

Machine Learning for econometrics

Statistical learning and regularized linear models

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

Today's program

- Last session: importance of causal variable status
- Today: **predictive inference** in high dimensions
 - ▶ Statistical learning basics
 - ▶ Regularized linear models for predictive inference
 - ▶ Hands-on with scikit-learn
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Today's program

- Last session: importance of causal variable status
- Today: **predictive inference** in high dimensions
 - Statistical learning basics
 - Regularized linear models for predictive inference
 - Hands-on with scikit-learn
- Next session:
 - Flexible models: Trees, Random Forests, Gradient Boosting
 - Practical scikit-learn

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

Statistical learning framework

Statistical learning, ie. predictive inference

Goal

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

Setting

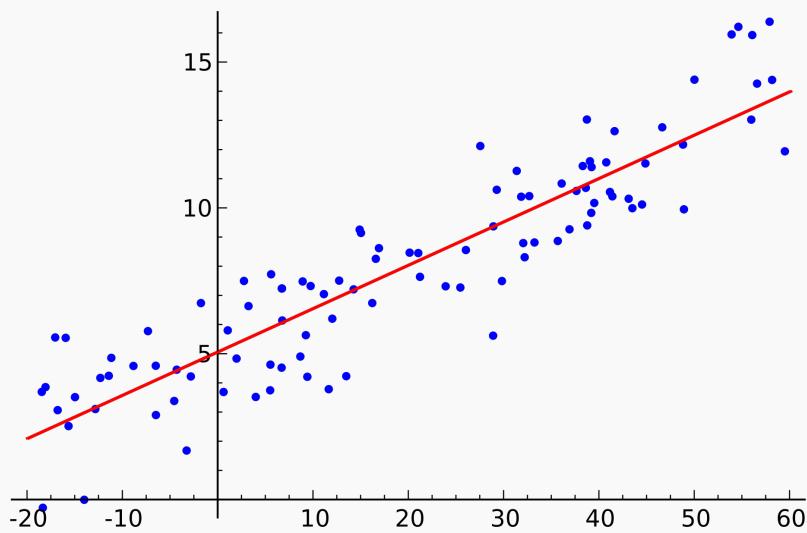
- Data: n pairs of (features, outcome), $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ identically and independently distributed (i.i.d.) from an unknown distribution P .
- Goal: find a function $\hat{f} : \mathcal{X} \rightarrow \mathcal{Y}$ that approximates the true value of y ie. for a new pair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

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

Vocabulary

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

Statistical learning, two classes of problems

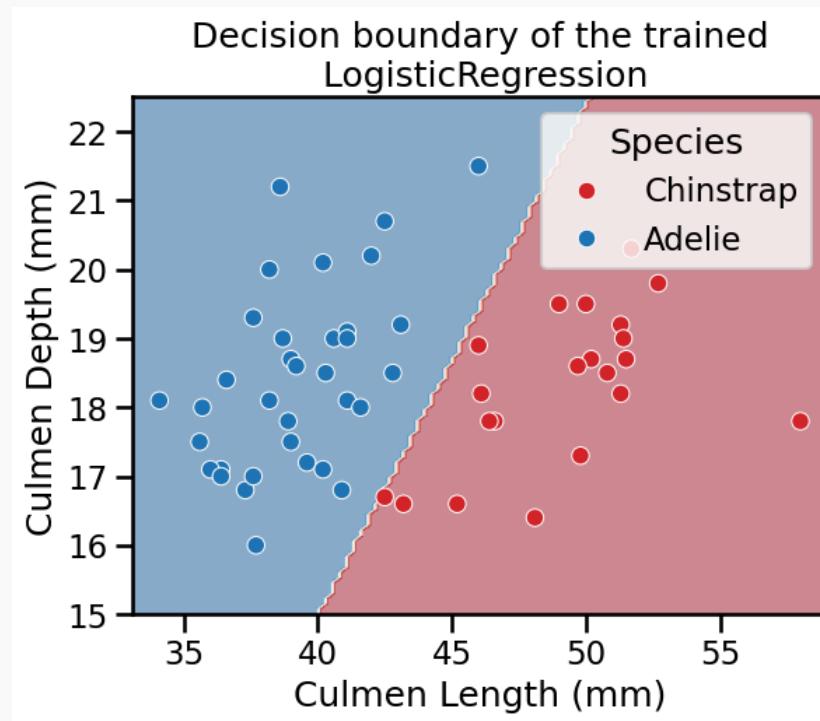


Regression

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

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

Statistical learning, two classes of problems



Classification

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

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

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

Motivation: why prediction?

Why do we need prediction for ?

Statistical inference

- Goal: infer some intervention effect with a causal interpretation
- Require to regress “away” the relationship between the treatment or the outcome and the confounders -> more on this in sessions on Double machine learning.

Predictive inference

- Some problems in economics requires accurate prediction without a causal interpretation (Kleinberg et al., 2015)
- Eg. Stratifying on a risk score (loan, preventive care, ...)

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

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?

Characteristics of the dataset that can lead 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 referencement dataset, individual file (INSEE): $n=19\ 735\ 576$; $p=88$ 🤝
- 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 examples from area with high dimensional data

Some examples

- The 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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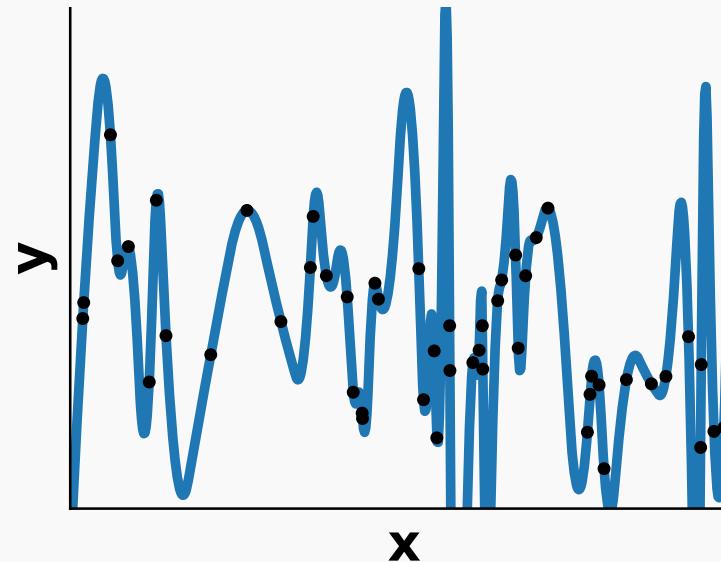
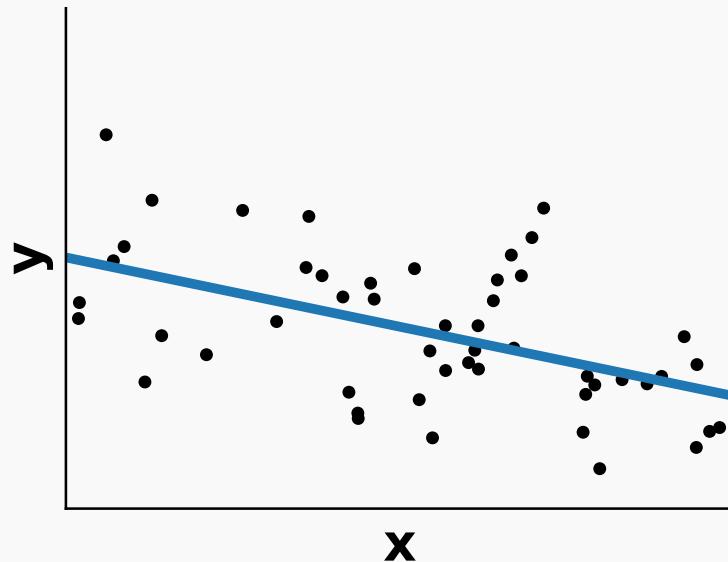
Other area

- 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 intu- tions

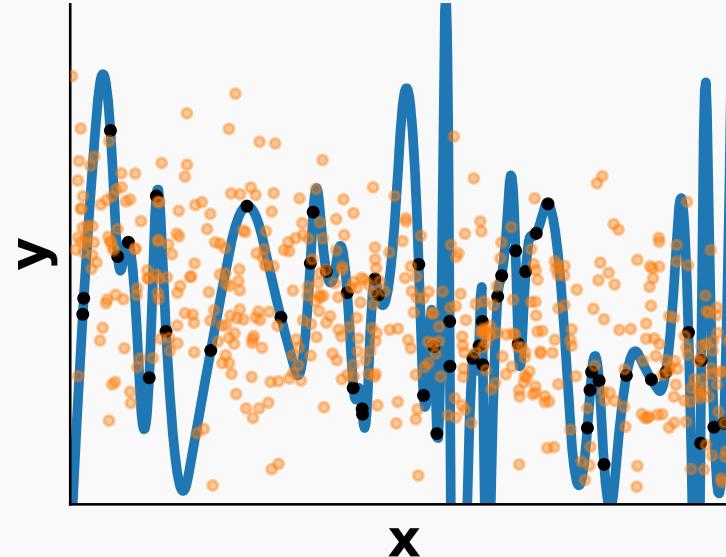
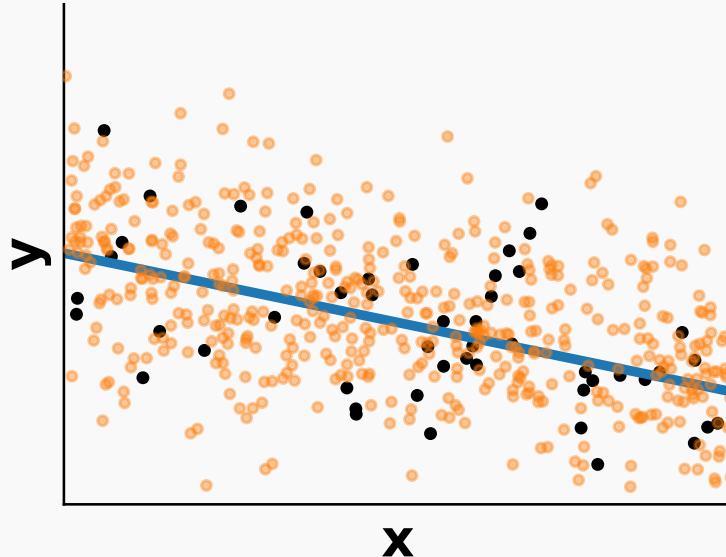
Under vs. overfitting

Which data fit do you prefer?



