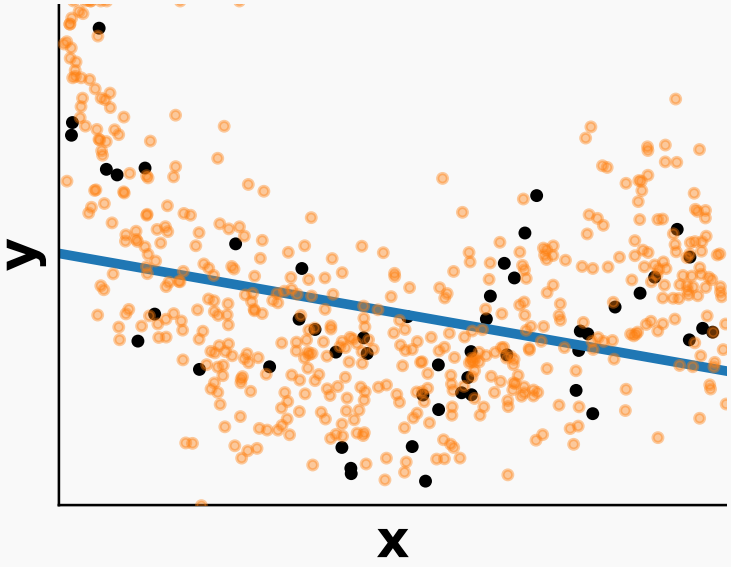

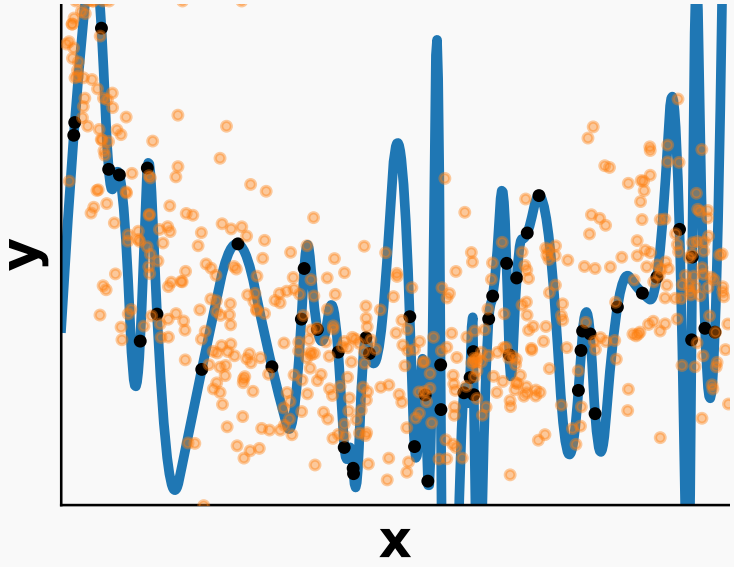

This trade-off is is called Bias variance trade-off.

- Let's recover it in the context of statistical learning theory.

Empirical Risk Minimization

Loss function

A loss function ℓ defines the proximity between the predicted value $\hat{y} = f(x)$ and the true value y: $\ell(f(x), y)$

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Risk minimization

We look into a (finite) family of candidate functions $f \in \mathcal{F}$,

For the best possible function $f^\star$, ie f minimizing the risk or expected loss $\mathcal{E}(f) = \mathbb{E}\big[(f(x) - y)^2\big]$:

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Empirical risk minimization: estimation error

- In finite sample regimes, the expectation $\mathbb{E}$ is not accessible since we only have access to a finite number of data pairs
- In practice, we minimize the empirical risk or average loss $R_{\text{emp}} = \sum_{i=1}^{n} (f(x_i) - y_i)^2$:

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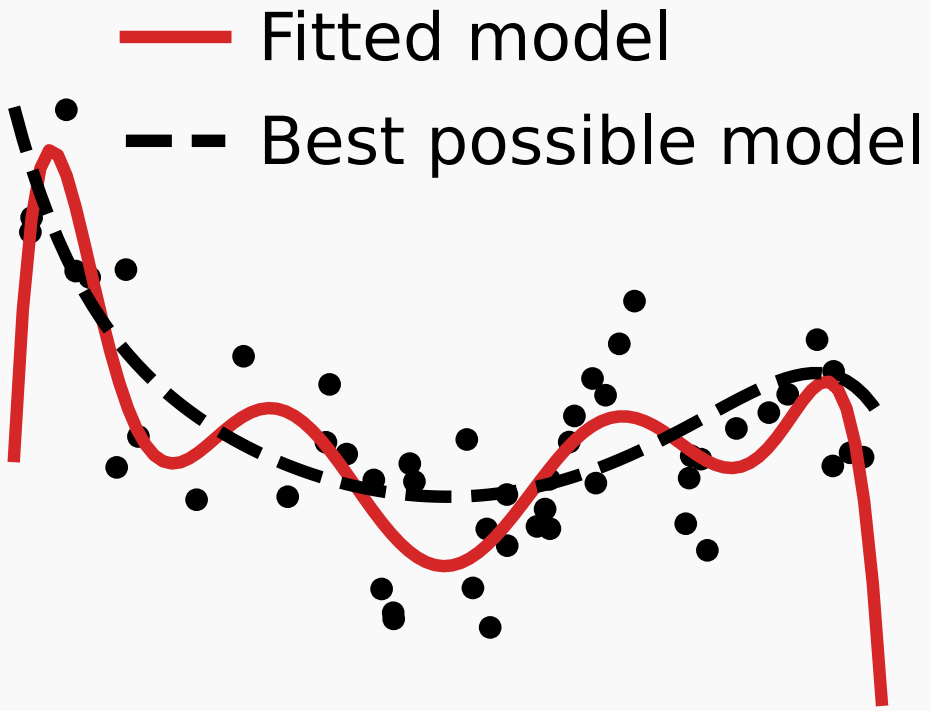
$$\hat{f} = \operatorname{argmin}_{f \in \mathcal{F}} \sum_{i=1}^{n} \left(f(x_i) - y_i\right)^2$$

- This creates the estimation error, related to sampling noise:

$$\mathcal{E}\left(\hat{f}\right) - \mathcal{E}(f^\star) = \mathbb{E}\left[\left(\hat{f}(x) - y\right)^2\right] - \mathbb{E}\left[\left(f^\star(x) - y\right)^2\right] \geq 0$$

High estimation error means overfit



Model is too complex

- The model is able to recover the true generative process
- But its flexibility captures noise

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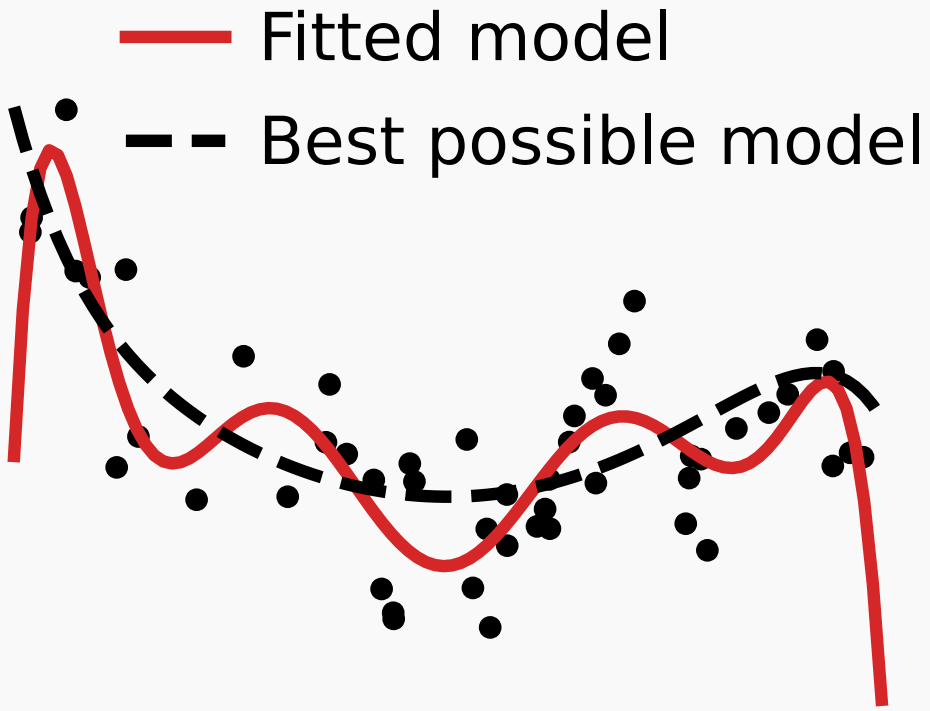

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Too much noise

Not enough data

Bayes error rate: Randomness of the problem

🪙 **Interesting problems exhibit randomness**

$y = g(x) + e$ with $E(e|x) = 0$ and $\text{Var}(e|x) = \sigma^2$

Bayes error rate: Randomness of the problem

🪙 Interesting problems exhibit randomness

$y = g(x) + e$ with $E(e|x) = 0$ and $\text{Var}(e|x) = \sigma^2$

🥇 $g(\cdot)$ is the best possible estimator

$g(\cdot)$ induces the Bayes error, the unavoidable error:

$$\mathcal{E}(g) = \mathbb{E}\big[(g(x) + e - g(x))^2\big] = \mathbb{E}\big[e^2\big] = \sigma^2$$

Empirical risk minimization: approximation error

In practice, the class of function in which the true function lies is unknown:

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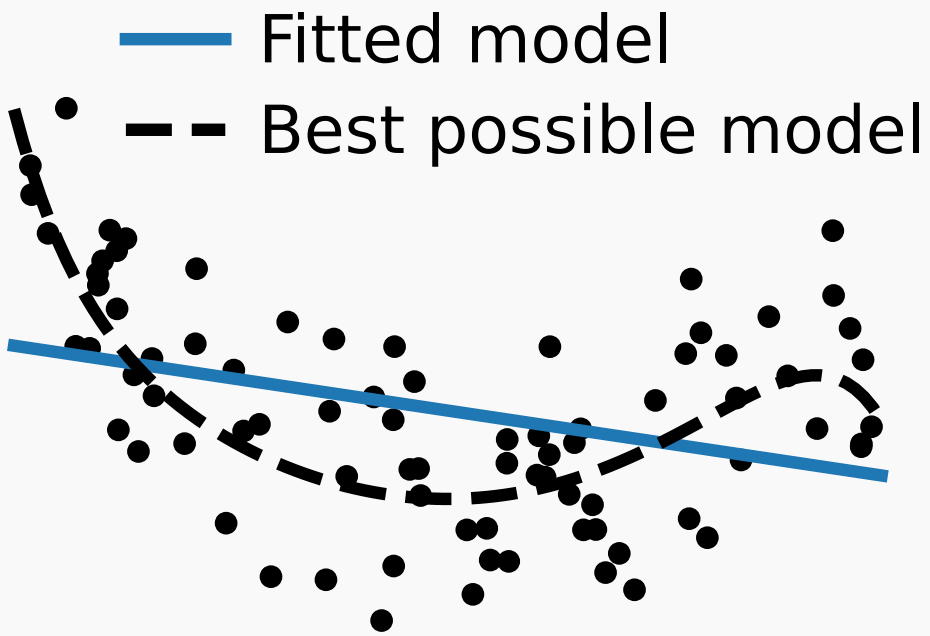
This creates the approximation error:

$$\mathcal{E}(f^\star) - \mathcal{E}(g) = \mathbb{E}\Big[(f^\star(x) - y)^2\Big] - \mathbb{E}\big[(g(x) - y)^2\big] \geq 0$$

High approximation error means underfit



Model is too simple for the data

- its best fit does not approximate the true generative process
- Yet it captures little noise

Low noise

Rapidly enough data to fit the model

Bias variance trade-off: Putting the pieces together

Decomposition of the empirical risk of a fitted model $\hat{f}$

$$\mathcal{E}\left(\hat{f}\right) = \underbrace{\mathcal{E}(g)}_{\text{Bayes error}} + \underbrace{\mathcal{E}(f^\star) - \mathcal{E}(g)}_{\text{approximation error}} + \underbrace{\mathcal{E}\left(\hat{f}\right) - \mathcal{E}(f^\star)}_{\text{estimation error}}$$

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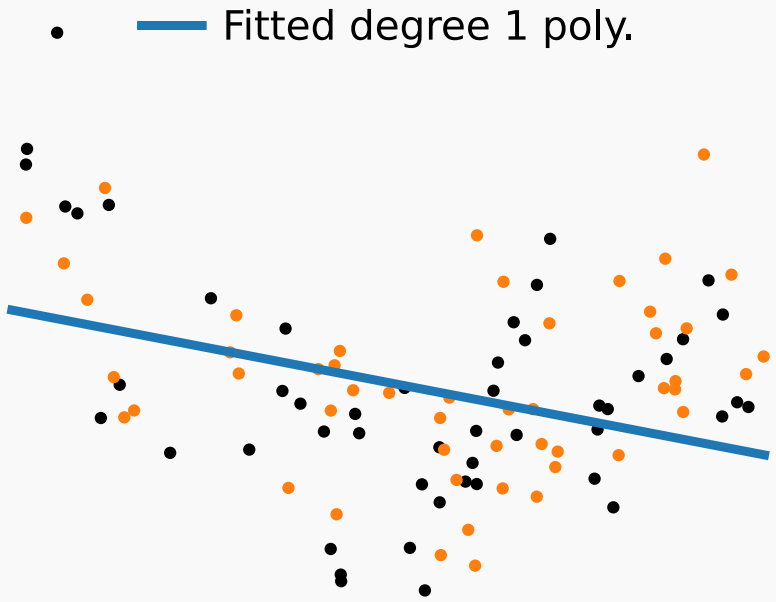
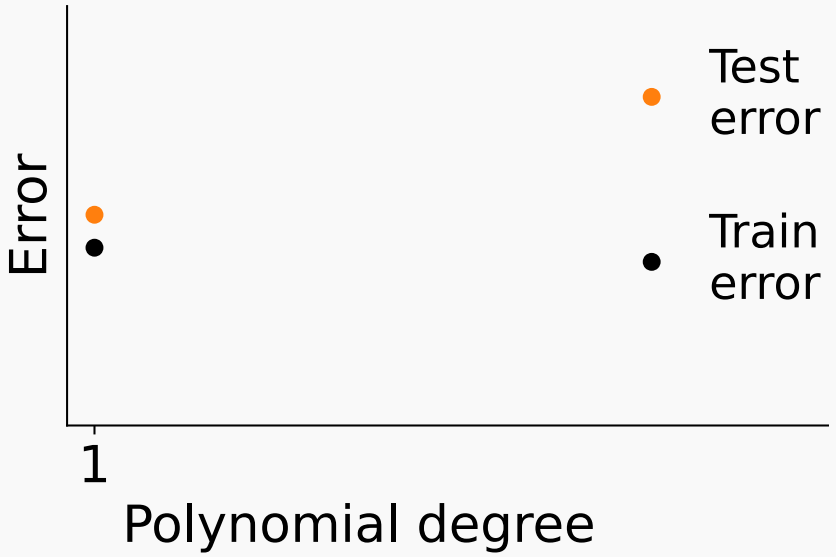
Controls on this trade-off

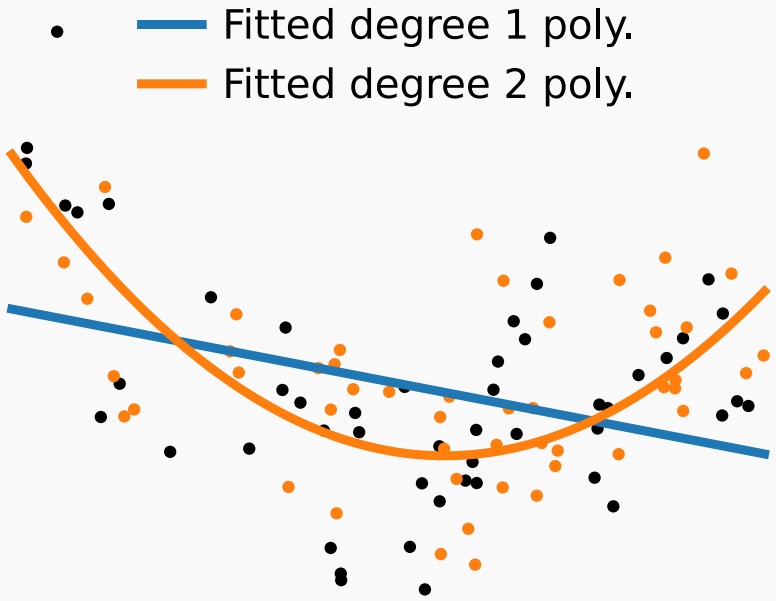
- Bigger candidate family (more complex models) $\mathcal{F}$: increases the estimation errors but decreases the approximation error.
- Smaller candidate family (simpler models): decreases the estimation error but increases the approximation error.
- Bigger sample size n: reduces estimation error and allows more complex models.