Under vs. overfitting

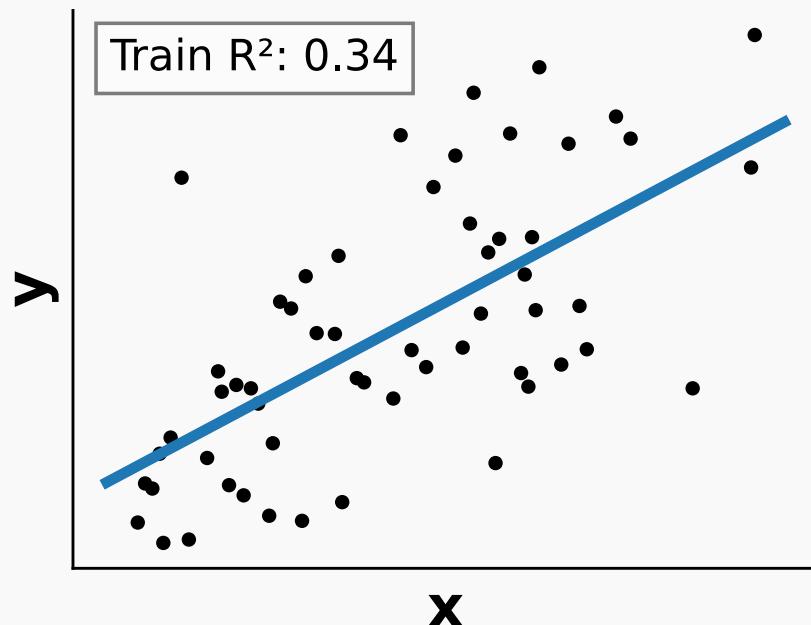
Which data fit do you prefer? (new data incoming)



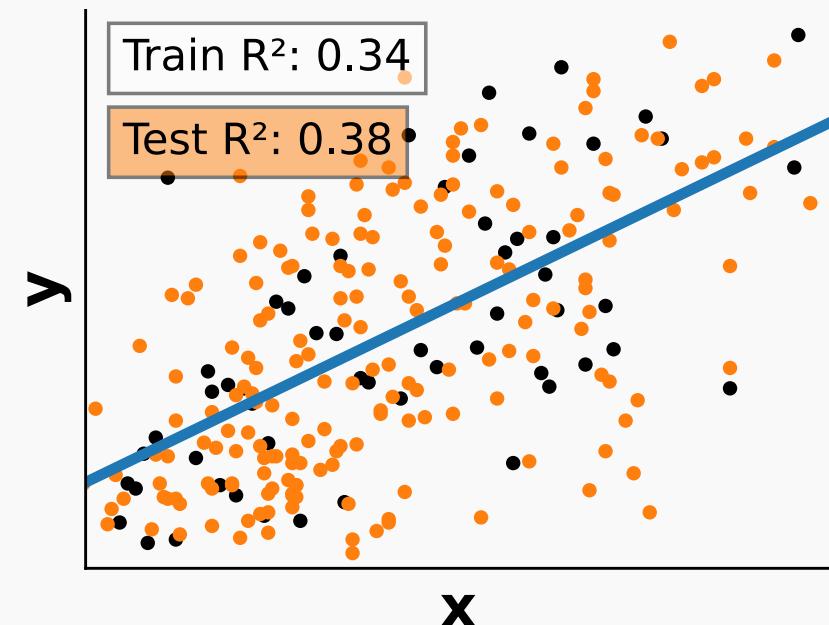
- Answering this question might be hard.
- Goal: create models that generalize.
- The good way of framing the question is: **how will the model perform on new data?**

Train vs test error: simple models

Measure the errors on the training data
= fitting



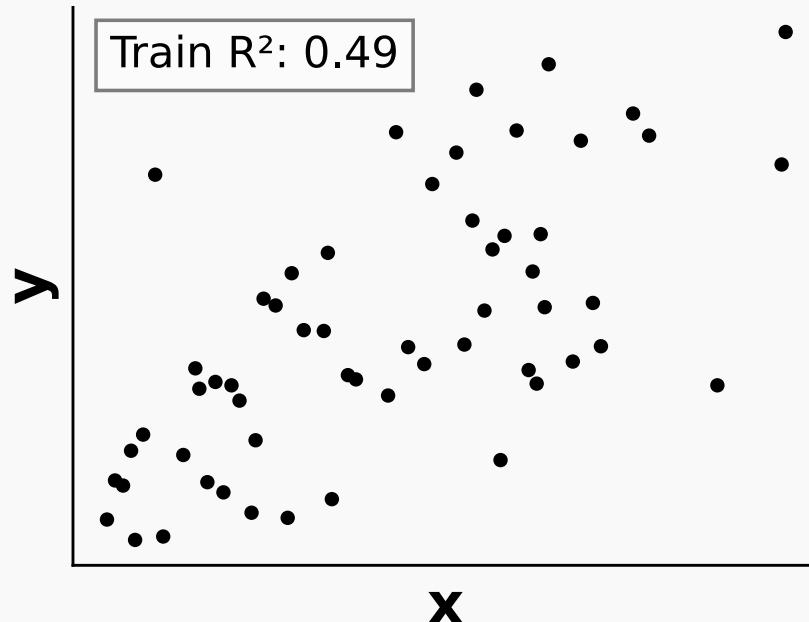
Measure the performances on test data
= generalization



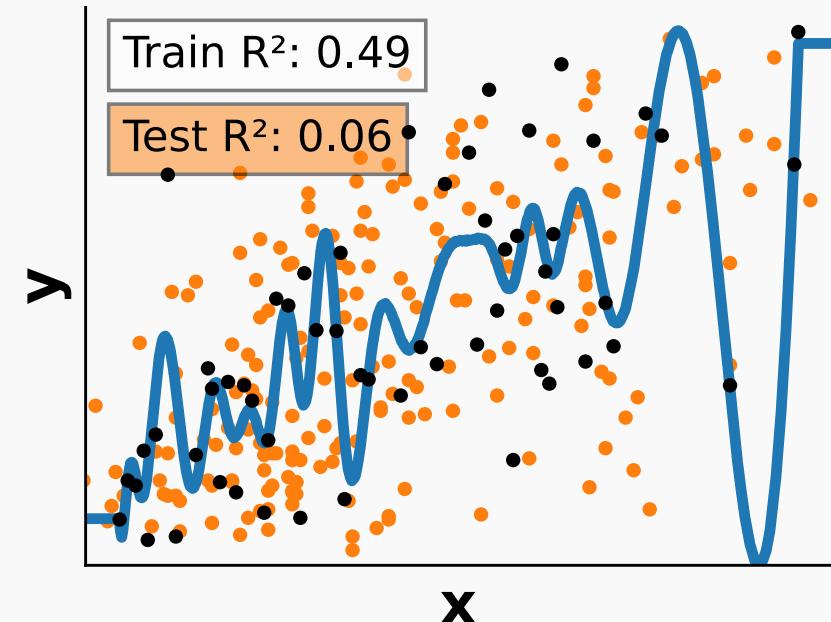
Here, no problem of overfitting: train vs test error are similar.

Train vs test error: flexible models

Measure the errors on the training data
= fitting

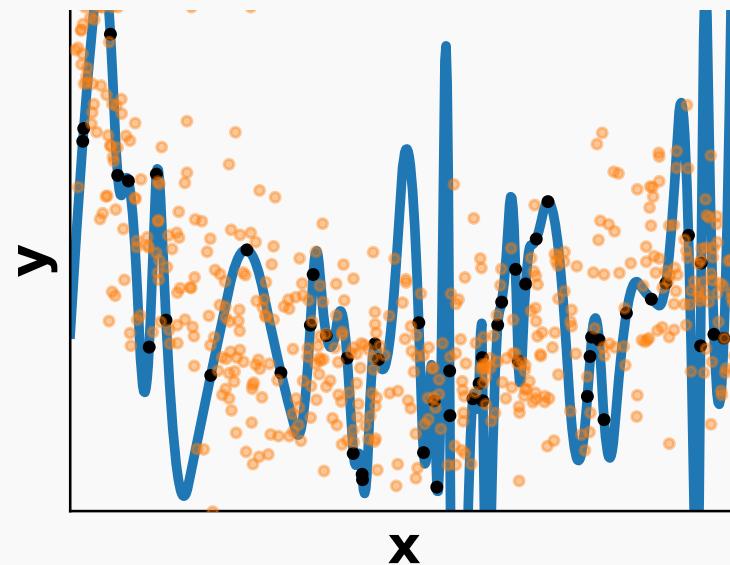
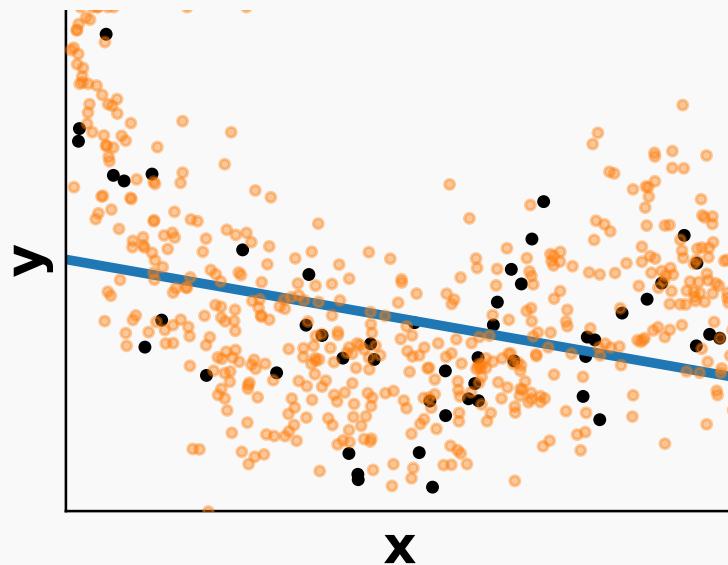


Measure the performances on test data
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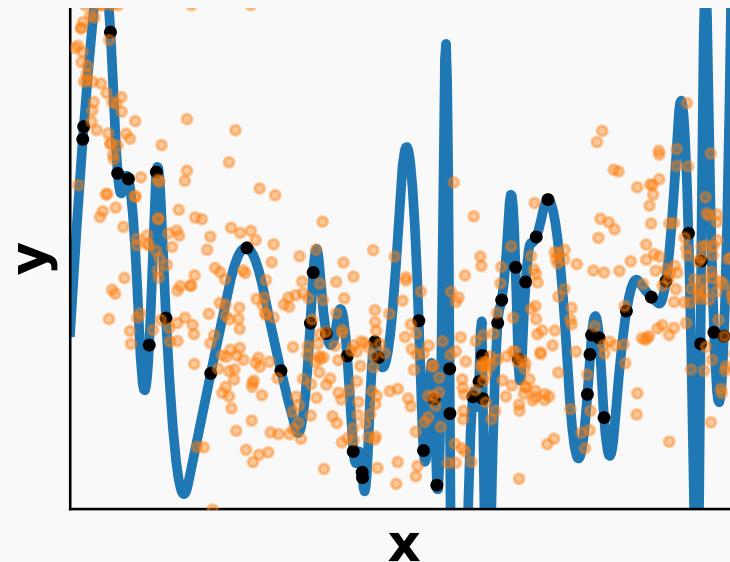
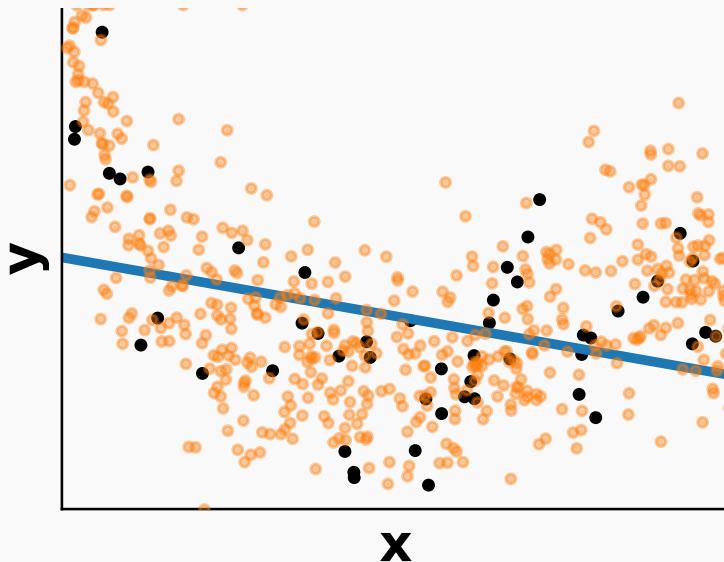


Overfitting: the model is too complex and captures noise.