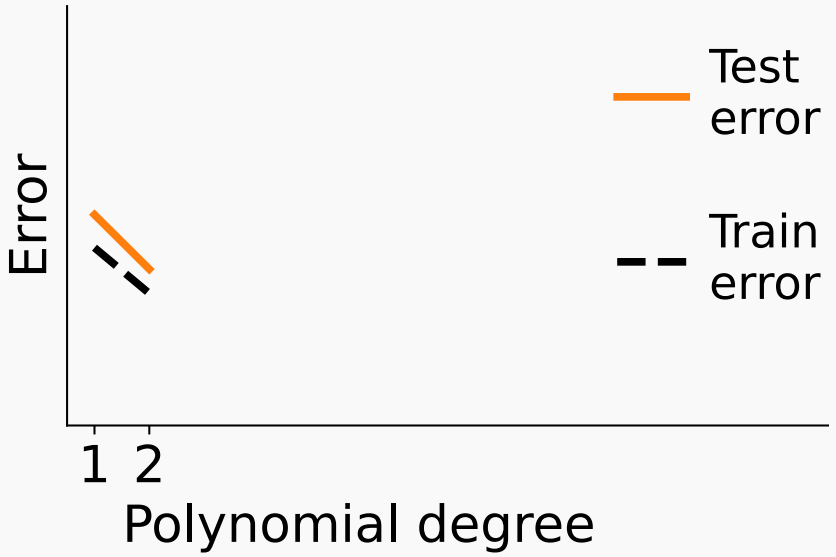
Train vs test error: increasing complexity



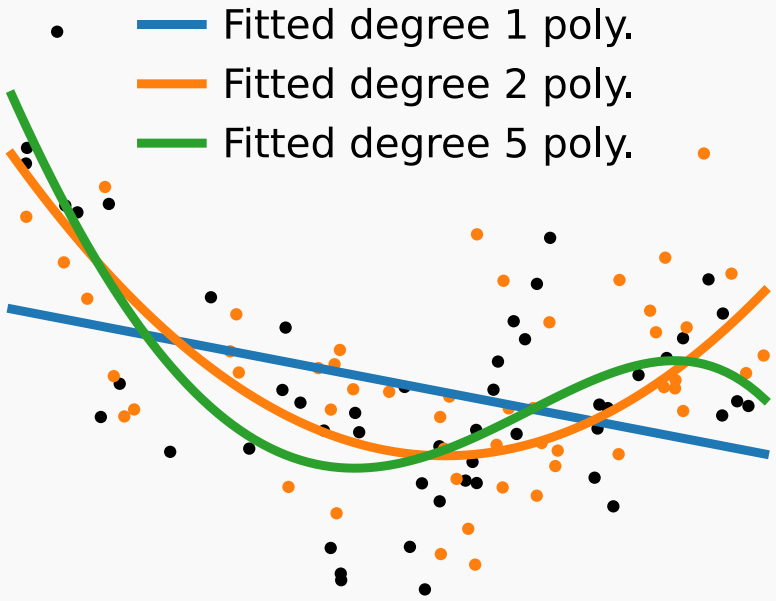


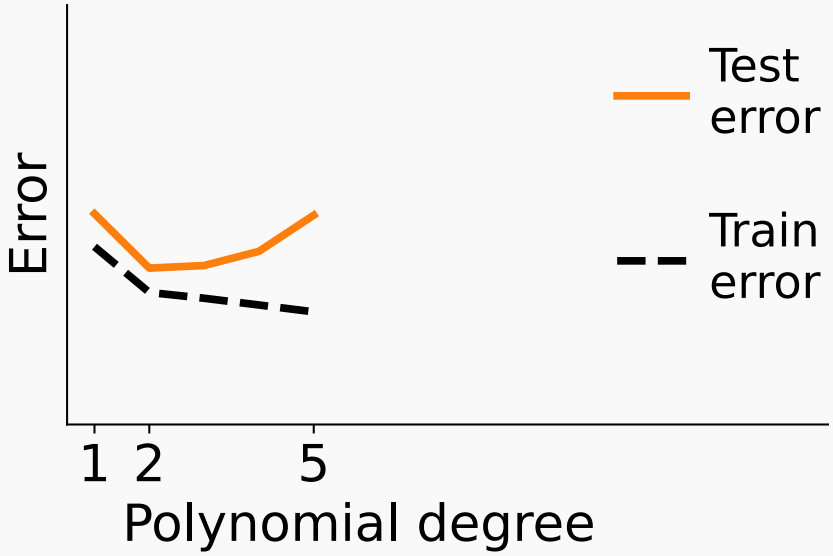
Train vs test error: increasing complexity



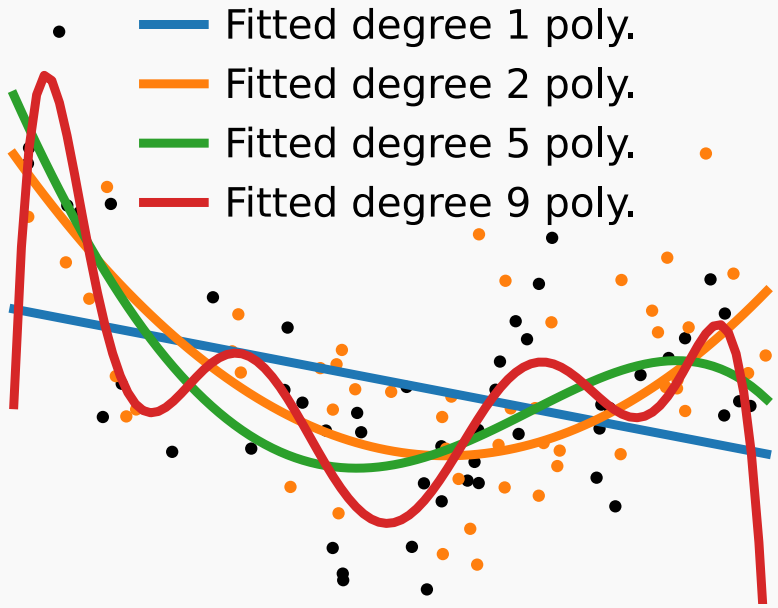


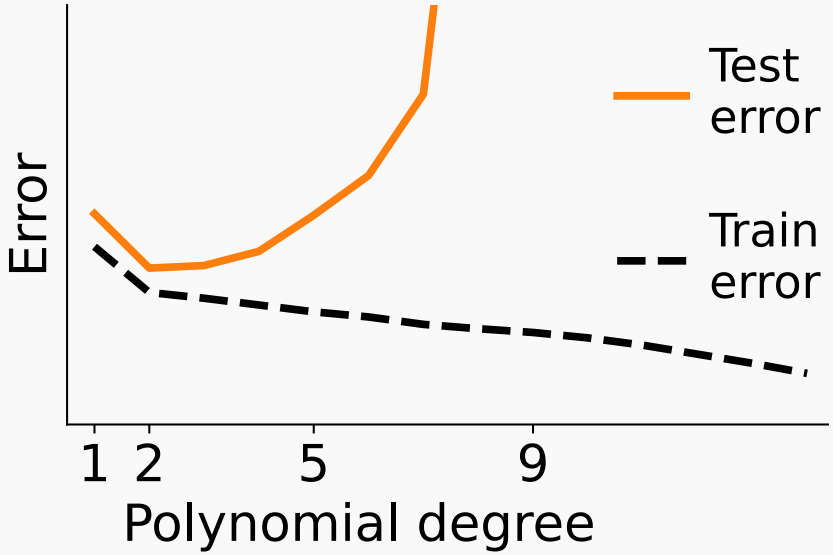
Train vs test error: increasing complexity



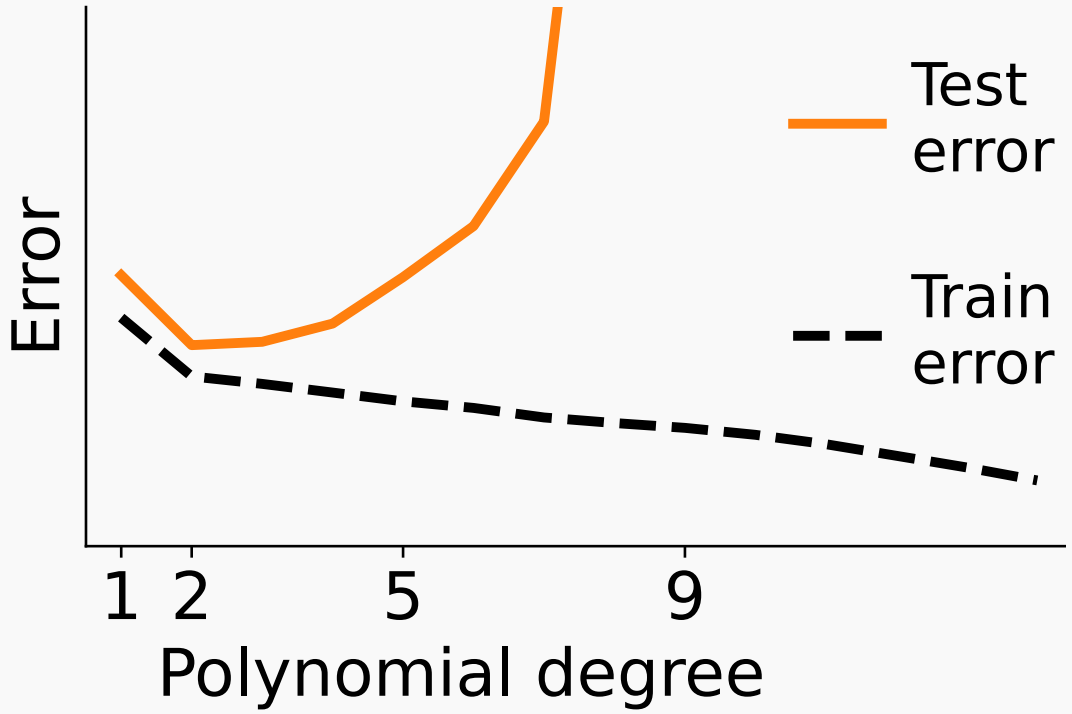


Train vs test error: increasing complexity



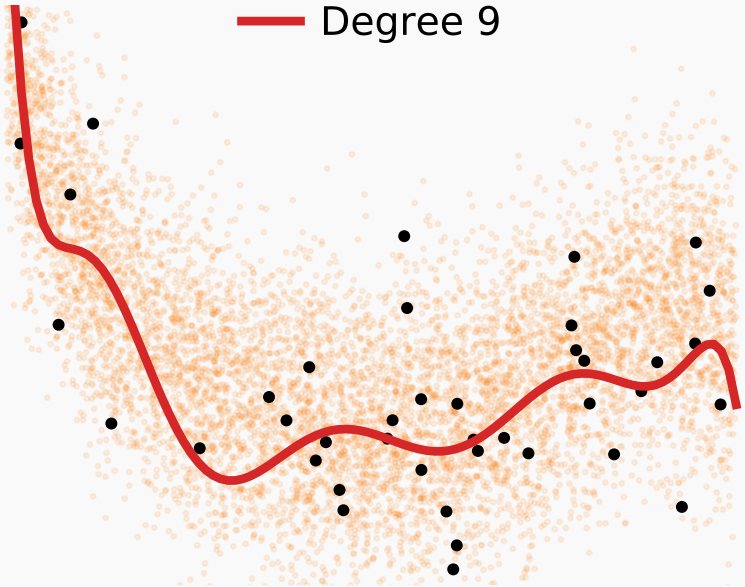


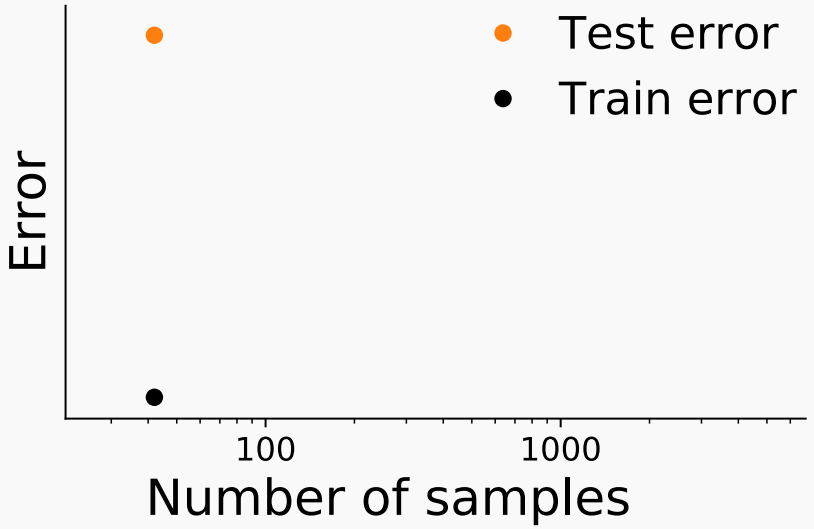
Train vs test error: increasing complexity



Underfit Sweet Spot Overfit

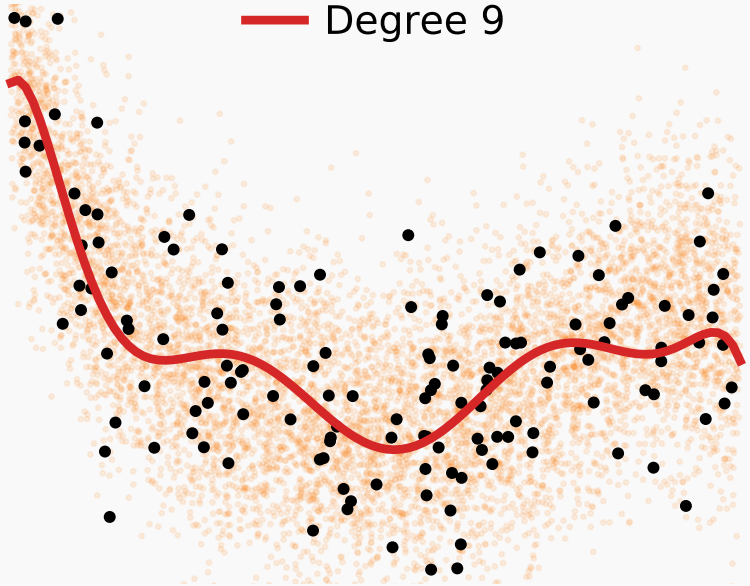
Varying sample size with a candidate family ($\mathcal{F}$ polynoms of degree 9)

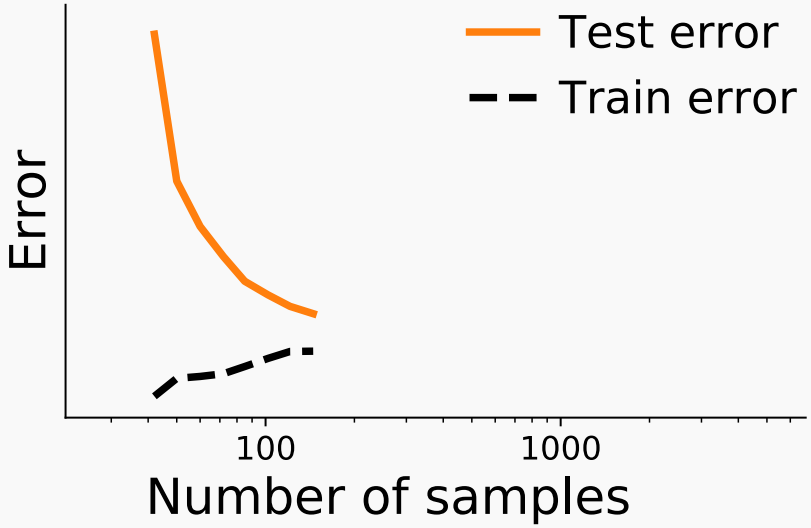




Overfit

Varying sample size with a candidate family ($\mathcal{F}$ polynoms of degree 9)