How to choose the complexity of the model?



How to choose the complexity of the model?



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

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

Empirical Risk Minimization

- Define a loss function ℓ that defines proximity between the predicted value $\hat{y} = f(x)$ and the true value y : $\ell(f(x), y)$
- Usually, for continuous outcomes, the squared loss is used: $\ell(f(x), y) = (f(x) - y)^2$
- We choose among a (finite) family of functions $f \in \mathcal{F}$, the best possible function f^* minimizes the **risk or expected loss** $\mathcal{E}(f) = \mathbb{E}[(f(x) - y)^2]$:

$$f^* = \operatorname{argmin}_{f \in \mathcal{F}} \mathbb{E}[(f(x) - y)^2]$$

Empirical risk minimization: estimation error

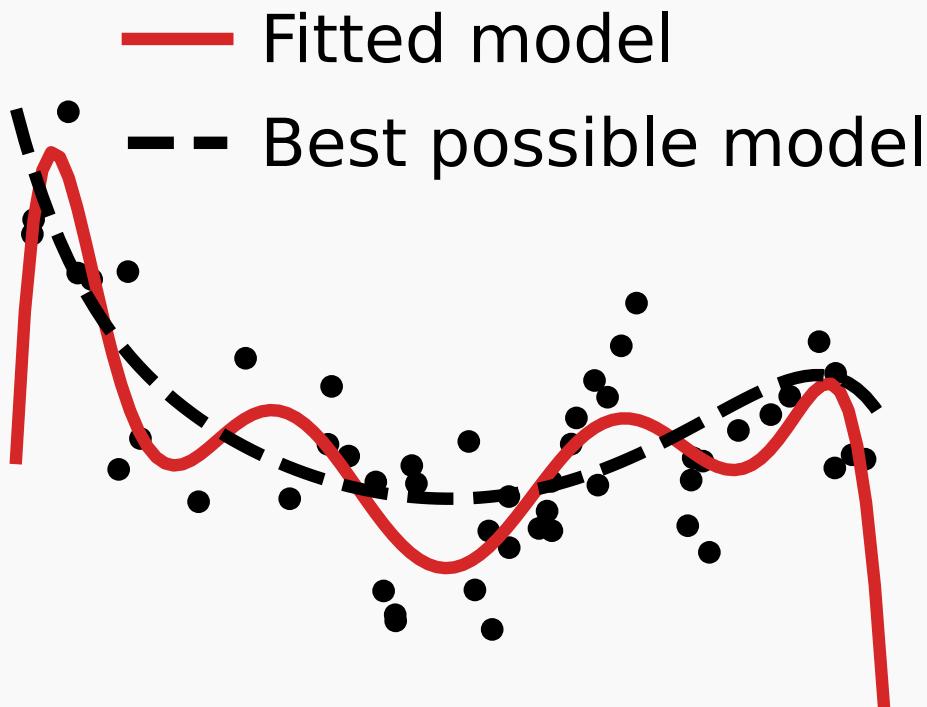
- In finite sample regimes, the expectation is not accessible since we only have access to a finite number of data pairs
- In practice, we minimize the **empirical risk** or average loss $R_{\text{emp}} = \sum_{i=1}^n (f(x_i) - y_i)^2$:

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

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

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

High **estimation error** means overfit



Model is too complex

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

Too much noise

Not enough data

Bayes error rate: Randomness of the problem

- Interesting problems exhibit randomness

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

- The best possible estimator is $g(\cdot)$, yielding the Bayes error, the unavoidable error:

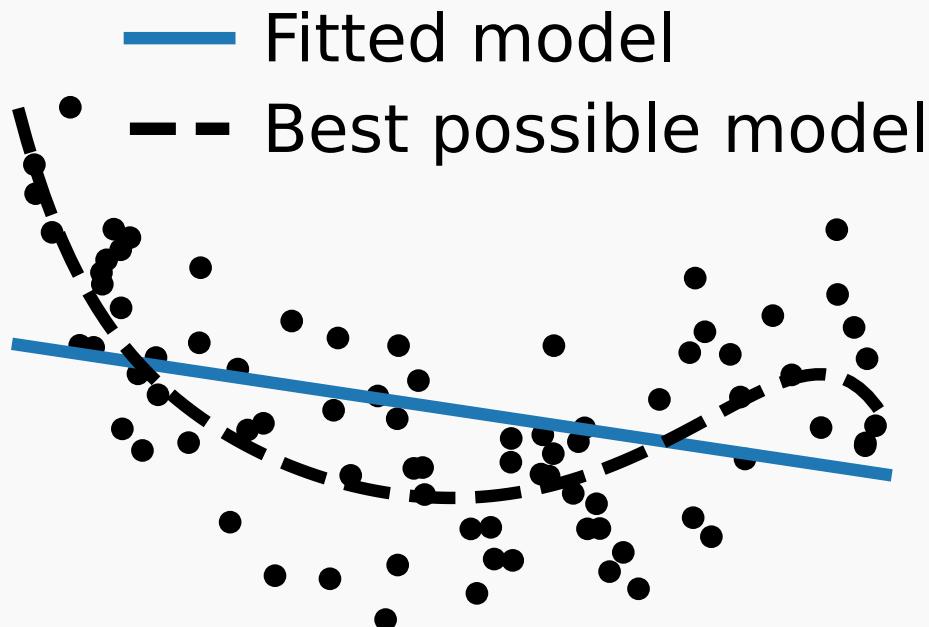
$$\mathcal{E}(g) = \mathbb{E}[(g(x) + e - g(x))^2] = \mathbb{E}[e^2]$$

Empirical risk minimization: approximation error

- In practice you don't know the class of function in which the true function lies : $y \approx g(x)$: Every model is wrong !
- You are choosing the best possible function in the class of functions you have access to: $f^* \in \mathcal{F}$ eg. linear models, polynomials, trees, ...
- This creates the **approximation error**:

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

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}

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

Bias variance trade-off: Putting the pieces together

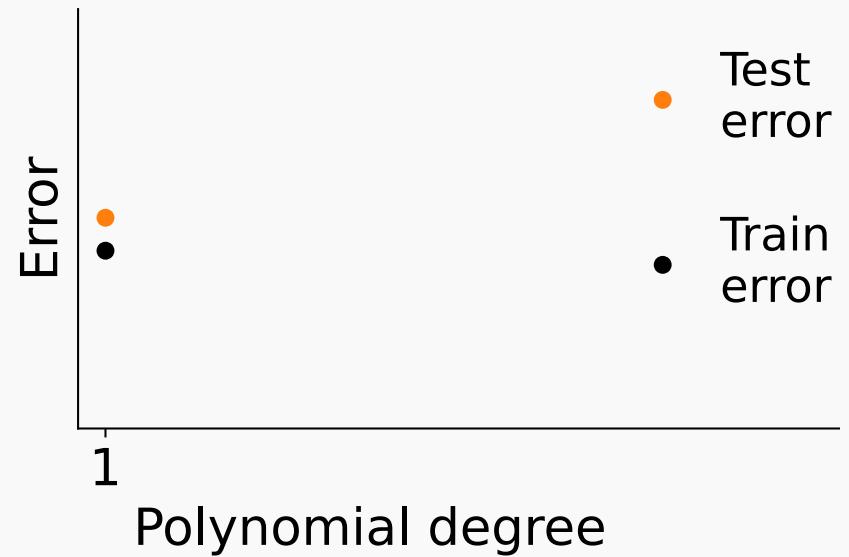
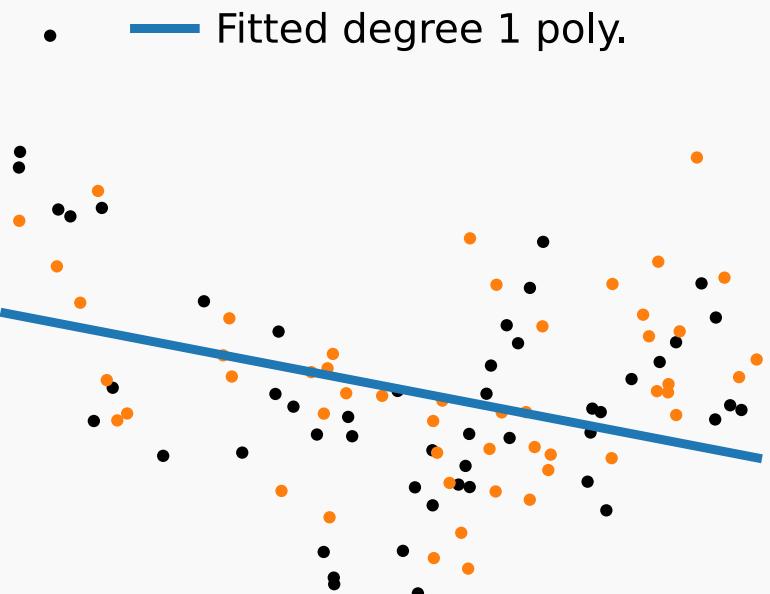
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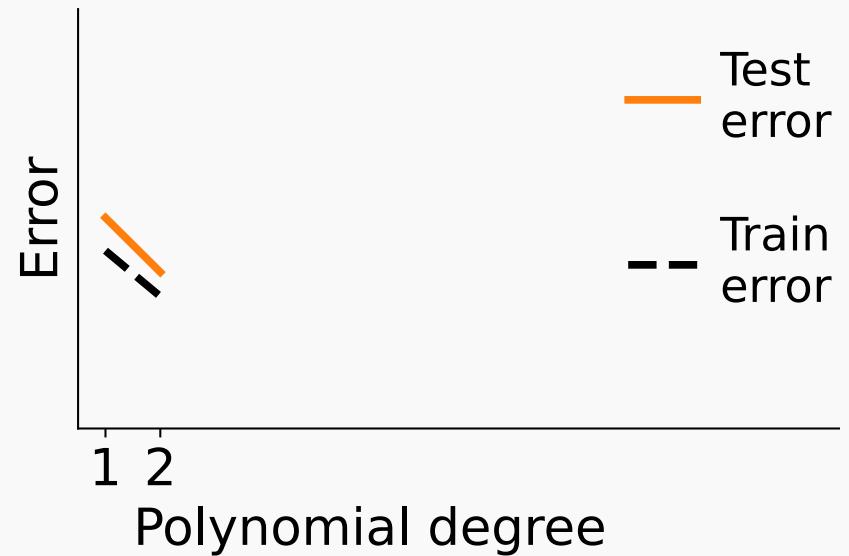
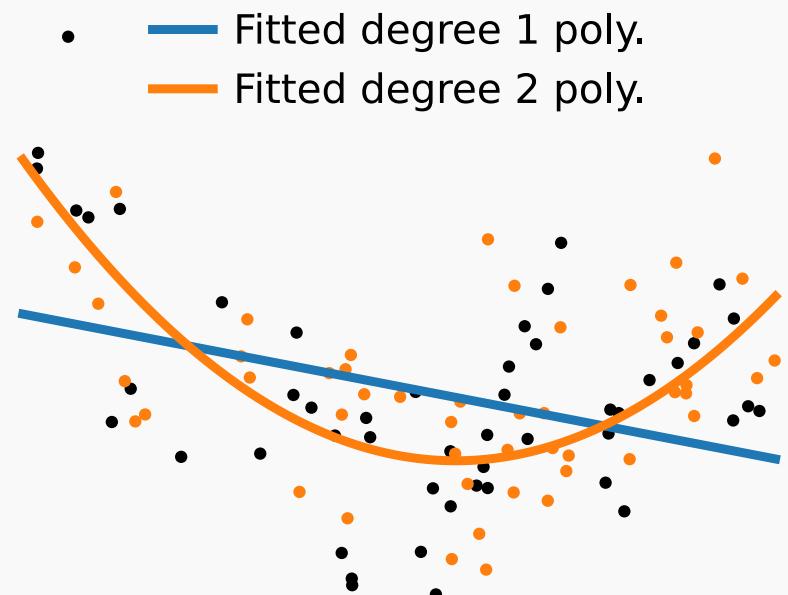
Controls on this trade-off

- Increase/decrease the size of the hypothesis family : \mathcal{F} ie. more or less complex models.
- Increase your sample size: n ie. more observations.