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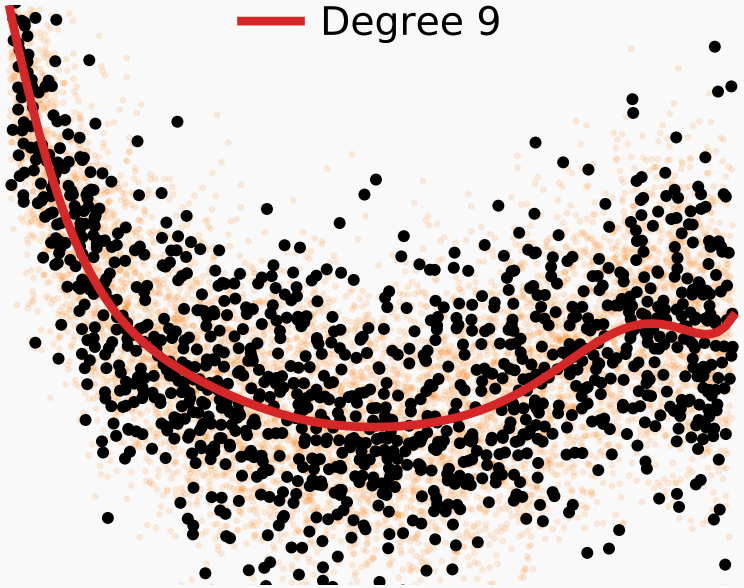
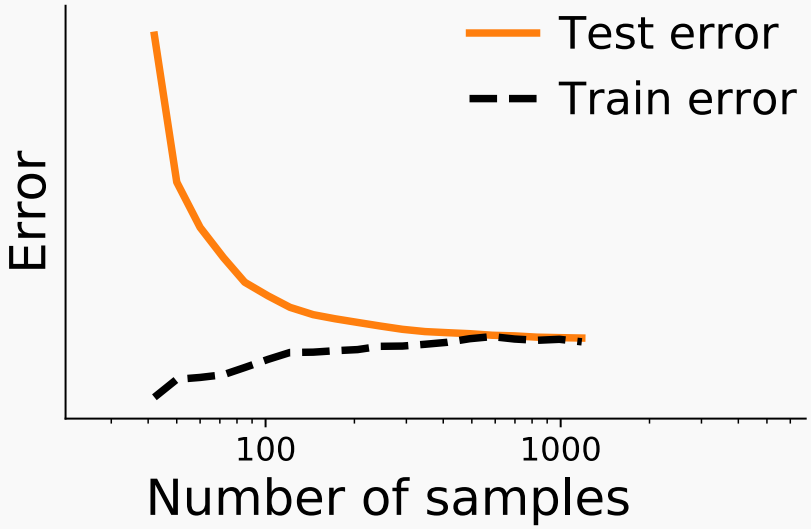
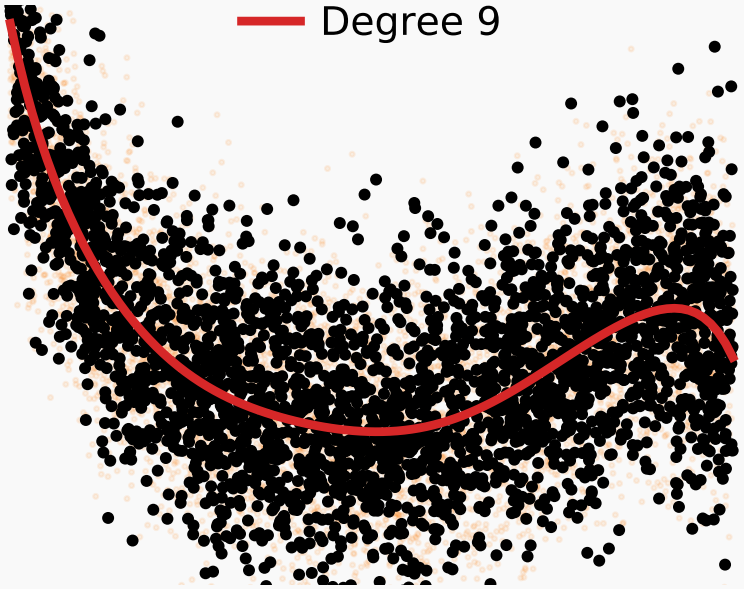
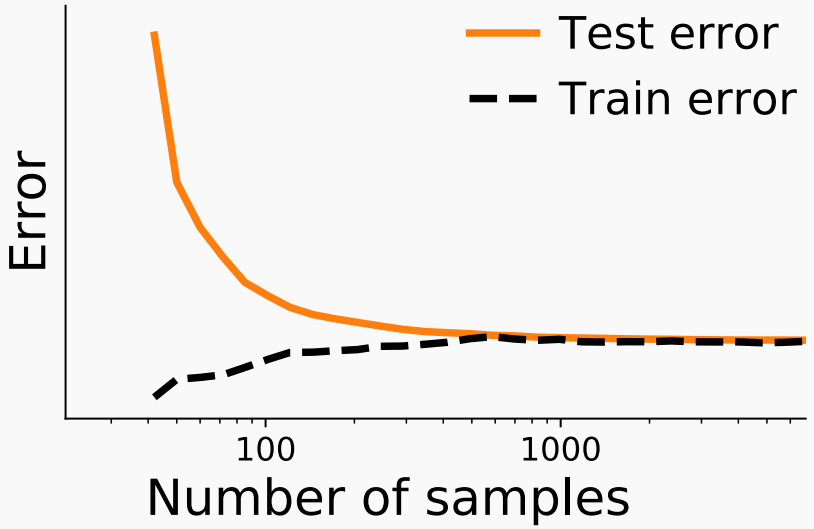




Sweet spot?

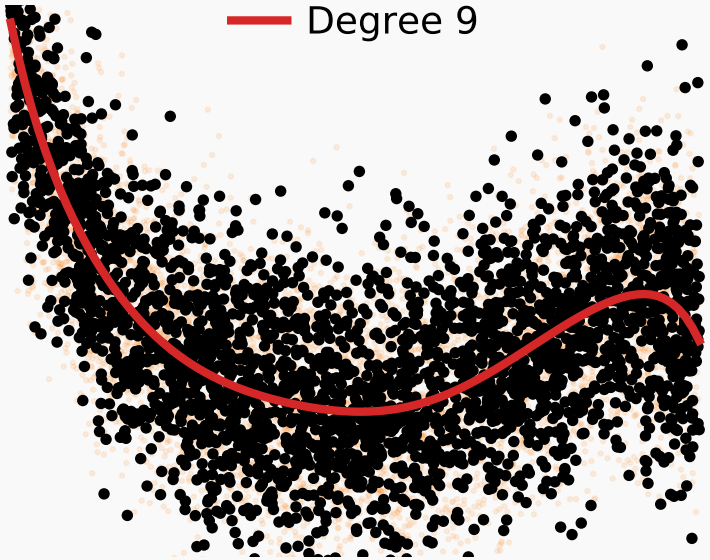
Varying sample size with a candidate family ($\mathcal{F}$ polynoms of degree 9)





Diminishing returns?

Varying sample size with a candidate family ($\mathcal{F}$ polynoms of degree 9)



The error of the best model trained on unlimited data.

Here, the data is generated by a polynomial of degree 9.

We cannot do better.

Prediction is limited by noise: Bayes error.

Common model families suited to tabular data

Today

- Regularized linear models: Lasso and Ridge
- Hands-on with scikit-learn

Next session

- Practical model selection: Cross-validation
- Flexible models: Trees, Random Forests, Gradient Boosting
- Practical scikit-learn

Regularized linear models for predictive inference

Reminder: Linear regression

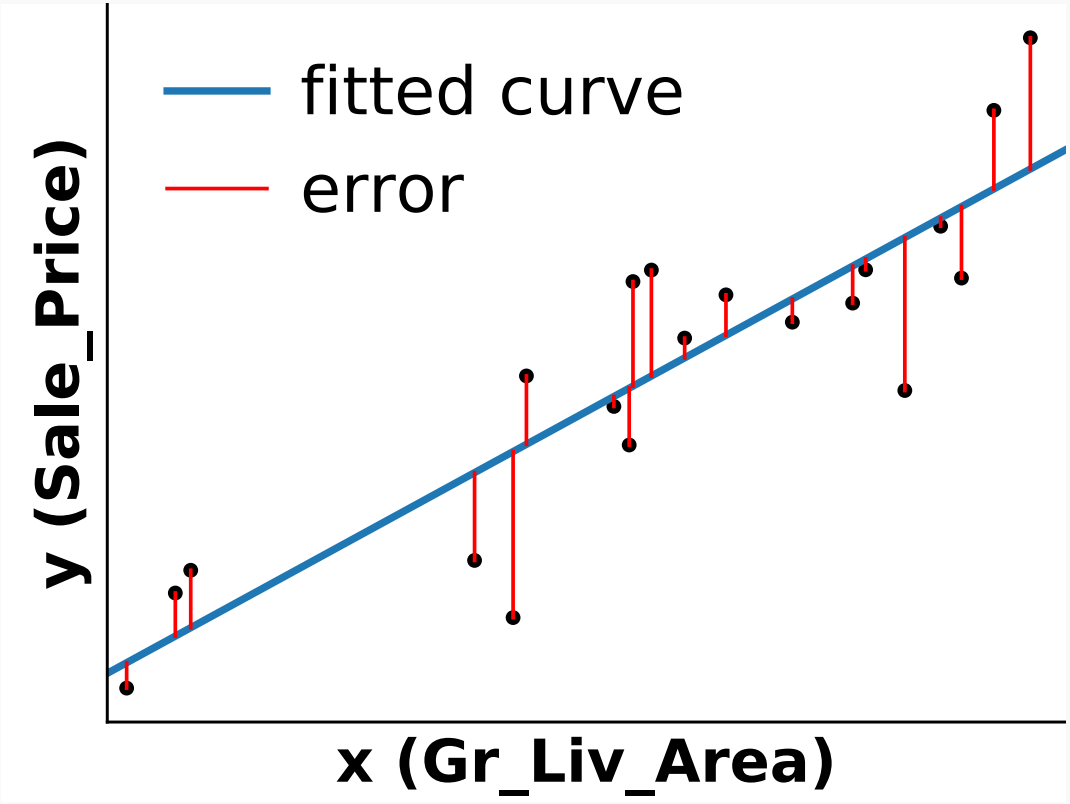
y is a linear combination of the features $x \in \mathbb{R}^p$

$$Y_i = X_i^T \beta_0 + \varepsilon_i$$

- ε the random error term (noise), often assumed $\varepsilon_i \mid X \sim \mathcal{N}(0, \sigma^2)$
- $\beta_0 \in \mathbb{R}^{p \times 1}$ the *true* coefficients.

Reminder: Linear regression

$$Y_i = X_i^T \beta_0 + \varepsilon_i$$



Common metrics

- Mean Squared Error: MSE $= \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2$
- R-squared, : $R^2 = 1 - \frac{\sum_{i=1}^{n}\left(Y_i - \widehat{Y}_i\right)^2}{\sum_{i=1}^{n}\left(Y_i - \bar{Y}\right)^2}$ where $\bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$

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The proportion of variance explained by the model (perfect fit: $R^2 = 1$)

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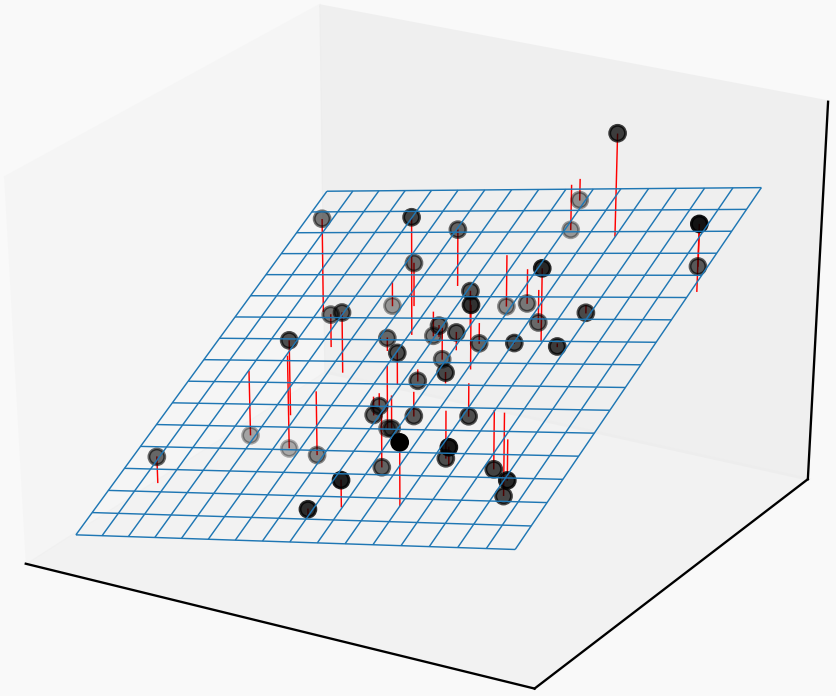
The proportion of variance explained by the model (perfect fit: $R^2 = 1$)

- Mean absolute error: $\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|Y_i - \hat{Y}_i|$

Linear regression: Illustration in two dimensions



Reminder: logistic regression for classification

The logit of the probability of the outcome is a linear combination of the features $X_i \in \mathbb{R}^p$:

$$\ln\left(\frac{p(Y_i=1|X_i)}{p(Y_i=0|X_i)}\right) = X_i^T\beta_0$$

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Taking exponential of both sides, we get:

$$p(Y_i = 1|X_i, \beta_0) \stackrel{\text{def}}{=} p(X_i, \beta_0) = \frac{1}{1+\exp(-X_i^T \beta_0)}$$

The statistical model is a Bernoulli 🪙 : $B(p(x, \beta_0))$

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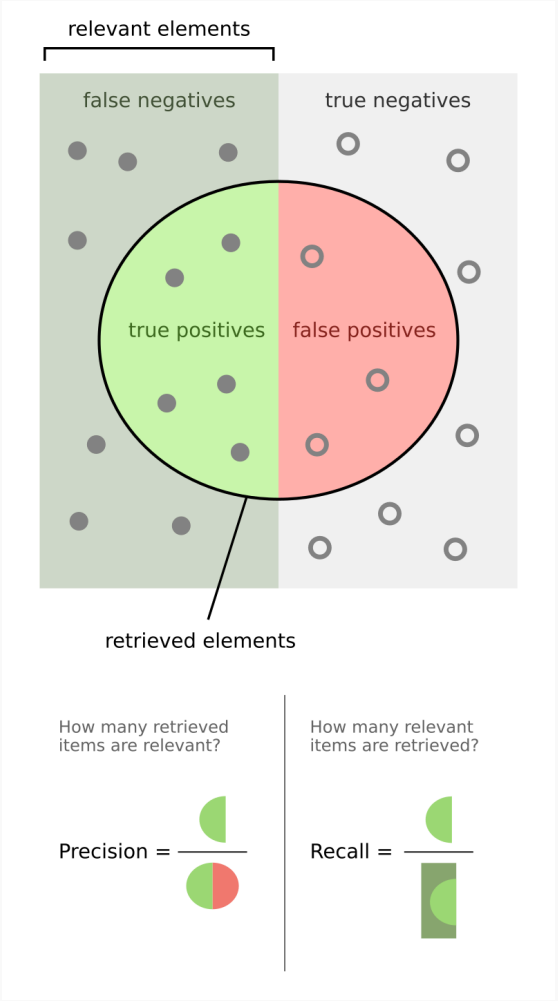
The statistical model is a Bernoulli 🪙 : $B(p(x, \beta_0))$

Model fitted by maximum likelihood with iterative optimization (Hastie, 2009): eg. coordinate descents (liblinear), second order descent (Newton's method), gradient descent (SAG)...