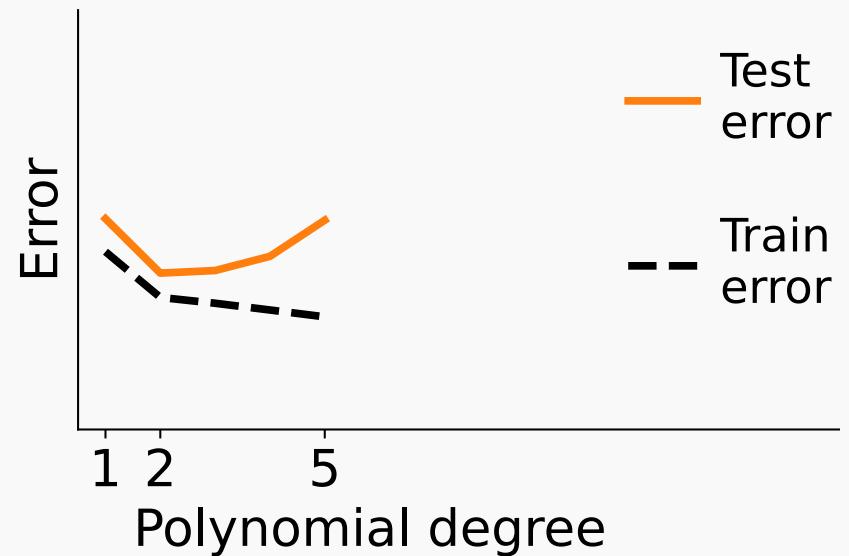
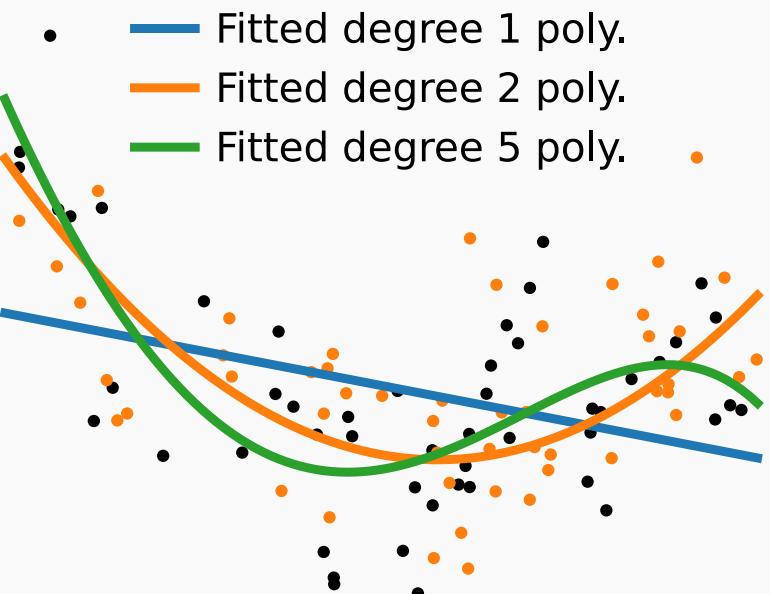
Train vs test error: increasing complexity



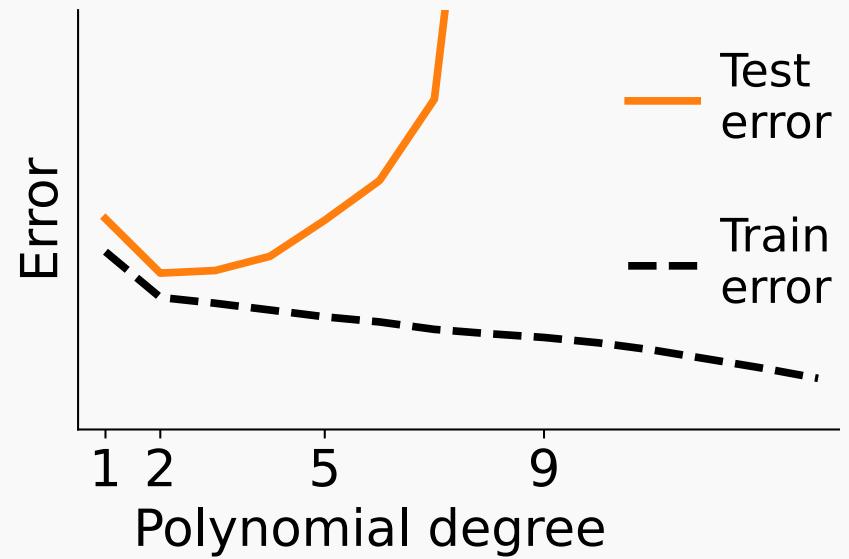
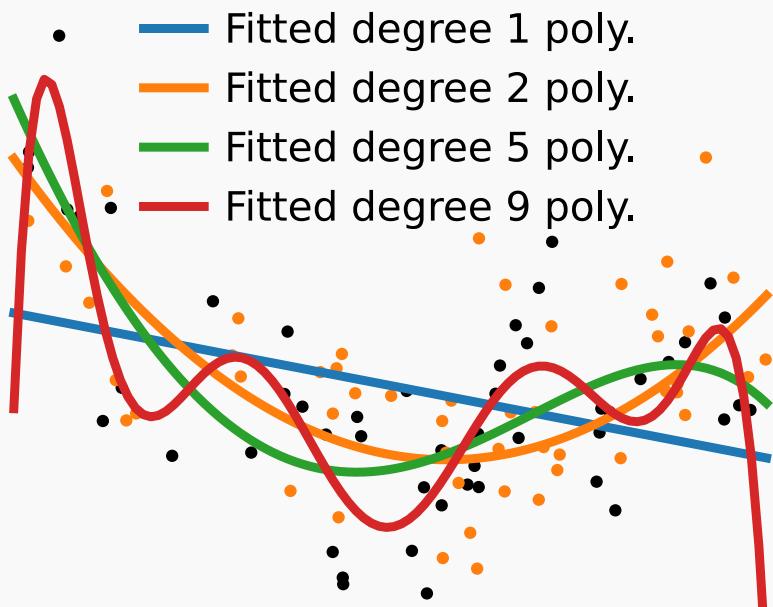
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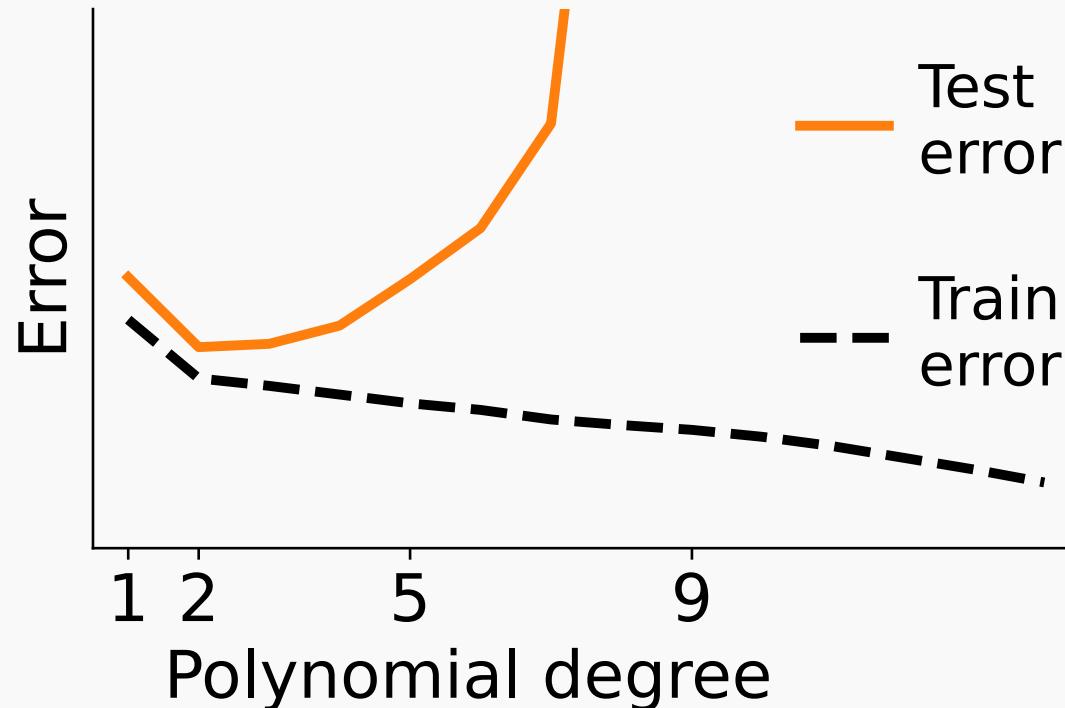
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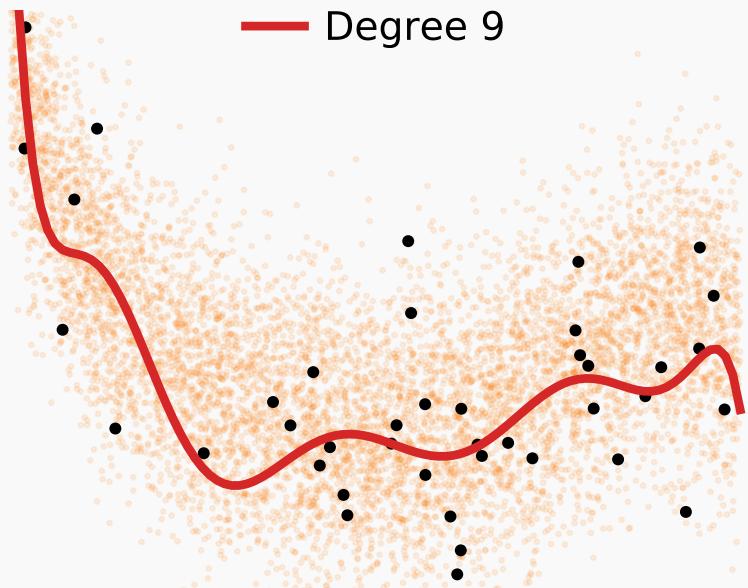