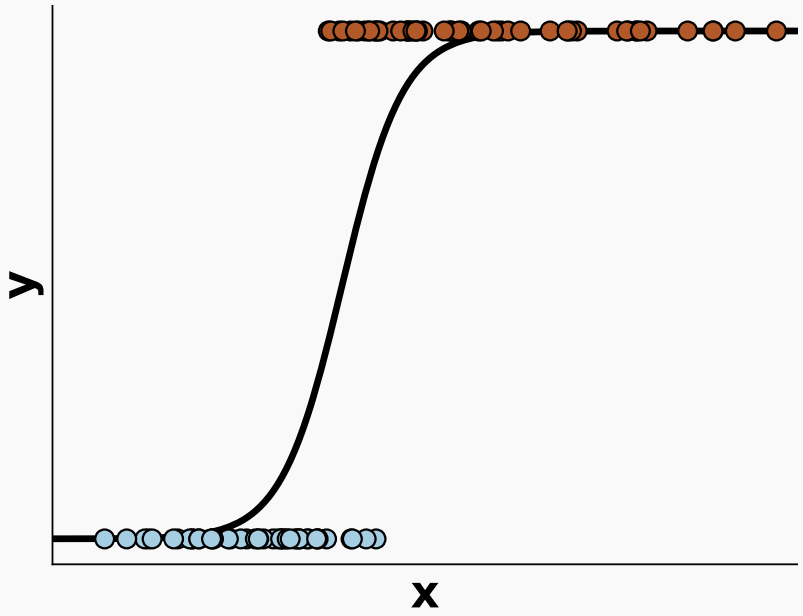
Reminder: classification, logistic regression

Common metrics

- Accuracy $= \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left(Y_i = \hat{Y}_i\right)$
- Precision: Precision $= \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$
- Recall: Recall $= \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$
- Brier score loss: $\mathrm{BSL} = \frac{1}{n}\sum_{i=1}^{n} \left(Y_i - p_i\right)^2$

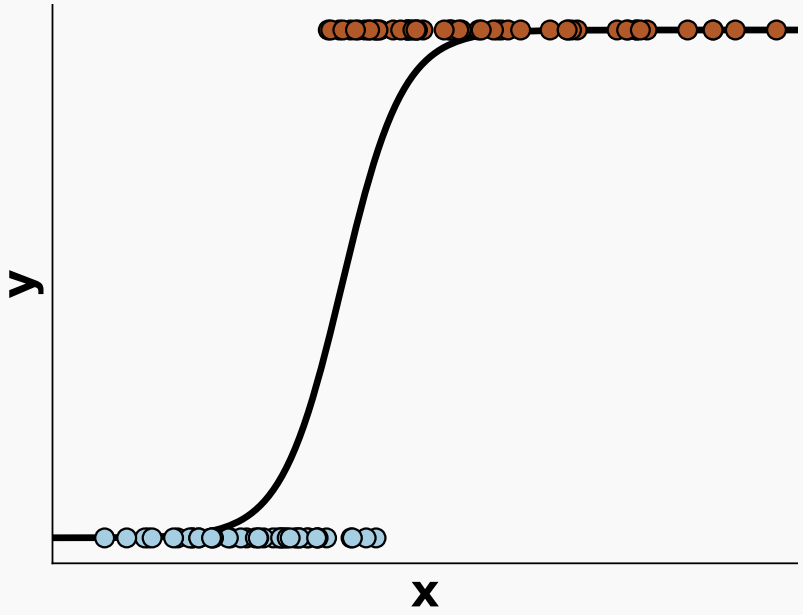


Logistic regression: Illustrations

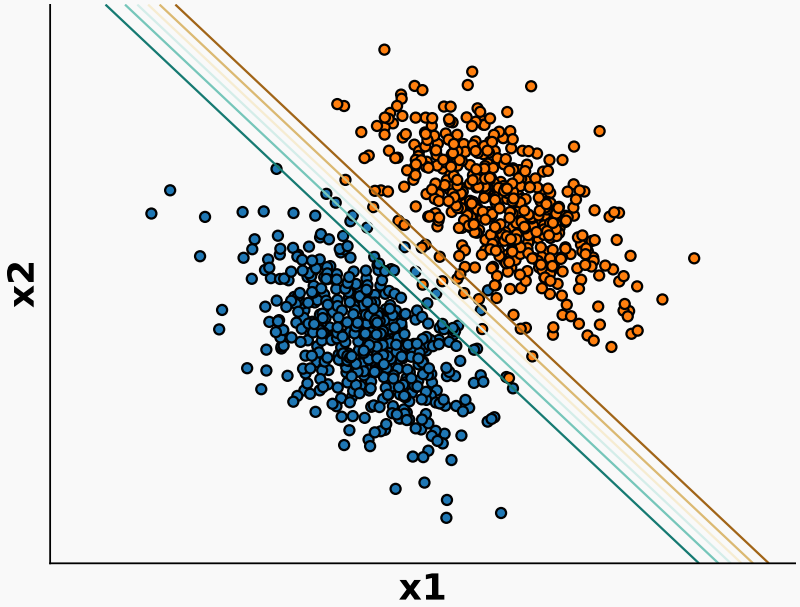


Logistic regression in one dimension.

Logistic regression: Illustrations

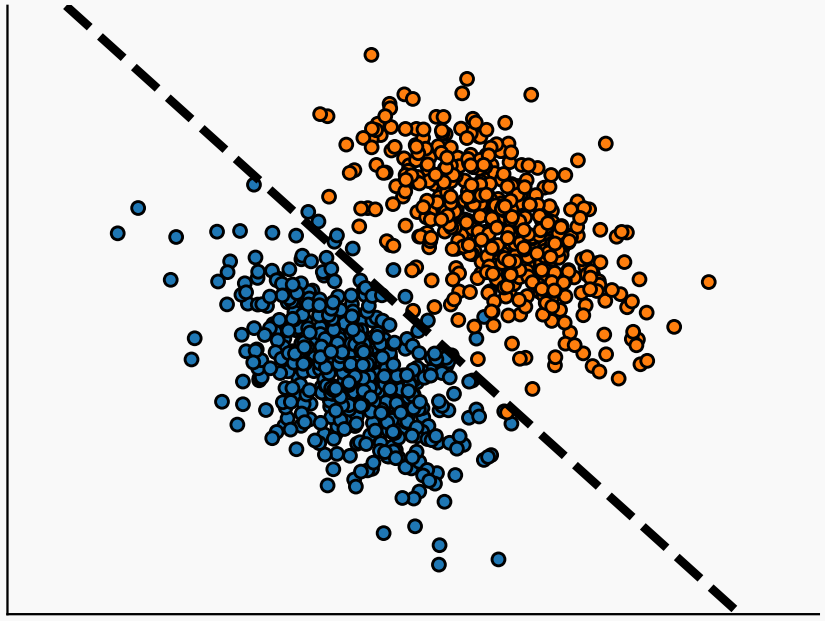


Logistic regression in one dimension.



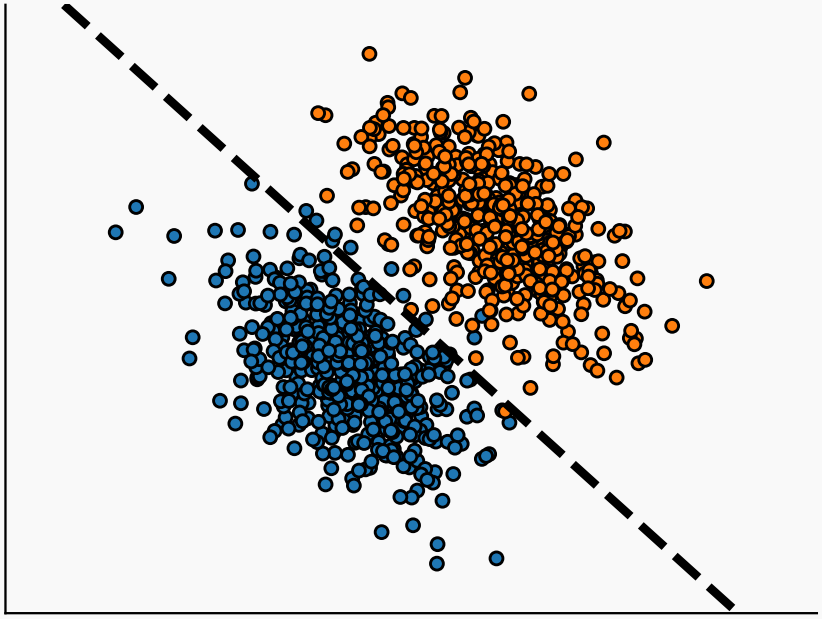
Logistic regression in two dimensions.

Linear models are not suited to all data

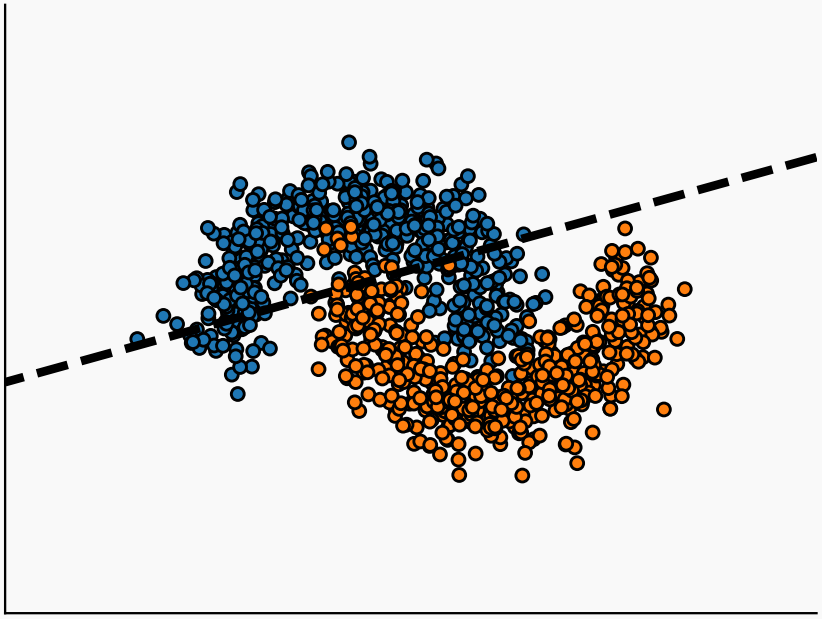


Almost linearly separable data.

Linear models are not suited to all data



Almost linearly separable data.



Data not linearly separable.

Linear model pros and cons

Pros

- Converge quickly
- Hard to beat when n_features is large but we still have n_samples >> n_features
- Linear models work well if
  - the classes are (almost) linearly separable
  - or the outcome is (almost) linearly related to the features.

Linear model pros and cons

Cons

Sometimes

- the best decision boundary to separate classes is not well approximated by a straight line.
- there are important non-linear relationships between the features and the outcome.

Linear model pros and cons

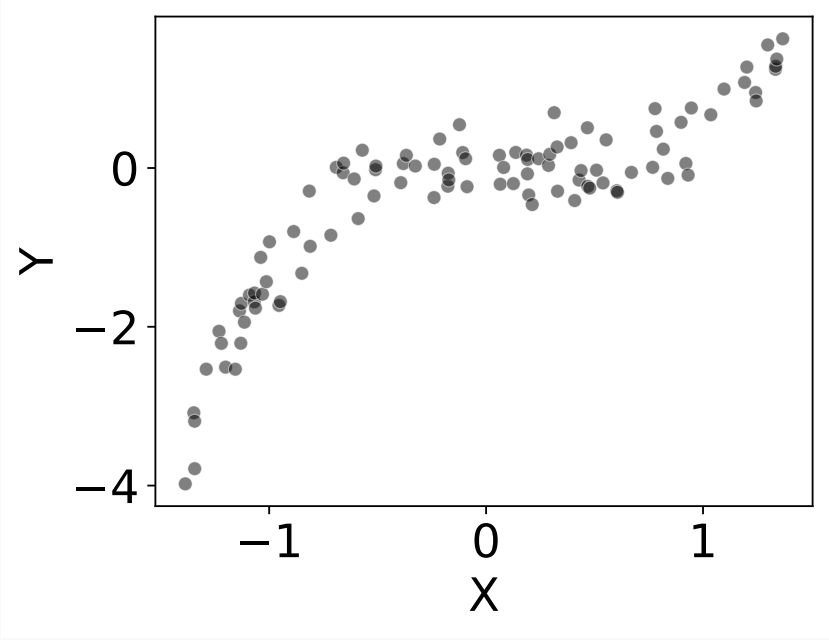
Cons

Sometimes

- the best decision boundary to separate classes is not well approximated by a straight line.
- there are important non-linear relationships between the features and the outcome.

💡 Either use non-linear models, or perform transformations on the data, to engineer new features.

Transformation of the features: Example

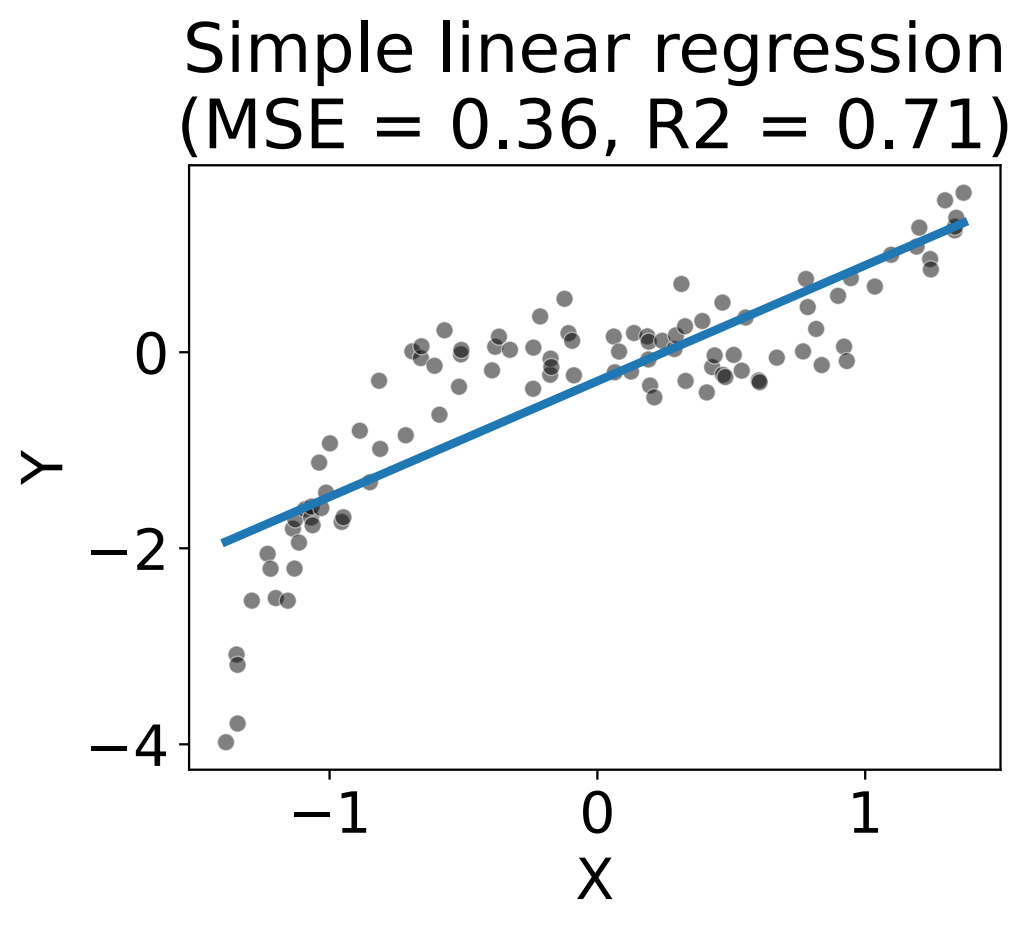


Non-linear relationship between the features and the outcome

True data generating process:

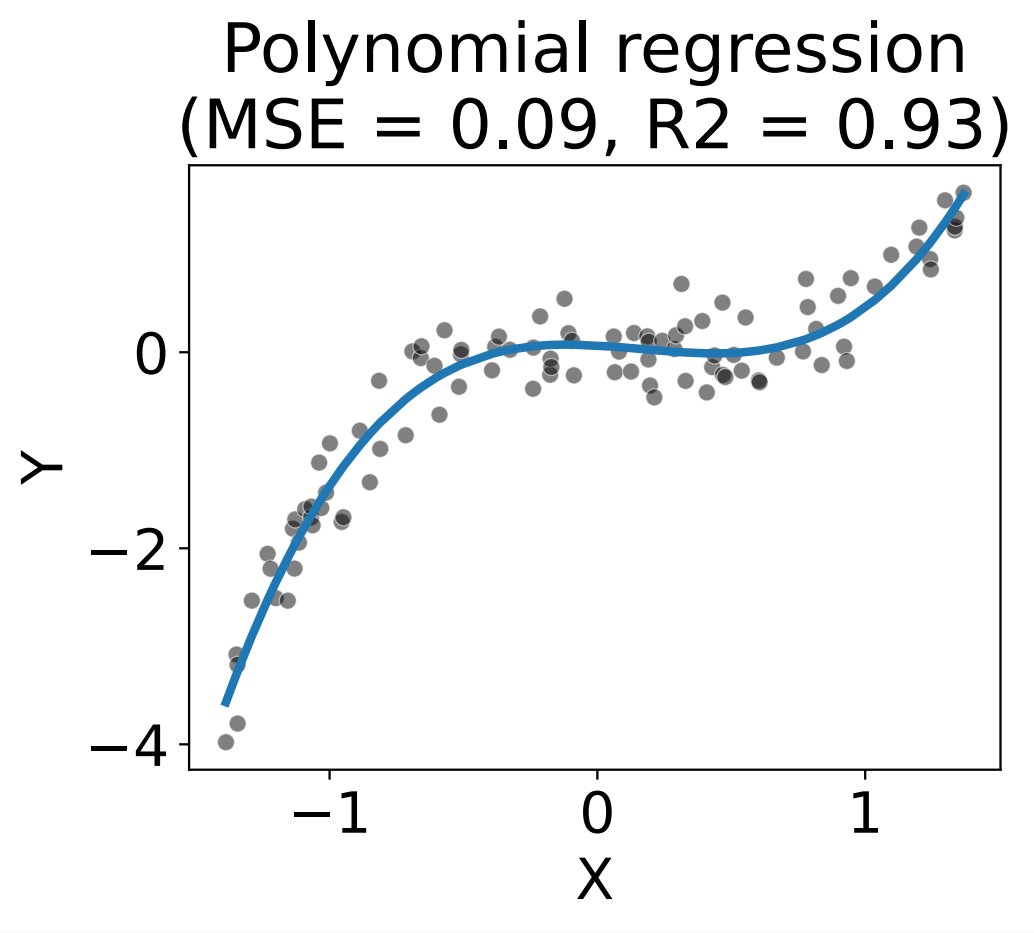
$Y = X^3 - 0.5 \times X^2 + \varepsilon$

Transformation of the features: Example



Vanilla linear regression fails to capture the relationship.

Transformation of the features: Example



Solution:

- Expand the feature space with polynoms of the features:

  $$X = [X, X^2, X^3]$$

- Run a linear regression on the new feature space.

$$Y = [X, X^2, X^3]^T \hat{\beta}$$

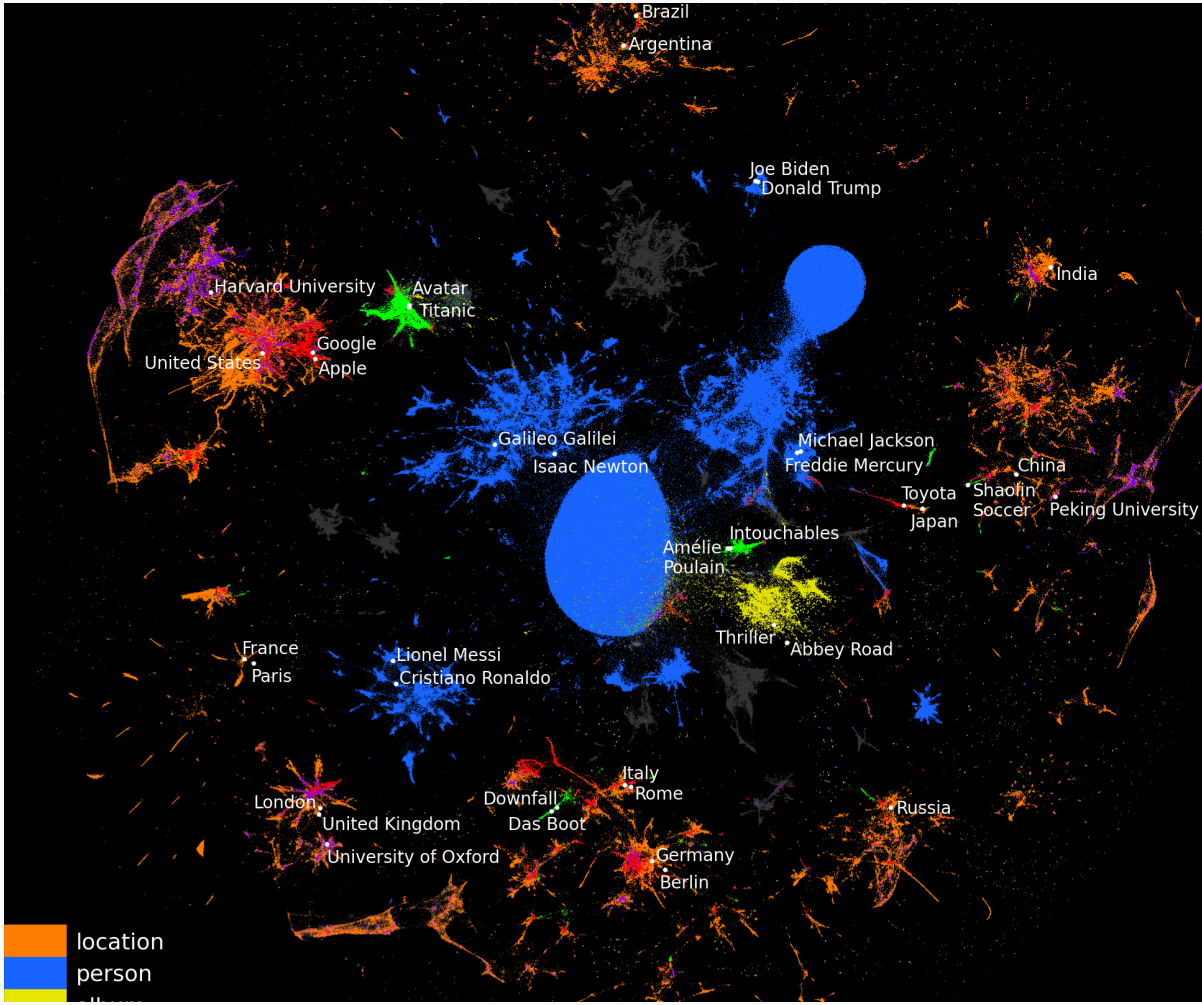
Takeaway on feature expansion

Feature expansion increase the family of models

- Linear model can underfit : when n_features small or the problem is not linearly separable.
- Feature expansion is an easy way to capture non-linear relationships.
- Different feature expansions exists: polynomial, log, splines, embeddings, kernels, ...

KEN (Cvetkov-Iliev et al., 2023): Relational Data Embeddings

Easy to use with skrub library



But Linear models can also overfit!

When

- p is large
- Many uninformative features

But Linear models can also overfit!

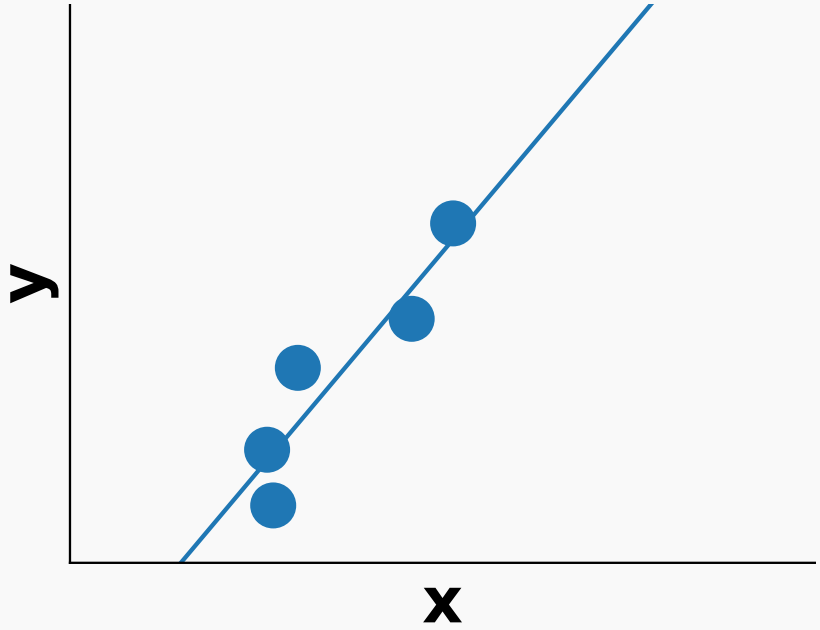
When

- p is large
- Many uninformative features

Solution

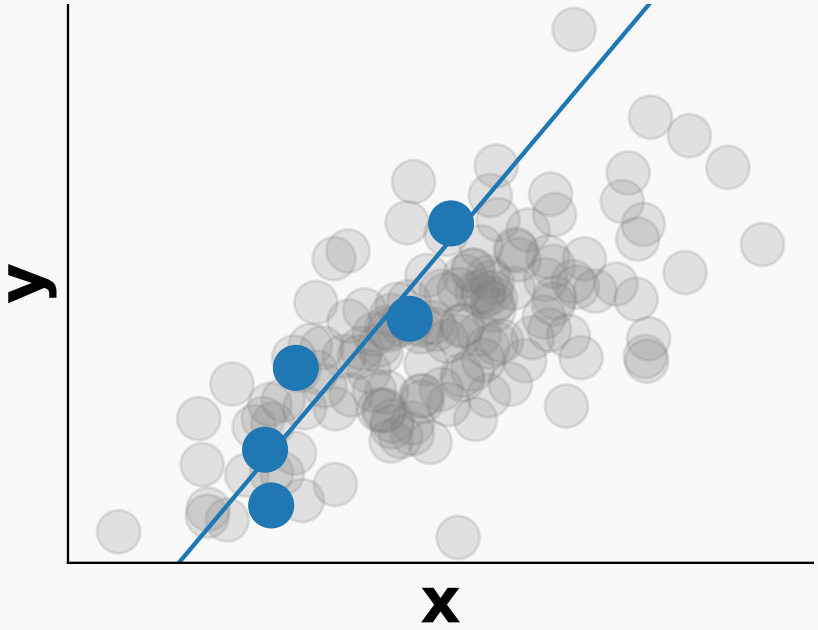
- Used regularized linear models: penalize extreme weights
- Statistically, this allows biased models but with lower variance.
- We will see: Lasso and Ridge but this is a general principle in machine learning.

Many features, few observations: illustration in 1D



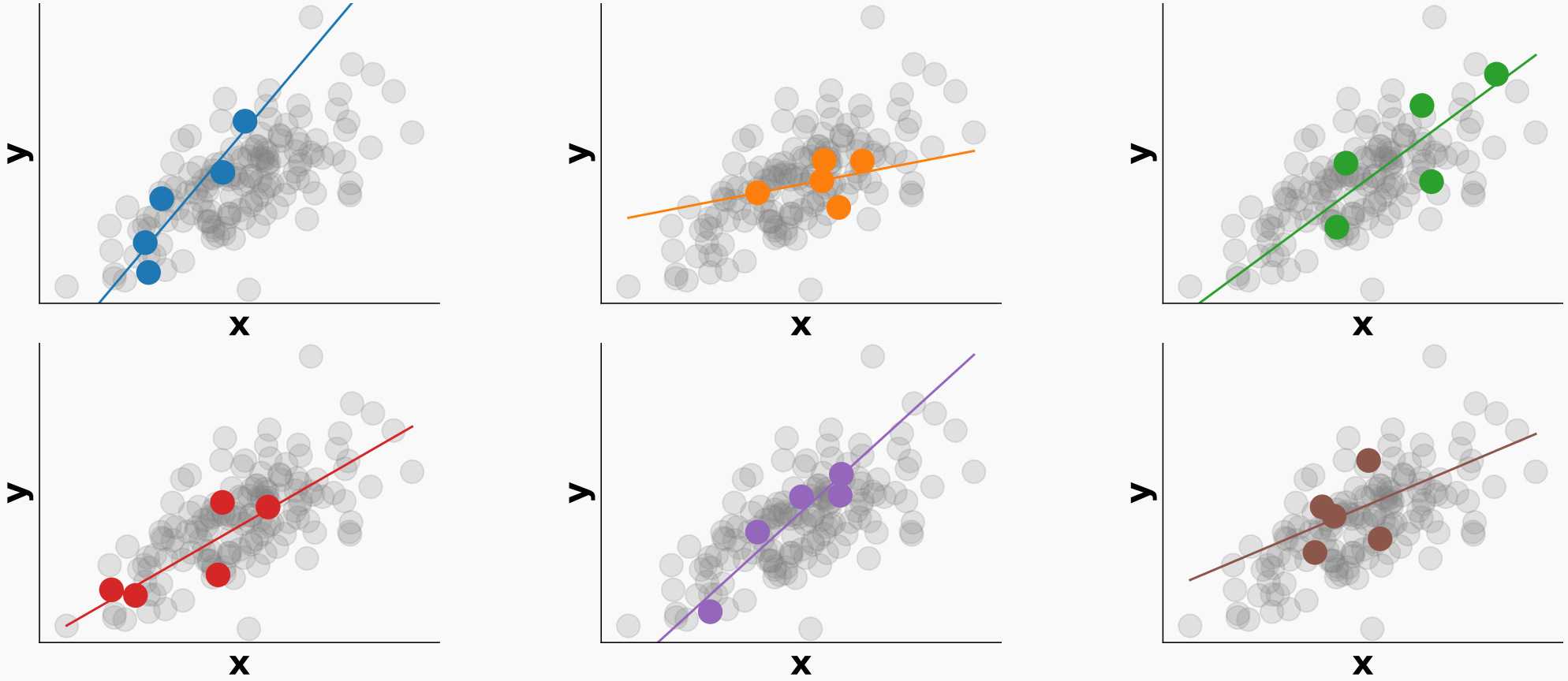
- Few observations with respect to the number of features.
- Fit a linear model without regularization.
-

Many features, few observations: illustration in 1D

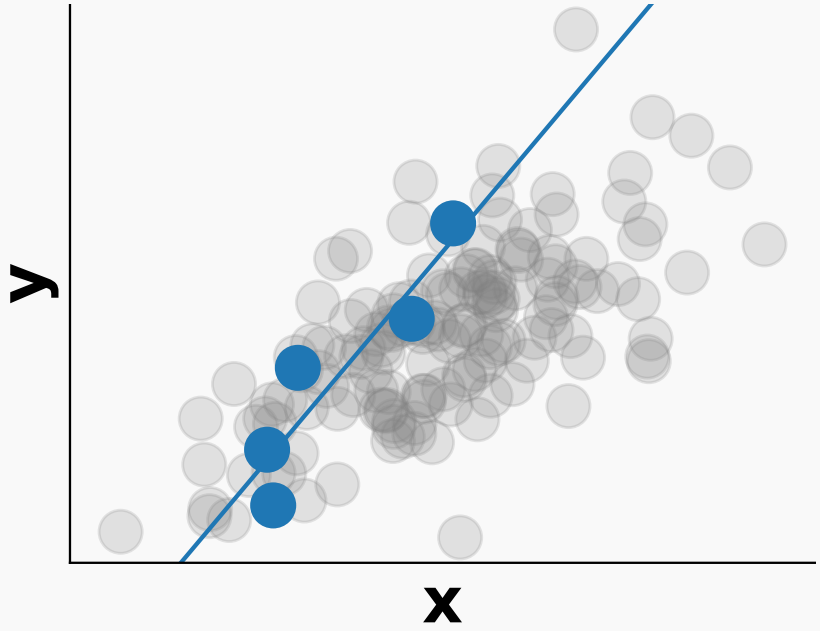


- Few observations with respect to the number of features.
- Fit a linear model without regularization.
- Linear model can overfit if data is noisy.

Sampling different training sets

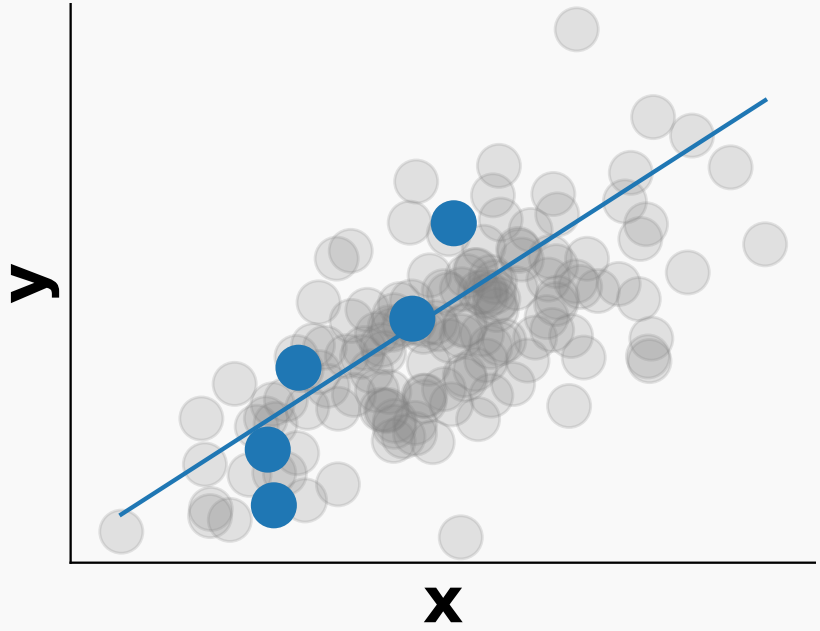


Bias variance trade-off with Lasso



Linear regression (no regularization)

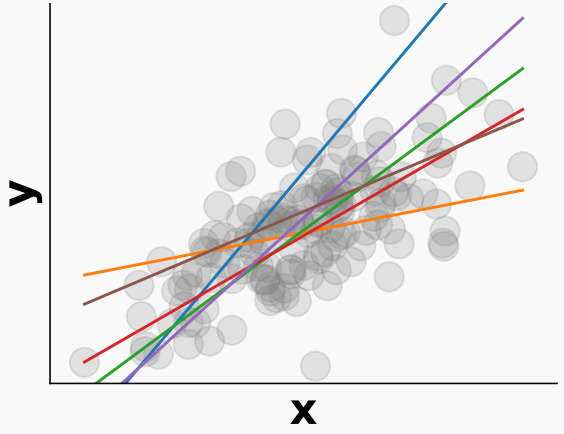
High variance, no bias.



Lasso (regularization): Shrink some coefficients of β.

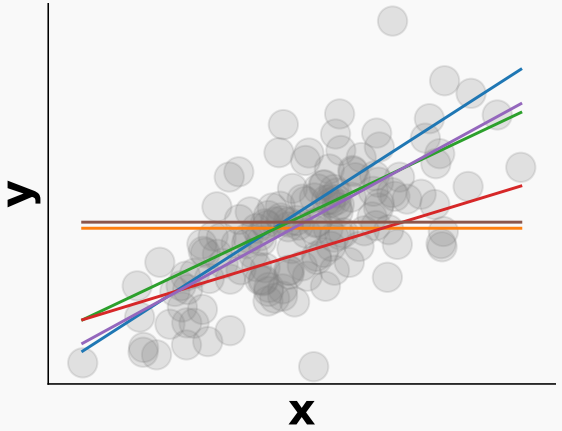
Lower variance, but bias.

Bias variance trade-off with Lasso

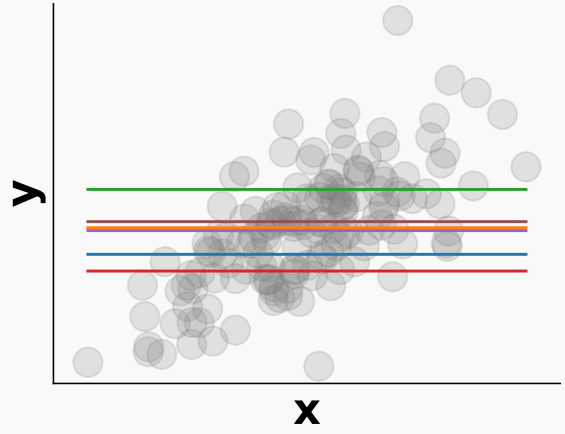


Too much variance

Not enough regularization



Best trade-off



Too much bias

Too much regularization

Many features, few observations

Assumption 1: Linear model with high dimension

$$Y = X\beta_0 + \varepsilon, \quad \varepsilon \perp\!\!\!\perp X \text{ and } X \in \mathbb{R}^{n \times p} \text{ with } n \ll p$$

Assumption 2: (approximate) sparsity

- The true β_0 is sparse: ie. many coefficients are zero or very close to zero.

Objective function of the Lasso

The lasso puts a constrainst of amplitude t on the L_1 norm of the coefficients:

$$\min_\beta \sum_{i=1}^n \left(\left(y_i - \beta^T x_i \right)^2 \right) \text{ st.} \sum_{j=1}^p |\beta_j| \leq t$$

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This is equivalent to the following optimization problem (using lagrangian multiplier):

$$\min_\beta \sum_{i=1}^n \left((y_i - \beta^T x_i)^2 \right) + \lambda \sum_{j=1}^p |\beta_j|$$

Objective function of the Lasso

The lasso puts a constrainst of amplitude t on the L_1 norm of the coefficients:

$$\min_\beta \sum_{i=1}^n \left((y_i - \beta^T x_i)^2 \right) \text{ st.} \sum_{j=1}^p |\beta_j| \leq t$$

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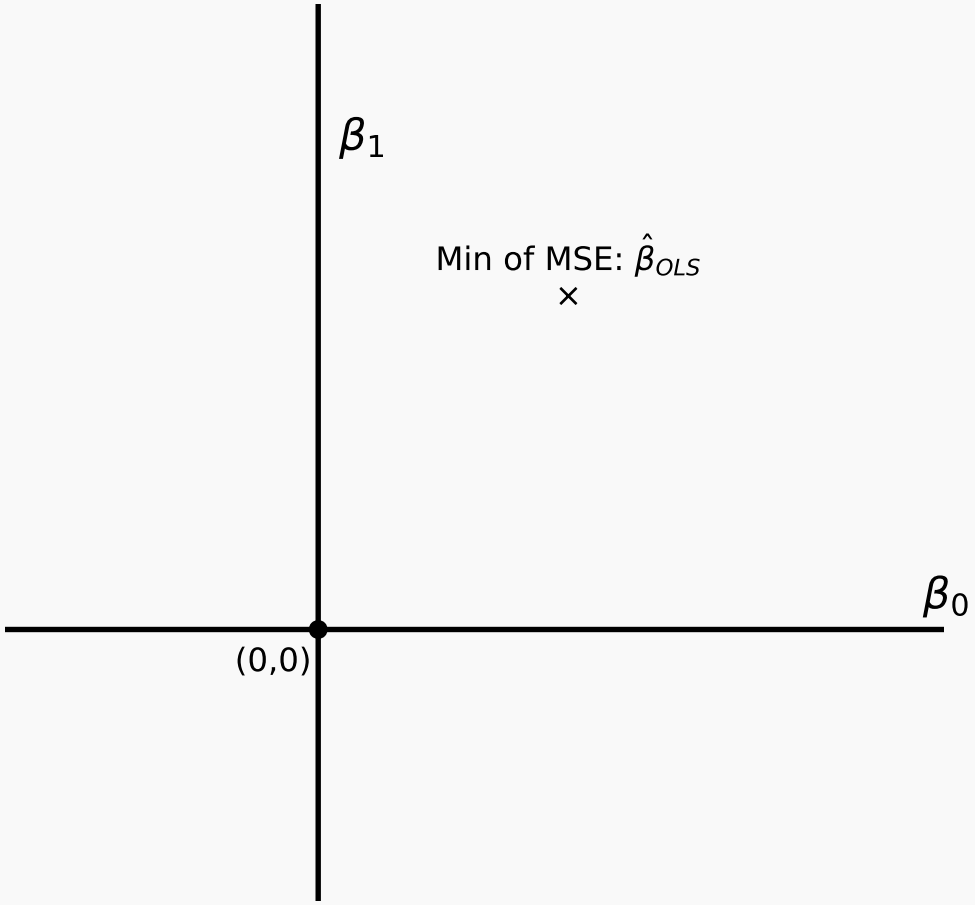
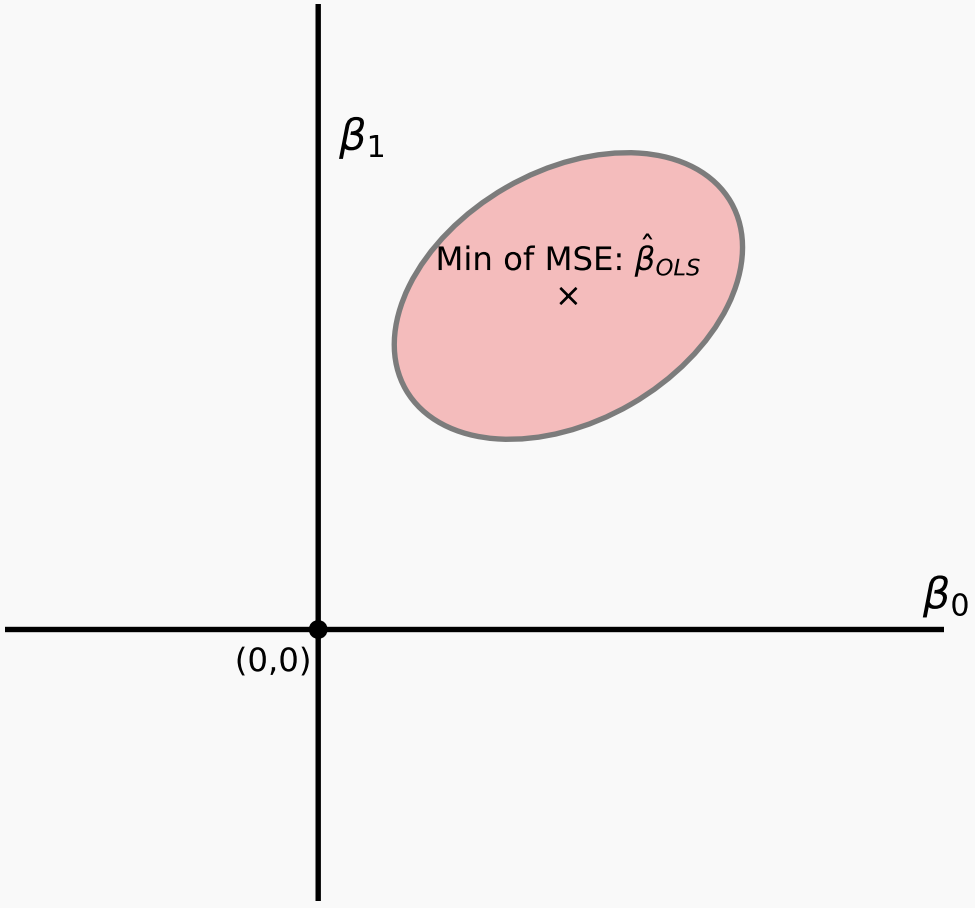
This penalty discourages large weights and can shrink certain weights to exactly *zero* (not clear yet why).

Why does Lasso shrink some coefficients to zero?



MSE as a function of the coefficients.

Why does Lasso shrink some coefficients to zero?



MSE as a function of the coefficients.

The MSE surface is an ellipsoid in β: Every point on the ellipsoid edge has the same MSE.

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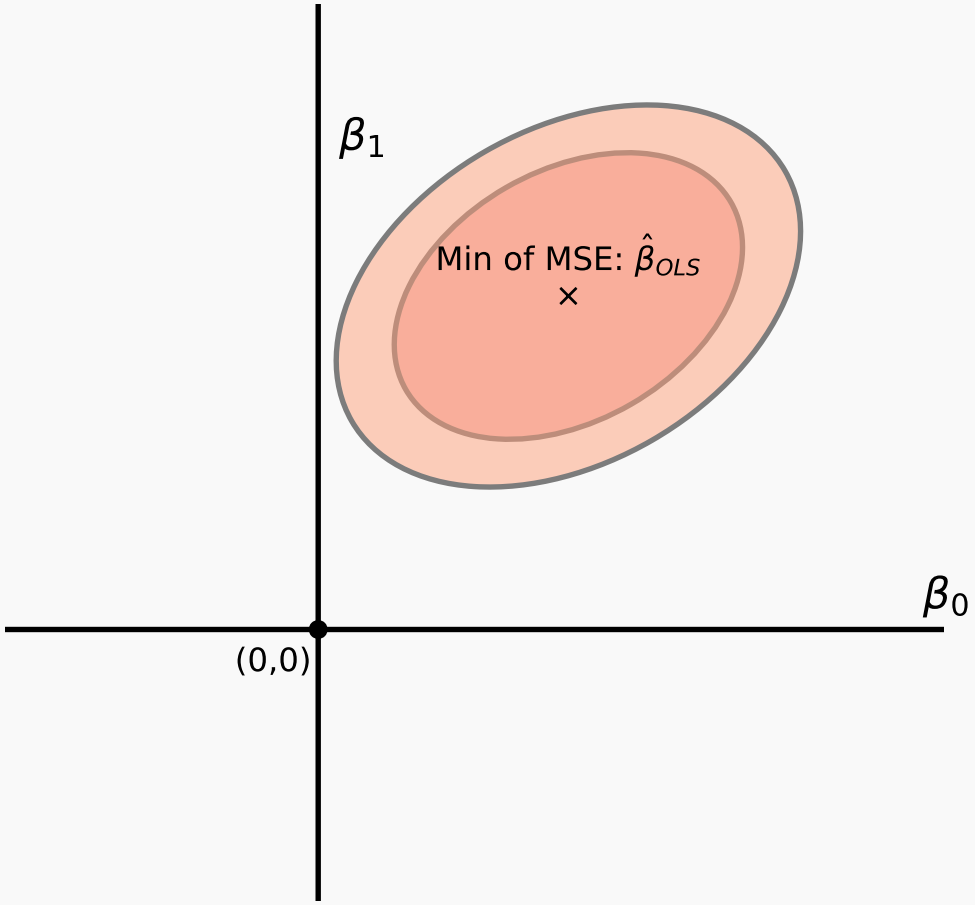

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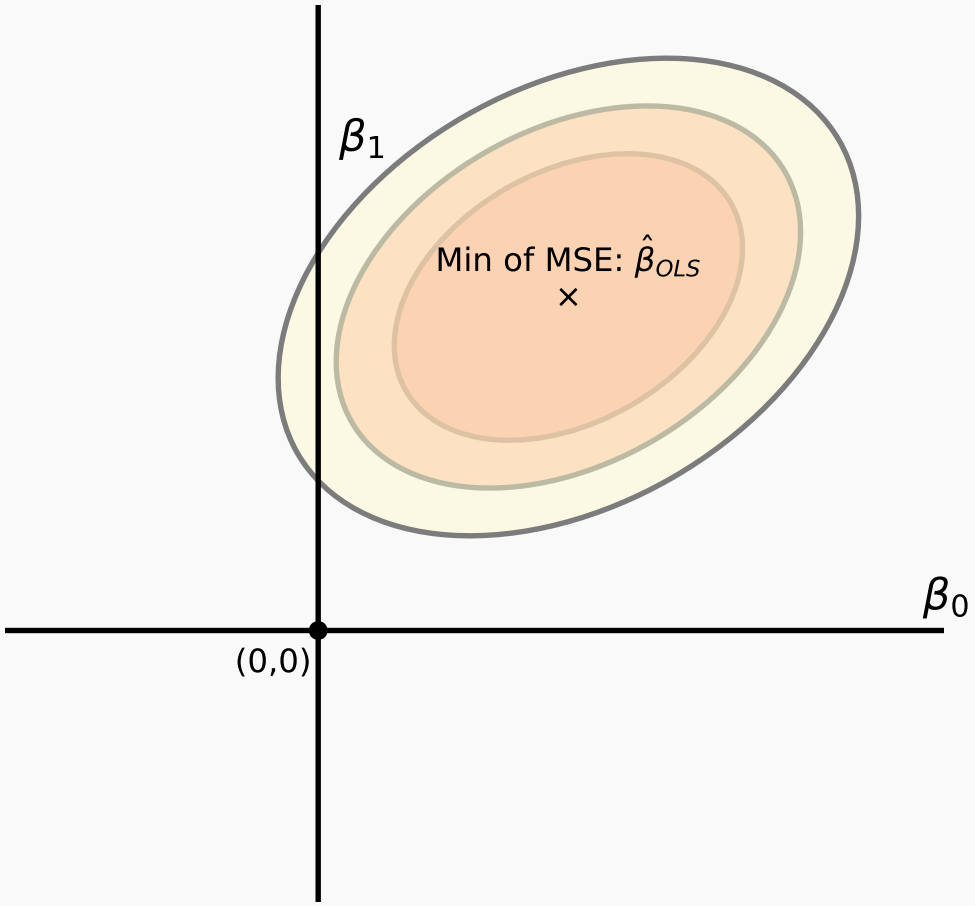