Train vs test error: increasing complexity

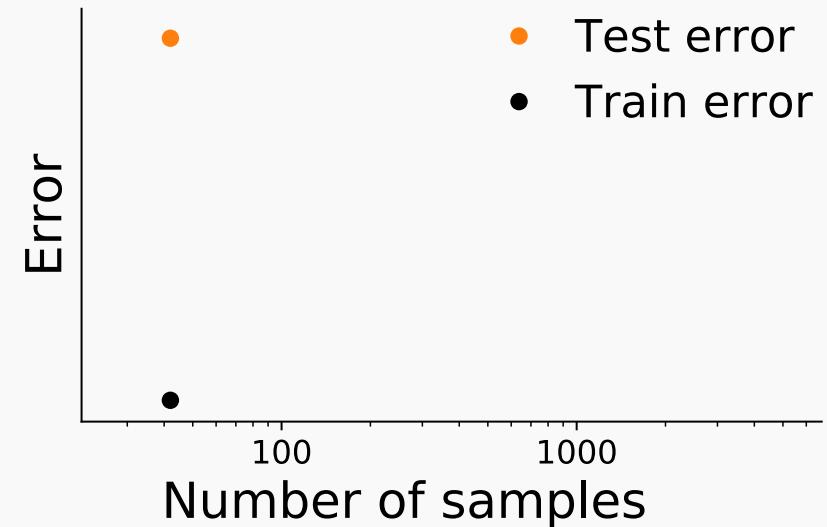


Underfit Sweet Spot Overfit

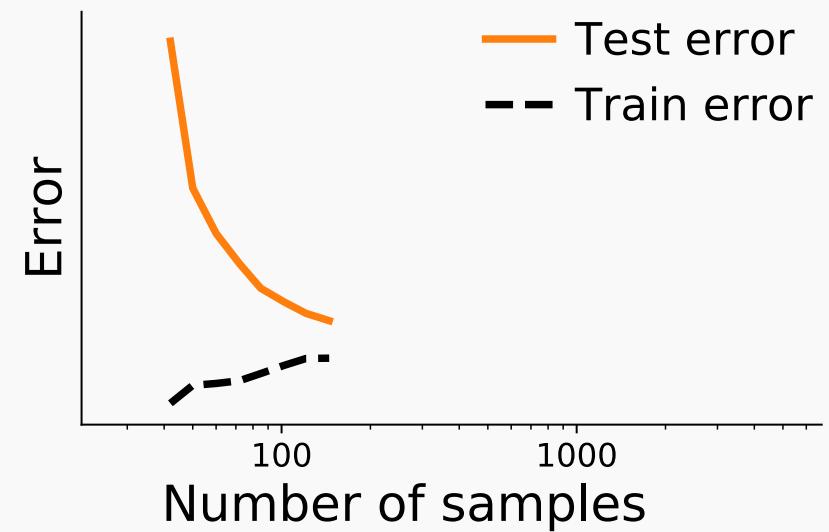
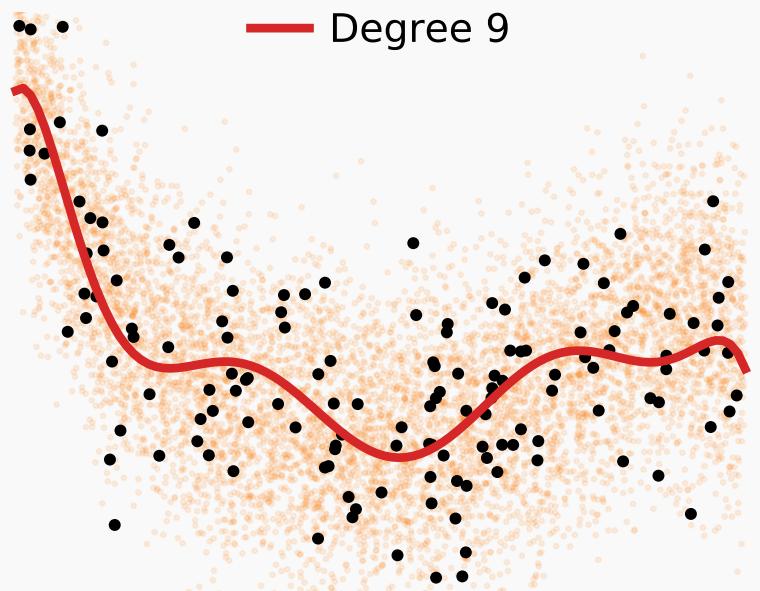
Varying sample size



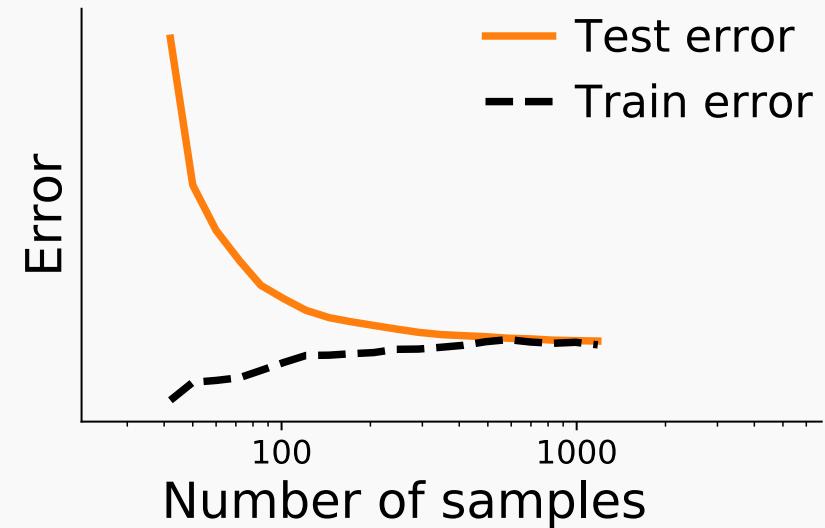
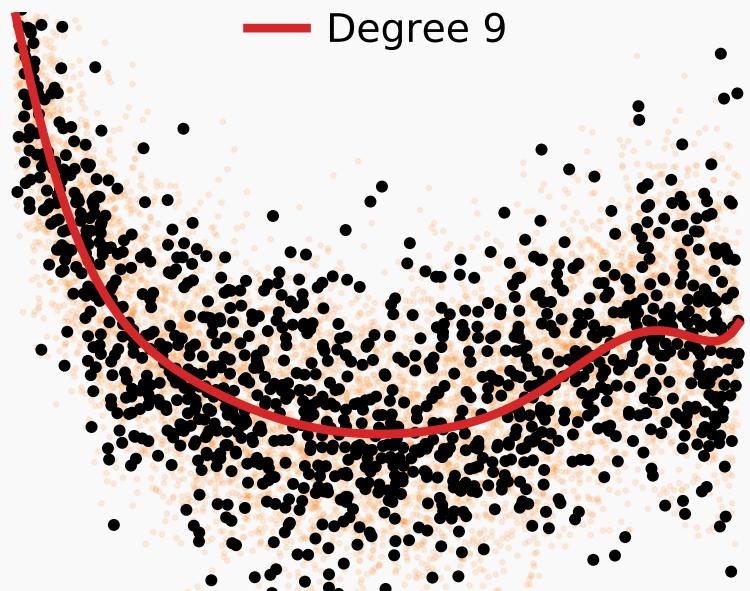
Overfit



Varying sample size

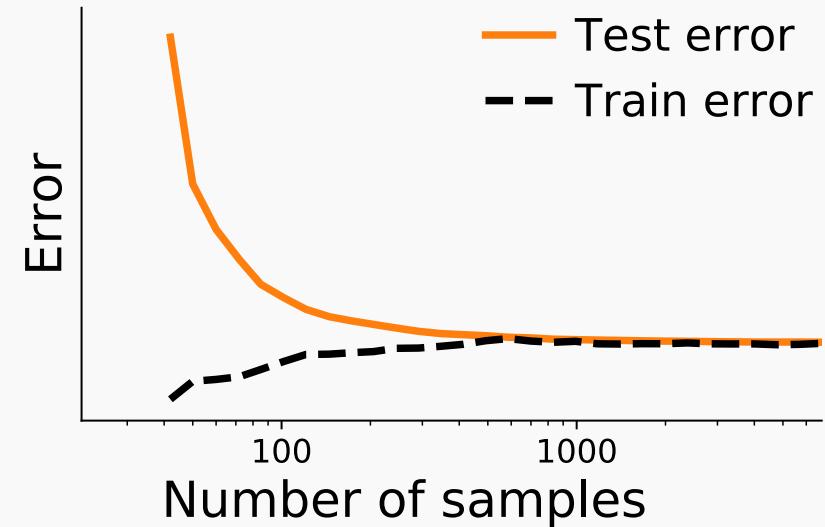
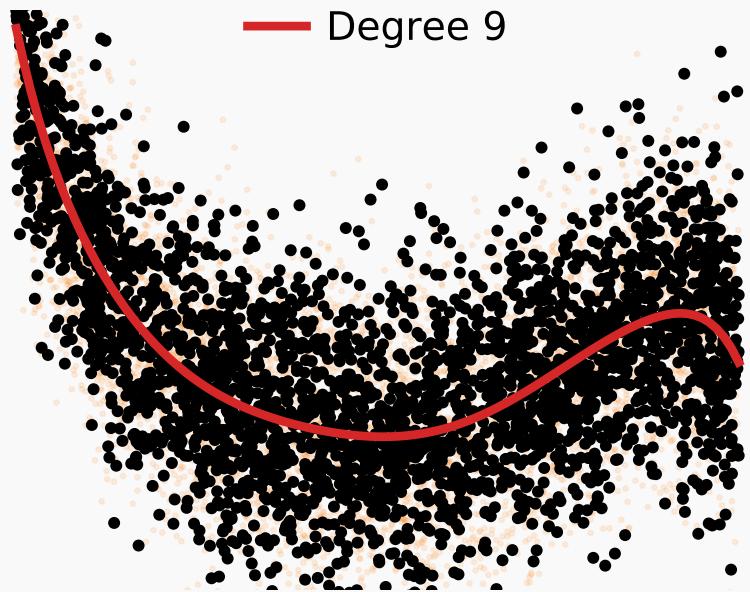


Varying sample size



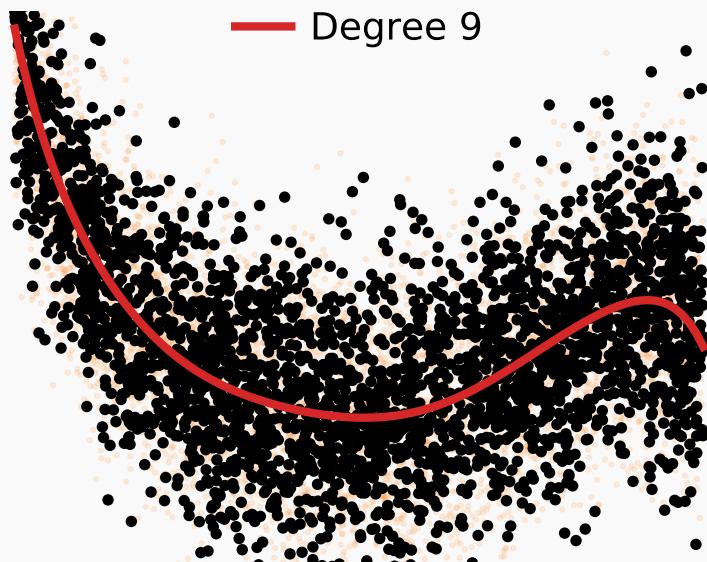
Sweet spot?