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Moving away from OLS solution

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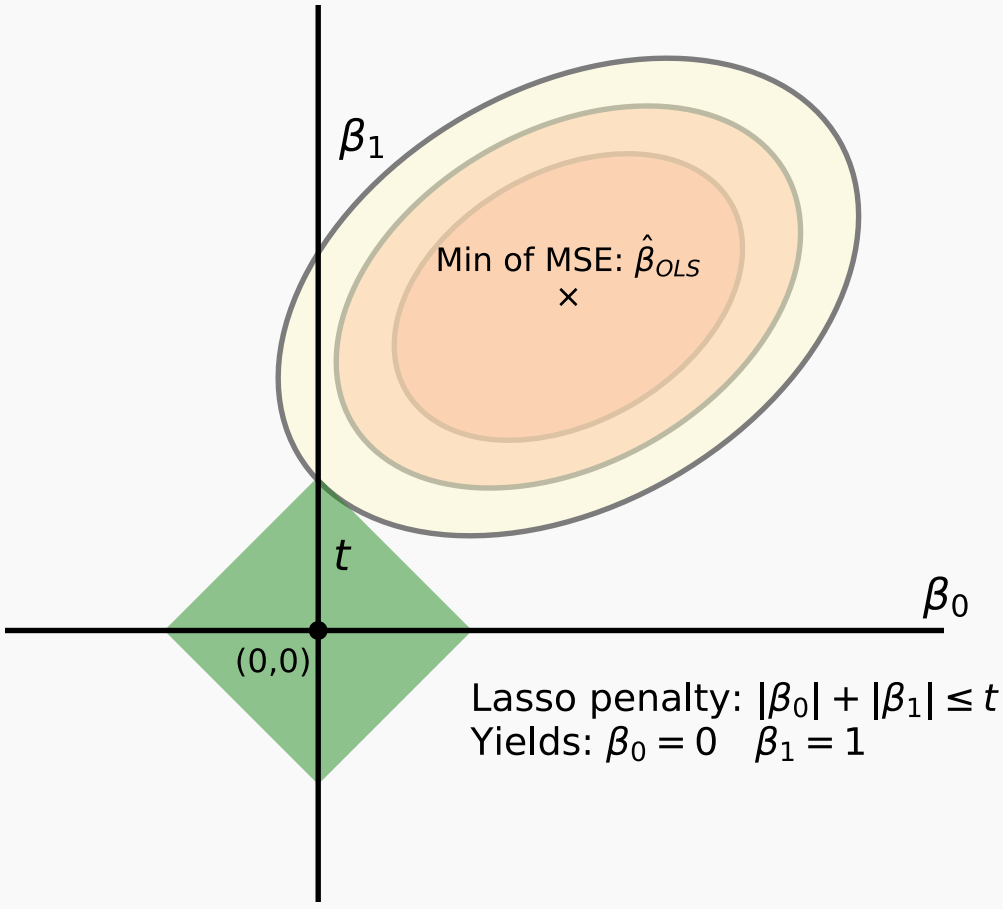

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The MSE surface is an ellipsoid in β: Every point on the ellipsoid edge has the same MSE.

Moving away from OLS solution

Until the ellipsoid respects the lasso penalty (green diamond).

Another regularized linear model: Ridge

Ridge puts a constrainst of amplitude t on the L_2 norm of the coefficients:

$$\min_\beta \sum_{i=1}^{n} \left((y_i - \beta^T x_i)^2 \right) \text{ st.} \sum_{j=1}^{p} \beta_j^2 \leq t$$

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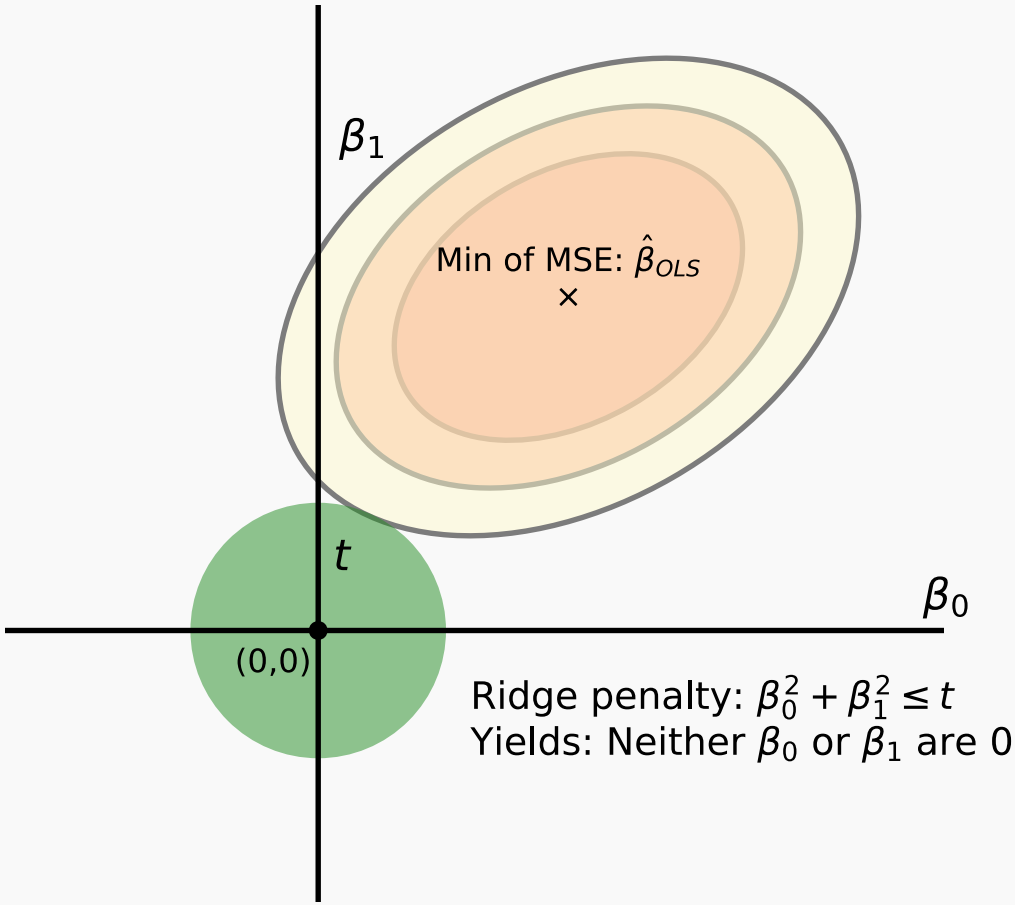
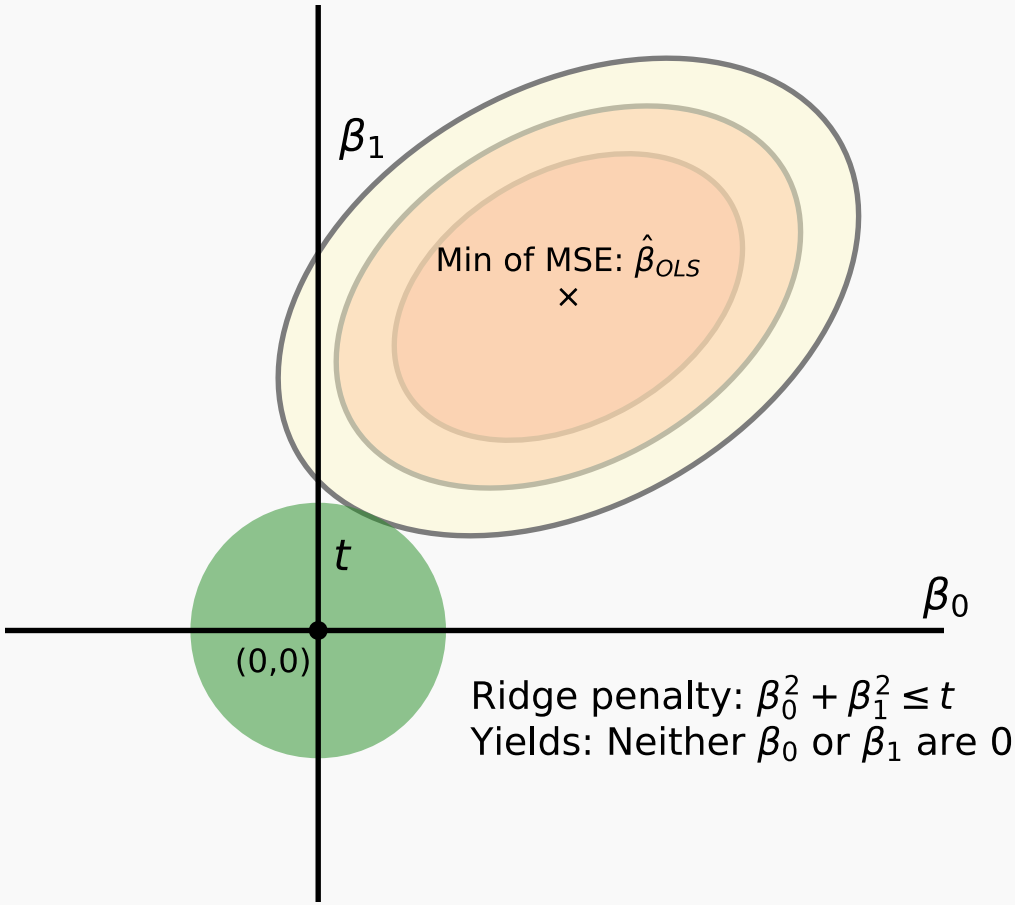
This penalty shrinks the coefficients towards zero and each other.

Illustration of Ridge penalty



The first contact between the ellipsoid and the circle is the solution of Ridge.

Illustration of Ridge penalty



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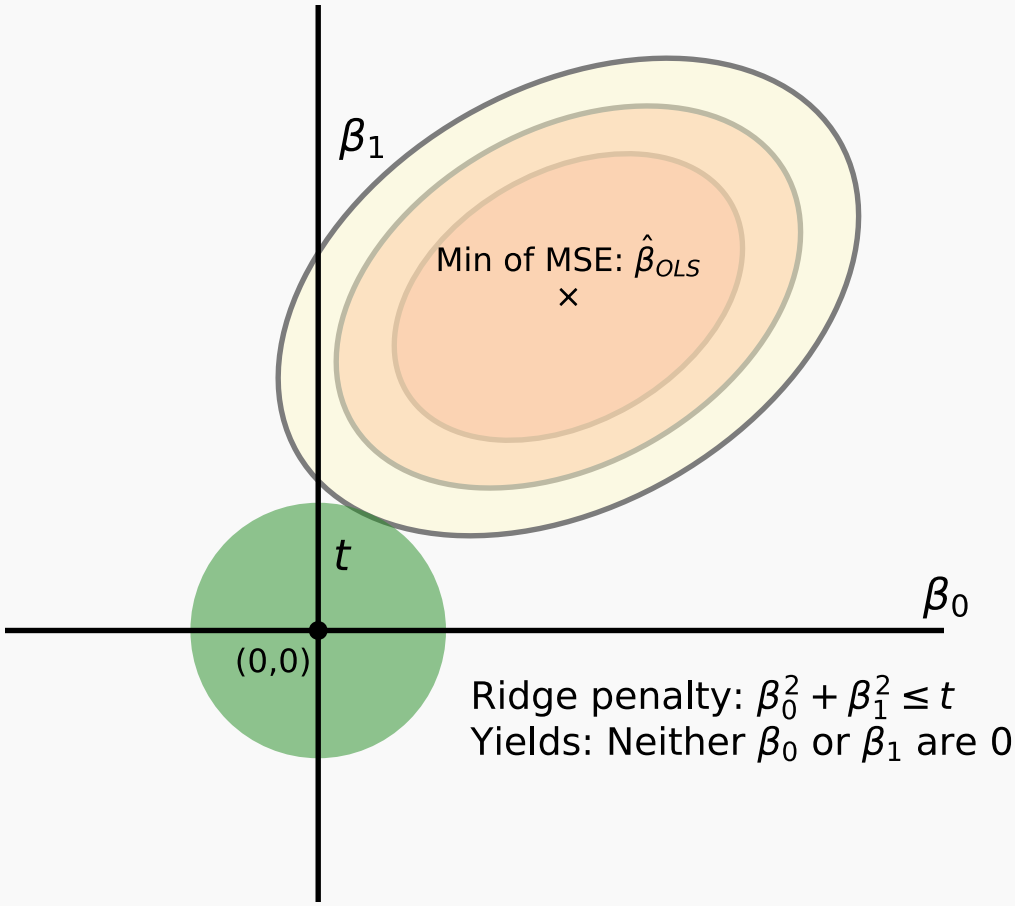

The first contact between the ellipsoid and the circle is the solution of Ridge.

Few chances than lasso to cross an axis.

Ridge insure smaller coefficients, but no exact zeros.

Importance of rescaling

Why rescale?

- The penalty term in the Lasso and Ridge is sensitive to the scale of the features.
- If the features are not on the same scale, the regularization will not be applied uniformly.
- The coefficients of the model will be biased towards the features with the largest scale.

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How to rescale?

- Gaussian hypothesis? Standard scaling: $X = \frac{X - \text{mean}(X)}{\text{std}(X)}$
- Non Gaussian? MinMax scaling: $X = \frac{X - \min(X)}{\max(X) - \min(X)}$

Log likelihood for Lasso classification

🔔 Log likelihood for vanilla logistic regression

$$p_{i,\beta} = \mathbb{P}[Y_i | X_i, \beta] = \frac{1}{1+\exp(-\beta^T X_i)}$$

$$L(\beta) = \frac{1}{N} \sum_{i=1}^{N} \log\left[p_{i,\beta}^{y_i} \left(1 - p_{i,\beta}\right)^{1-y_i}\right]$$

$$= \frac{1}{N} \sum_{i=1}^{N} [(y_i \beta^T X_i - \log[1 + \exp(\beta^T X_i)]$$

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Regularized linear models for classification

Log likelihood for Lasso classification

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How to choose lambda?

Theoretical garuantees

- See (Chernozhukov et al., 2024, Chap 3.2)

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- See (Chernozhukov et al., 2024, Chap 3.2) ⚠️ but assumptions are hard to check.

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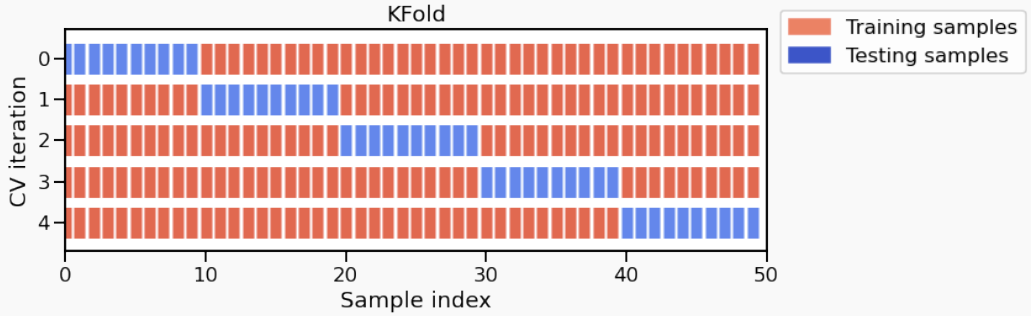
In practice

Use cross-validation: repeated train/test splits.