Varying sample size



Diminishing returns?

Varying sample size



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.

Remaining of this session (and the next)

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 variable of the error term.
- $\beta_0 \in \mathbb{R}^{p \times 1}$ the *true* coefficients.

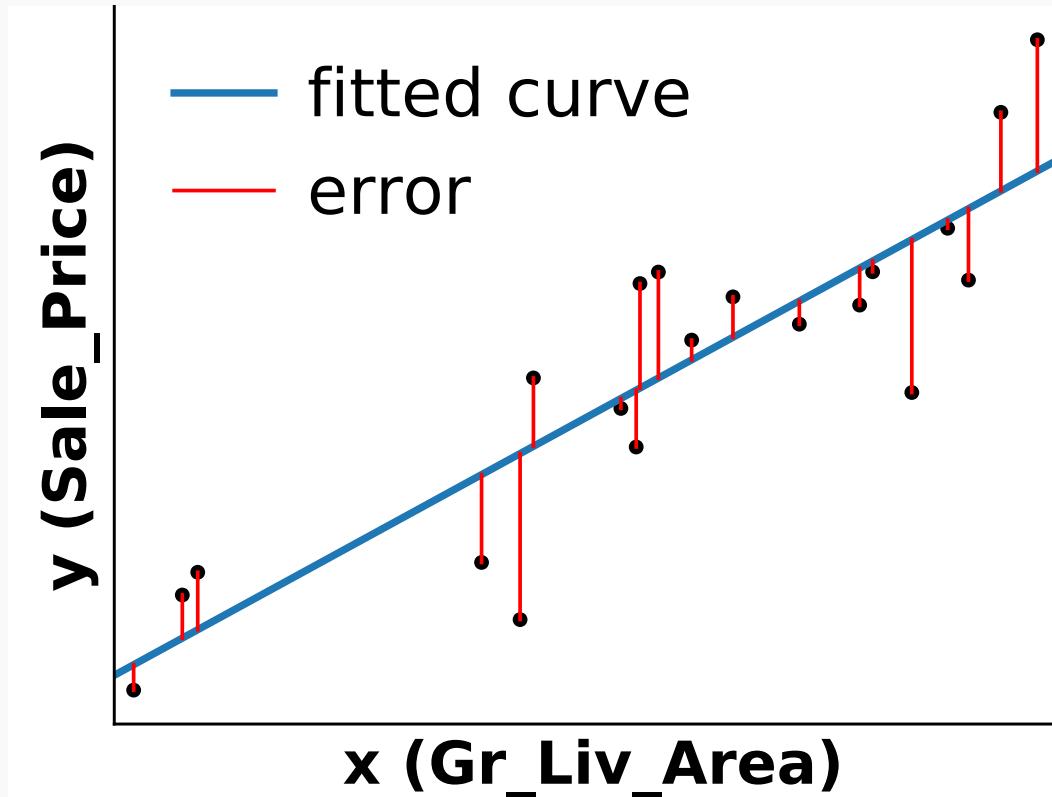
Usually, we assume that the errors are normally distributed and independent of X_i :

$$\varepsilon_i \sim \mathcal{N}(0, \sigma^2) \text{ and } \varepsilon_i \perp\!\!\!\perp X_i$$

Model are typically fitted by linear algebra methods (Hastie, 2009).

Reminder: Linear regression

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



Reminder: Linear regression

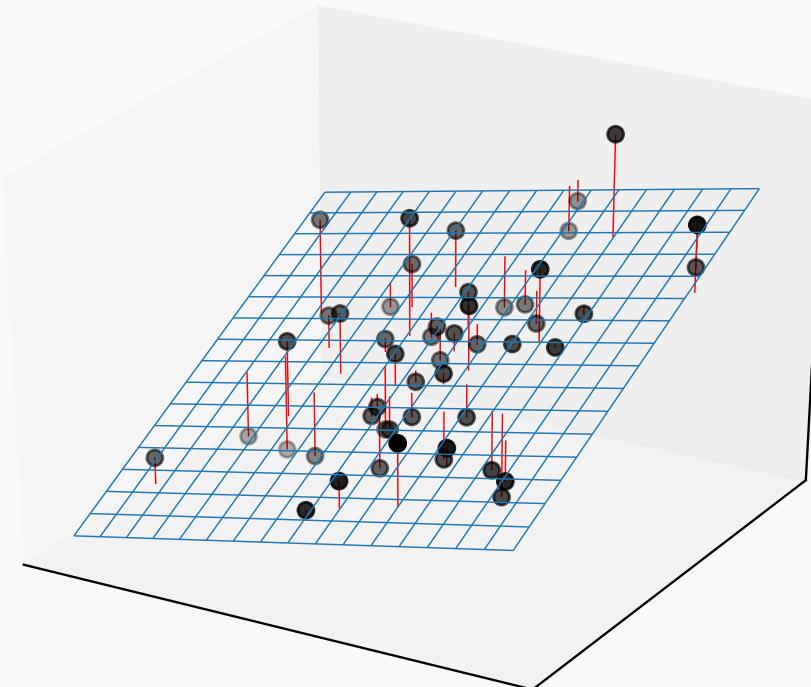
Common metrics

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

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

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

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 $X_i \in \mathbb{R}^p$:

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

Reminder: logistic regression for classification

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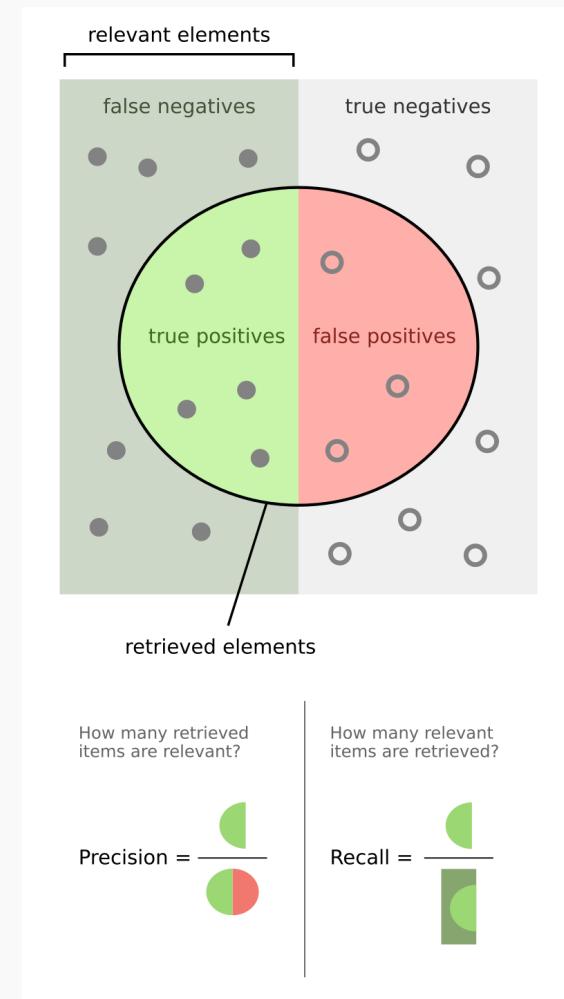
The statistical model is a Bernoulli  : $B(p(x, \beta_0))$

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

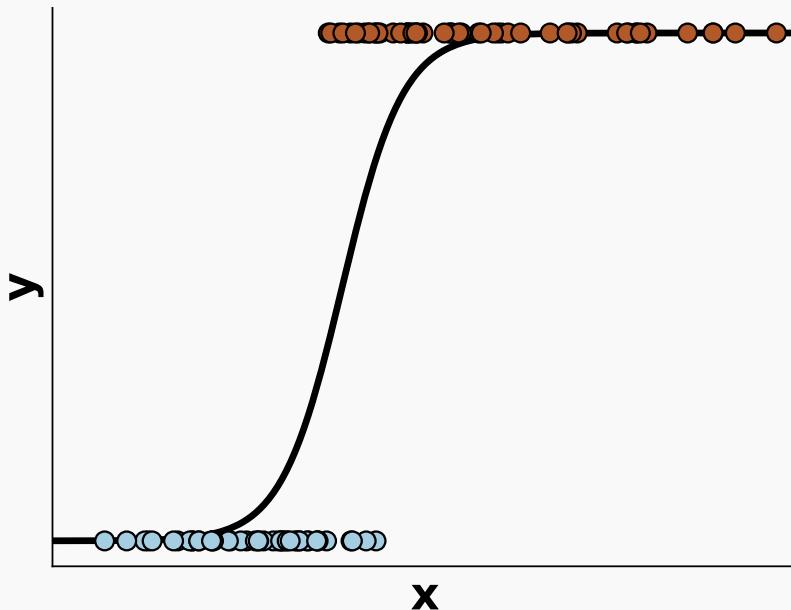
Reminder: classification, logistic regression

Common metrics

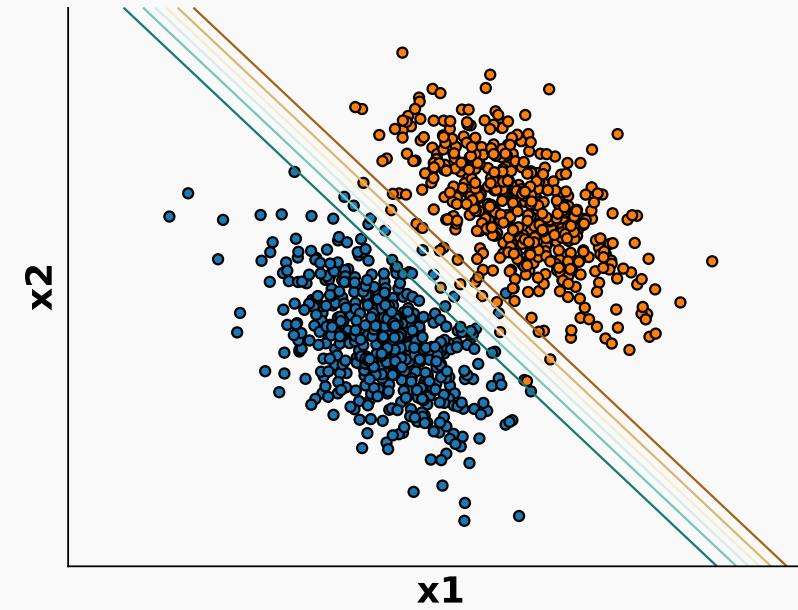
- Accuracy = $\frac{1}{n} \sum_{i=1}^n \mathbb{1}(Y_i = \hat{Y}_i)$
- Precision: Precision = $\frac{\text{TP}}{\text{TP} + \text{FP}}$
- Recall: Recall = $\frac{\text{TP}}{\text{TP} + \text{FN}}$
- Brier score loss: BSL = $\frac{1}{n} \sum_{i=1}^n (Y_i - p_i)^2$



Logistic regression: Illustrations

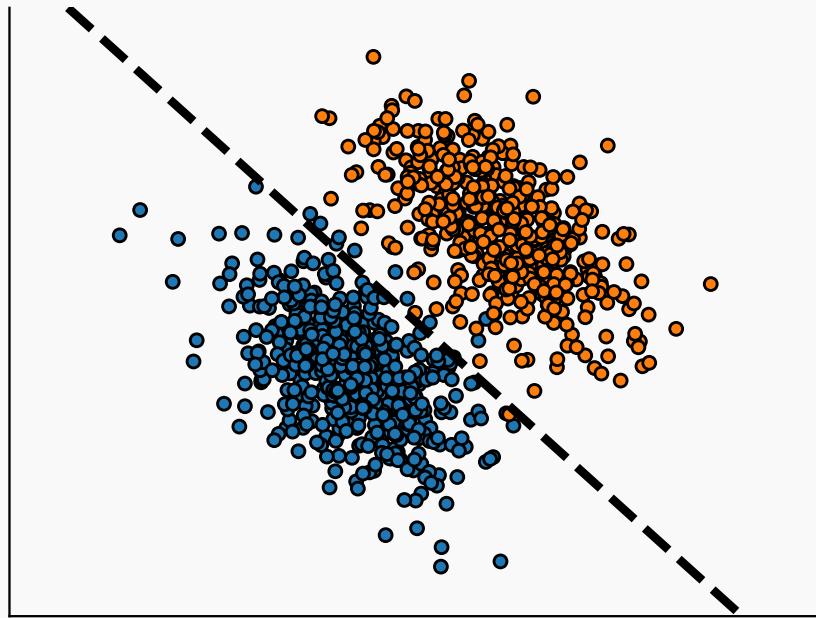


Logistic regression in one dimension.