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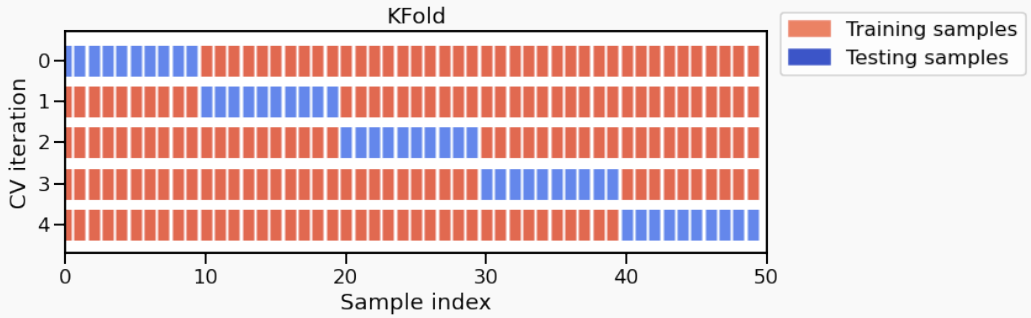
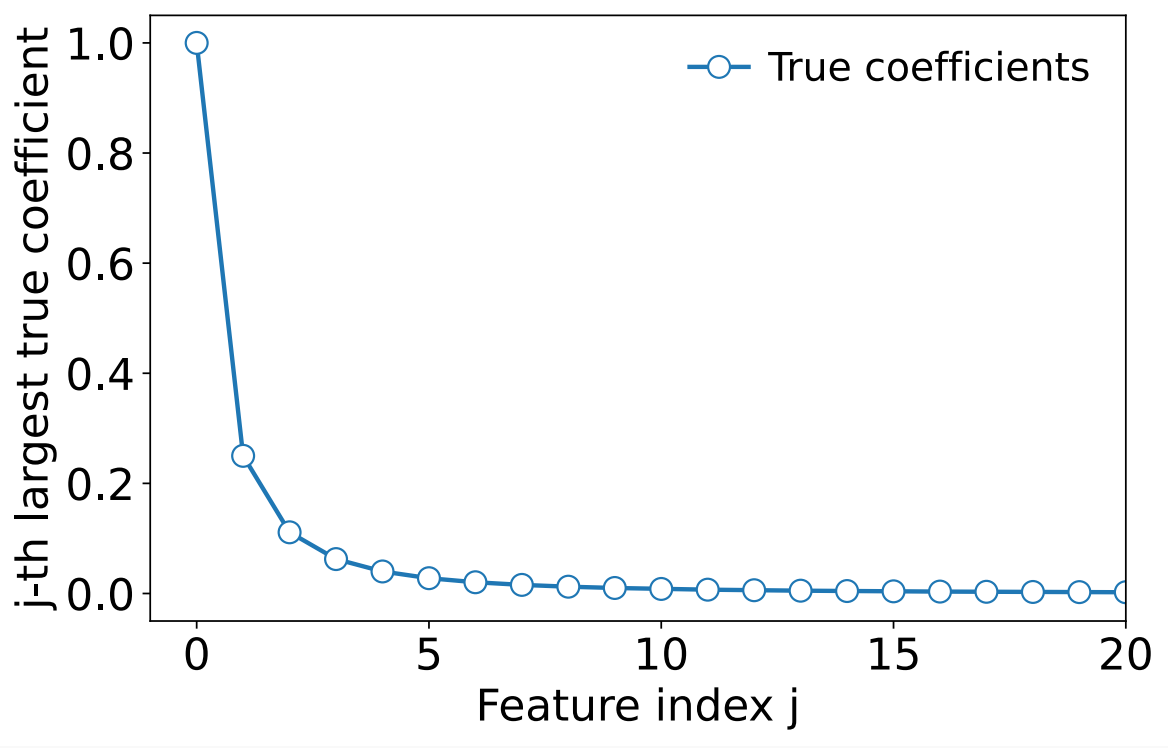


We will look into that in more details in the next session.

OLS Post-Lasso: fixing excessive shrunkage of coefficients



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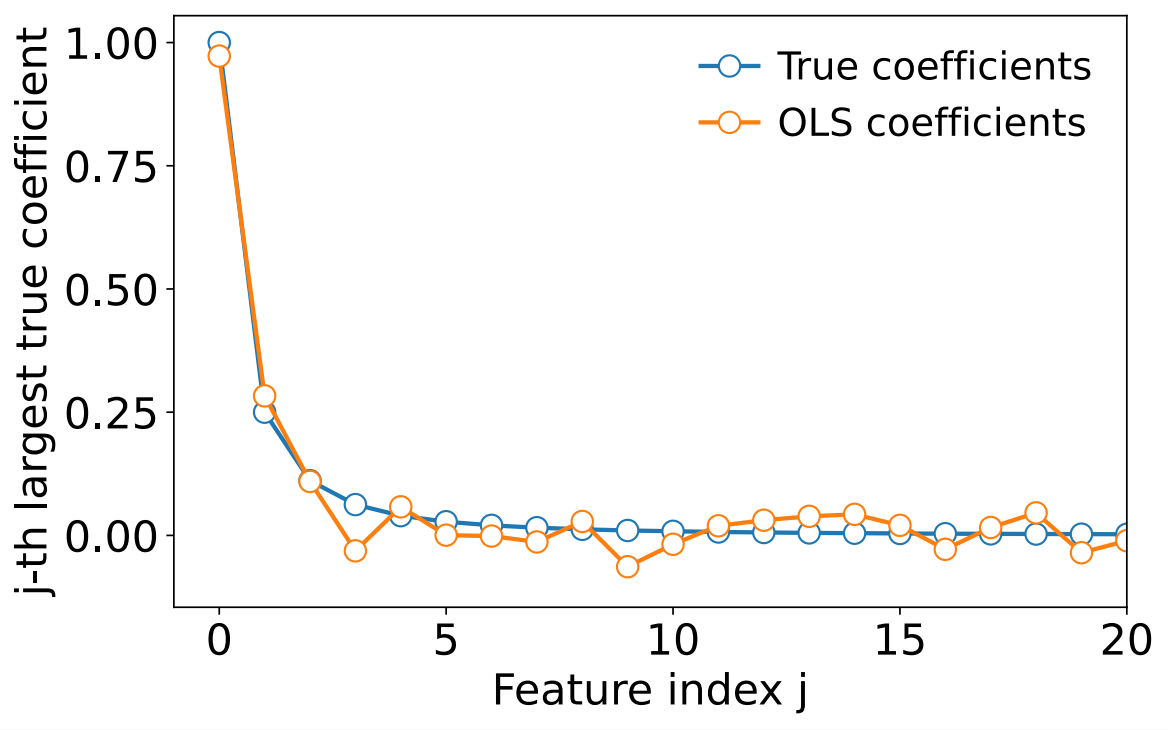

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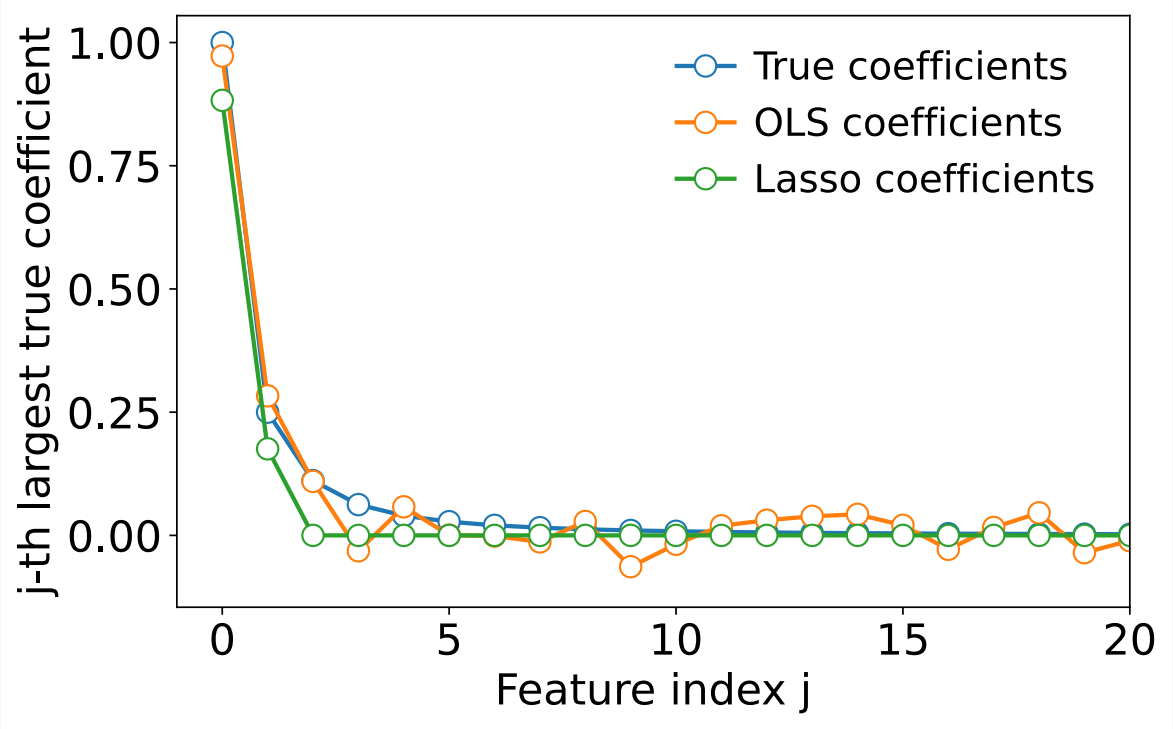

Lasso is good for true zero coefficients (on the right)

But not so good for true non-zeros coefficients (on the left)

OLS Post-Lasso

- 💡 Fit an OLS on the features selected by the Lasso (Belloni & Chernozhukov, 2013)

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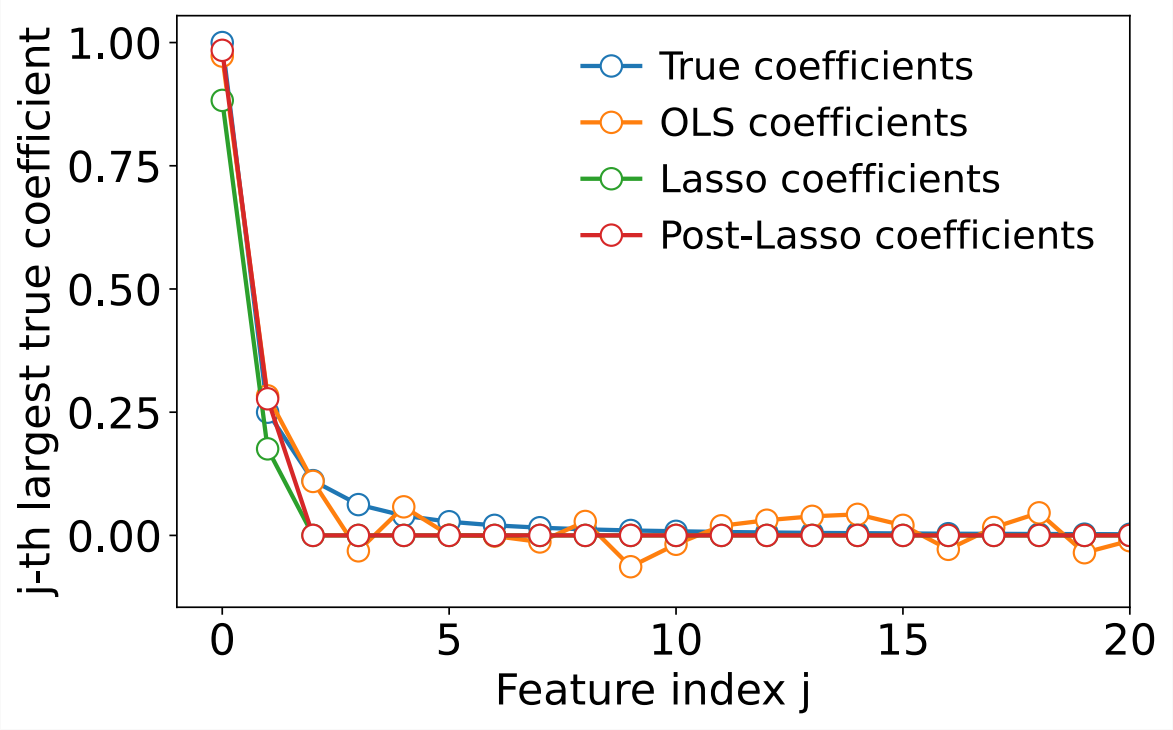

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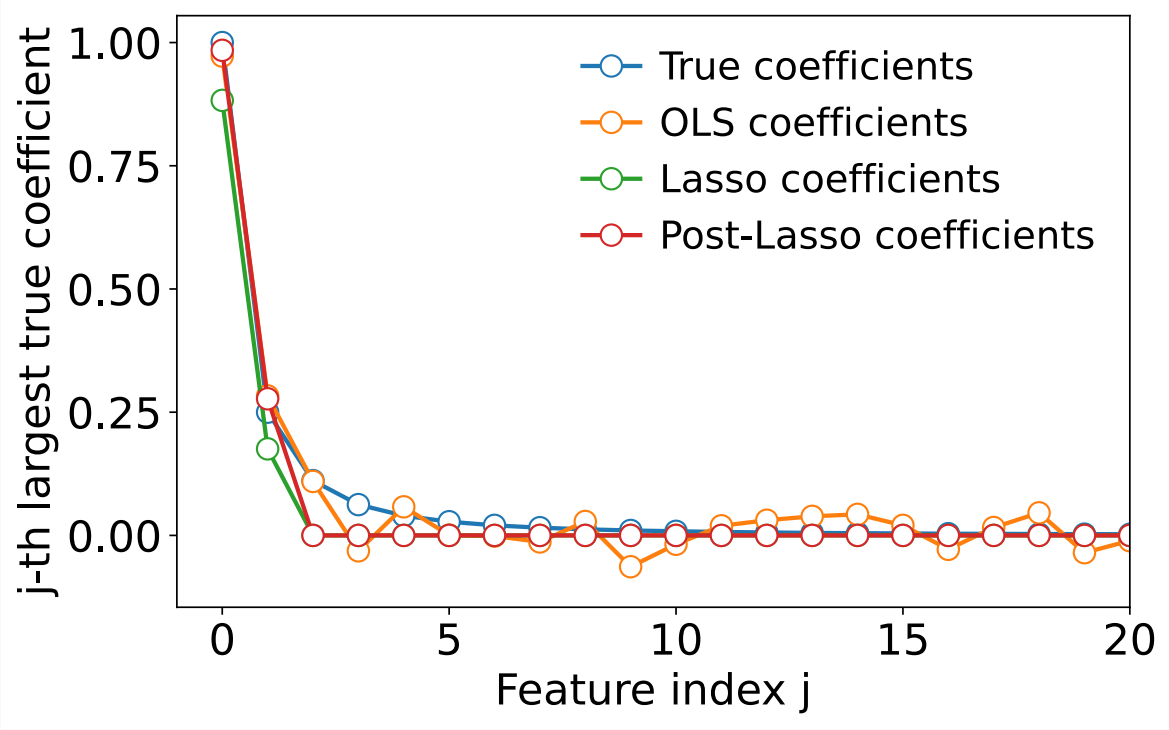

⚠️ Cross-validation should apply to the full procedure: Lasso + OLS, not only to the Lasso.

Take home messages: Bias-variance trade-off

High bias = underfitting

- systematic prediction errors
- the model prefers to ignore some aspects of the data
- mispecified models

High variance = overfitting

- prediction errors without obvious structure
- small change in the training set, large change in model
- unstable models

Take home messages: Lasso and Ridge

Lasso

- L1 penalty: sparsity
- Feature selection
- Unstable for correlated features

Ridge

- L2 penalty: shrinkage
- No feature selection
- Stable for correlated features

Short introduction to scikit-learn

- url: https://straymat.github.io/causal-ml-course/practical_sessions.html

Python hands-on: Common pitfalls in the interpretation of coefficients of linear models

To your notebooks 🧑‍💻 !

- url: https://straymat.github.io/causal-ml-course/practical_sessions.html

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Supplementary materials

Statistical model for lasso: approximate sparsity

Definition: Approximate sparsity

The sorted absolute values of the coefficients decay quickly.

$$|\beta|_{(j)} < Aj^{-a} \qquad a > \tfrac{1}{2}$$

for each j, where the constants a and A do not depend on the sample size n.