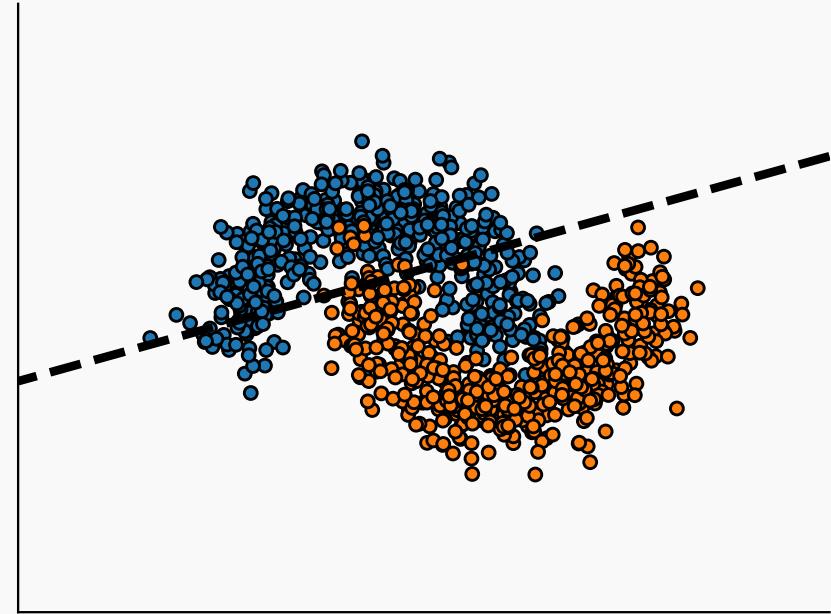


Logistic regression in two dimensions.

Linear models are not suited to all data



Almost linearly separable data.



Data not linearly separable.

Linear model pros and cons

Pros

- Converge quickly
- Hard to beat when n_{features} is large but we still have $n_{\text{samples}} \gg n_{\text{features}}$
- 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

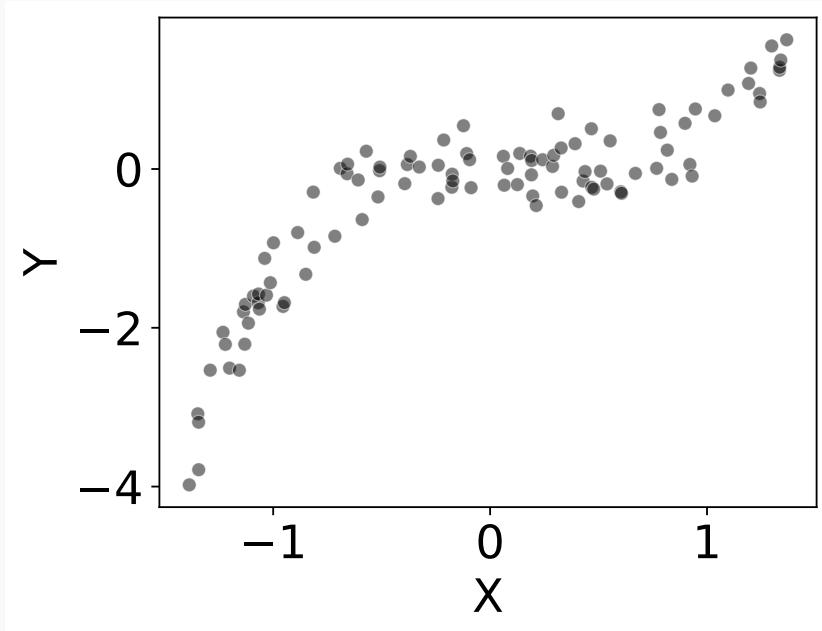
Sometimes

- the best decision boundary to separate classes is not well approximated by a straight line.
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Either use non-linear models, or perform transformations on the data, to engineer new features.

Transformation of the features: Example

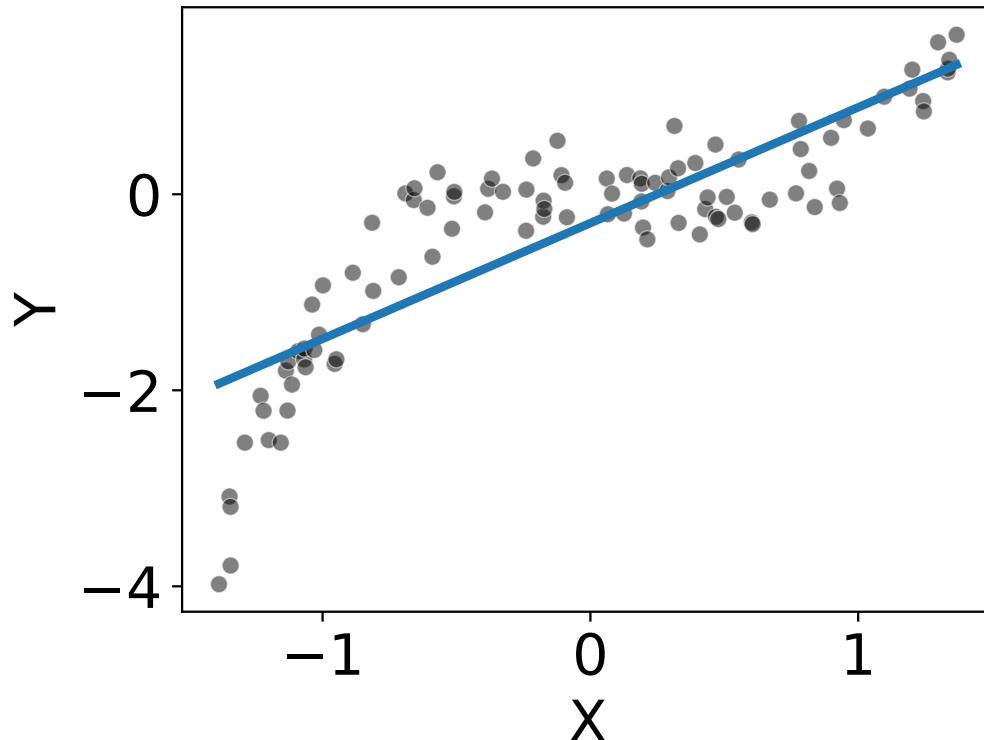


Non-linear relationship between the features and the outcome:

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

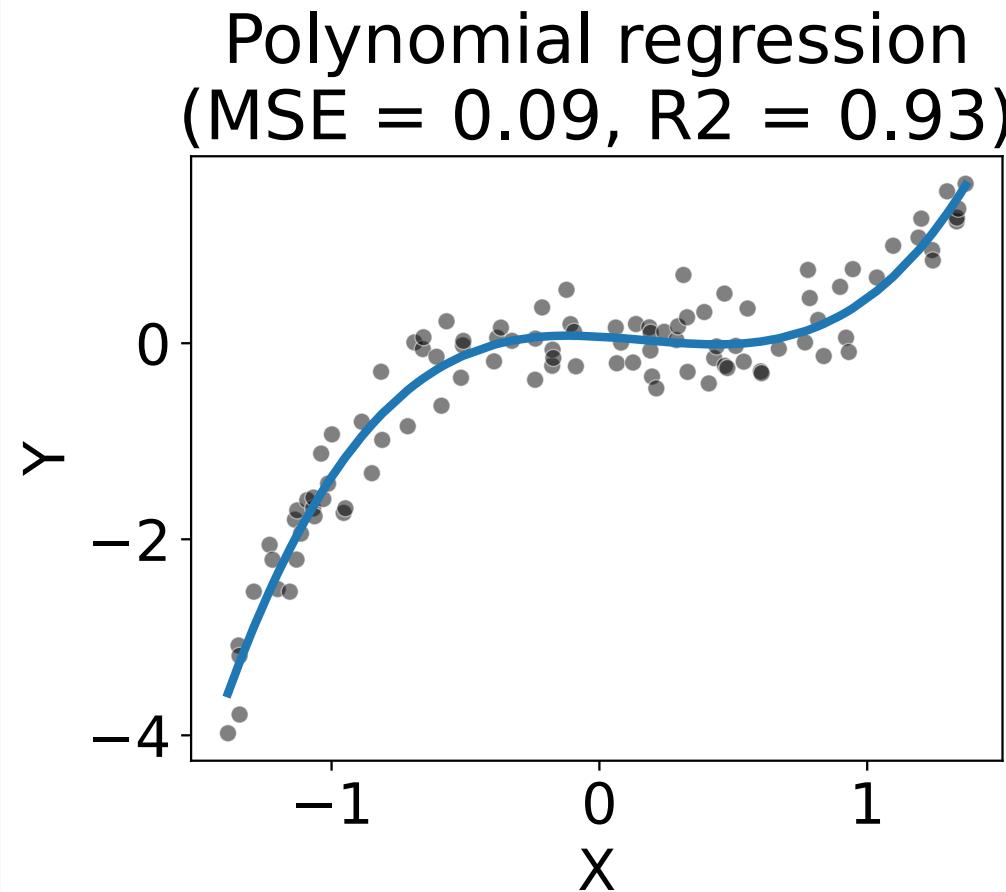
Transformation of the features: Example

Simple linear regression
(MSE = 0.36, R² = 0.71)



Vanilla Linear regression fails to capture the relationship.

Transformation of the features: Example



Solution:

- Expand the feature space with polynomials of the features:

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

- Run a linear regression on the new feature space.

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

Feature expansion increase the family of models

- Linear model can underfeat : 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, ...

Takeaway on feature expansion

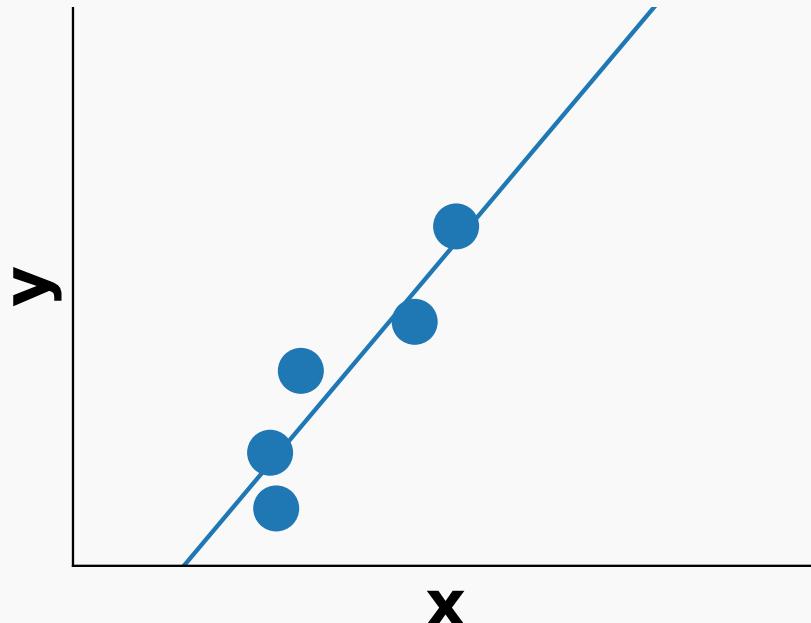
Feature expansion increase the family of models

- 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, ...

But...

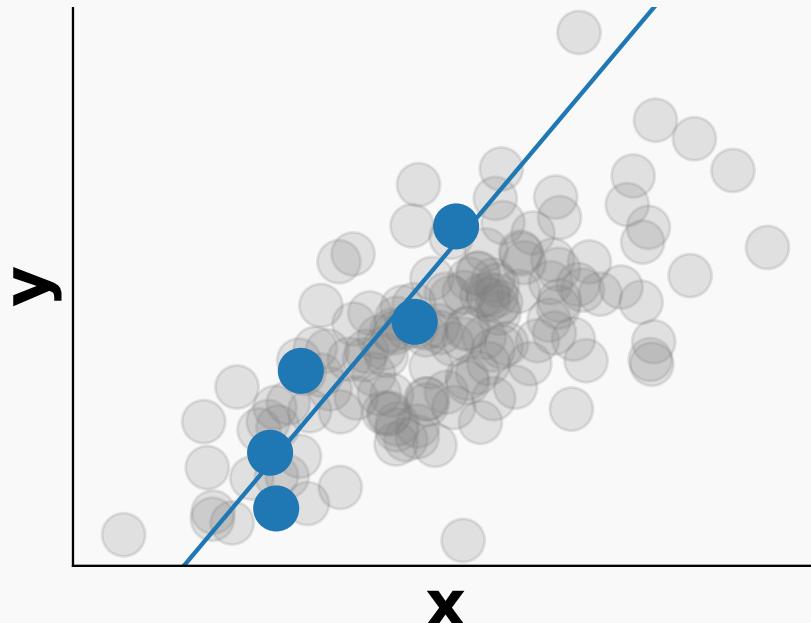
- Linear models can also overfit !
- When:
 - n_features is large
 - Many uninformative features

Many features, few observations: illustration in 1D



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

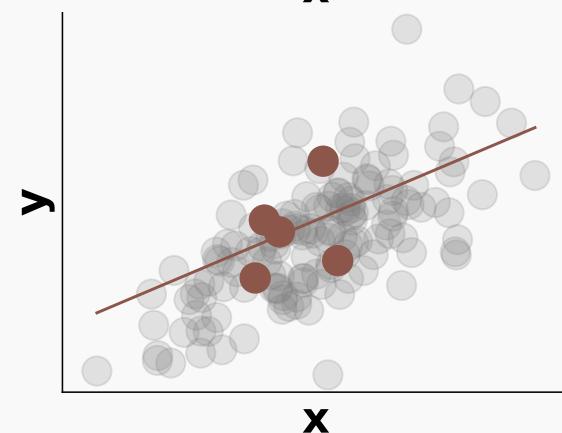
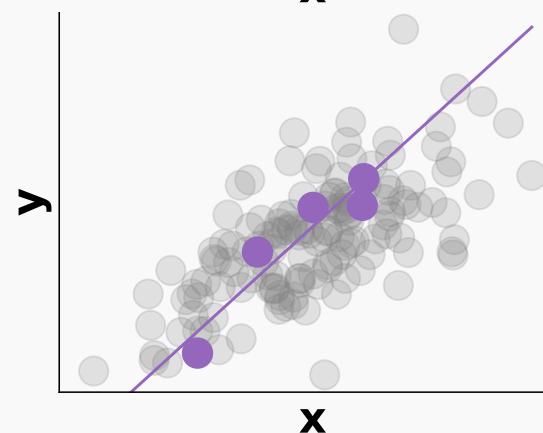
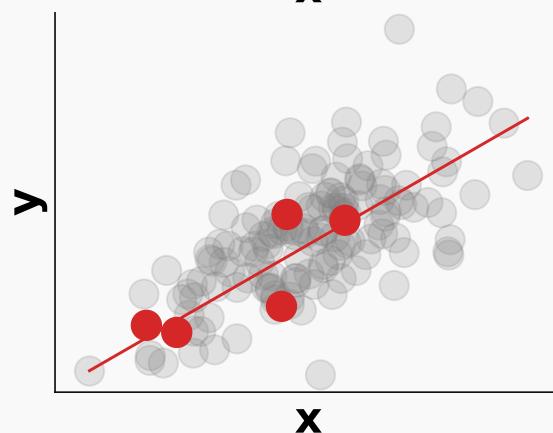
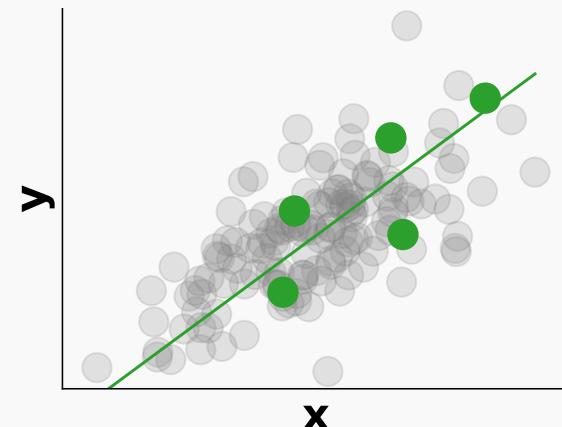
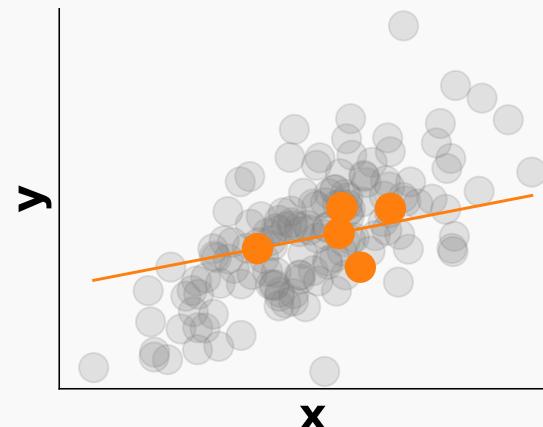
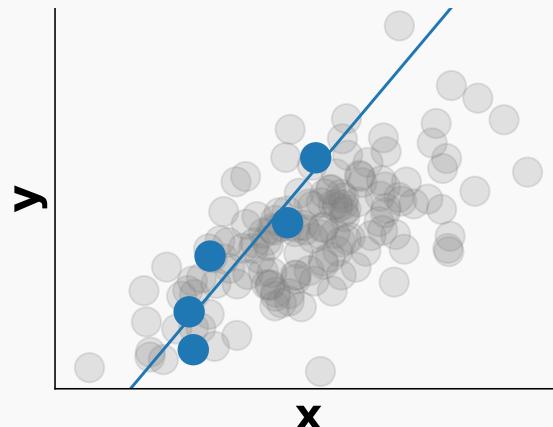
Many features, few observations: illustration in 1D



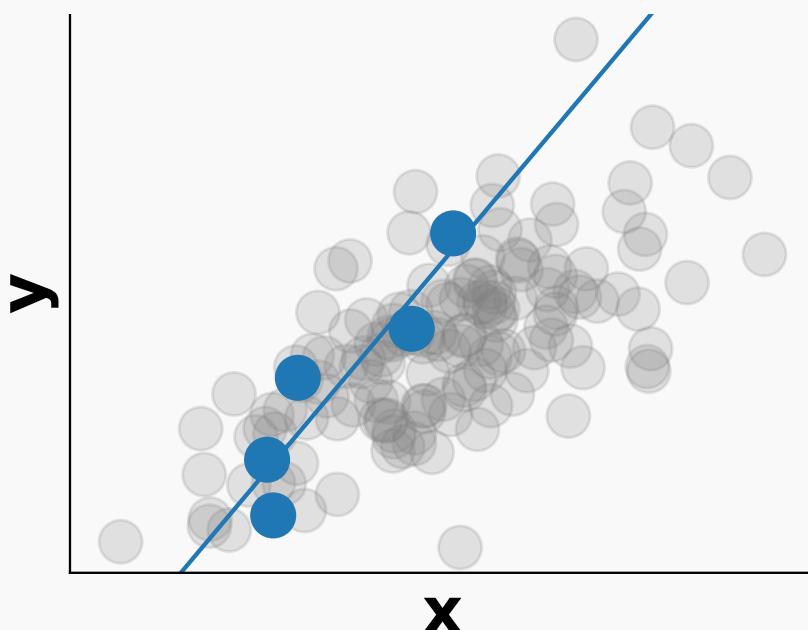
- Few observations with respect to the number of features.
- Fit a linear model without regularization.
- Linear model can overfit if data is noisy.

Many features, few observations: illustration in 1D

Sampling different training sets

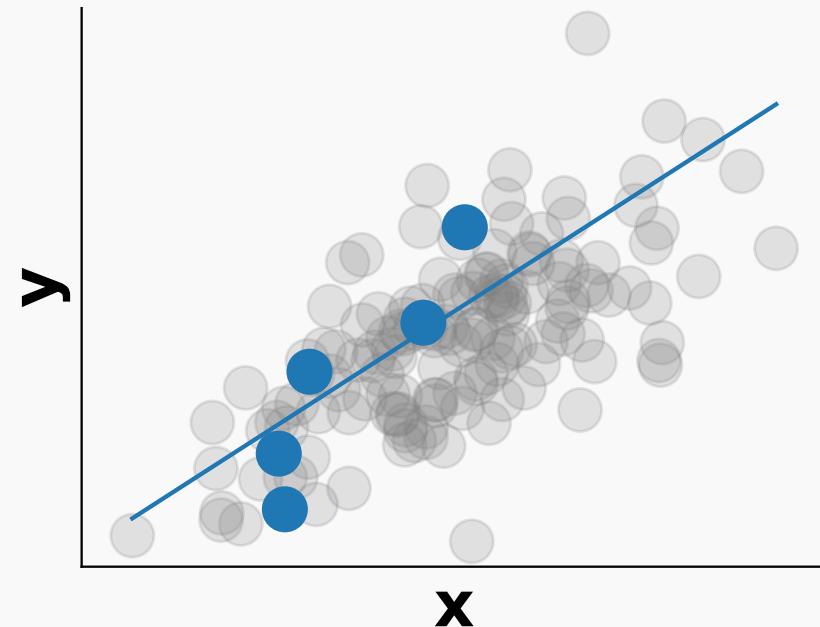


Bias variance trade-off with Lasso



Linear regression (no regularization)

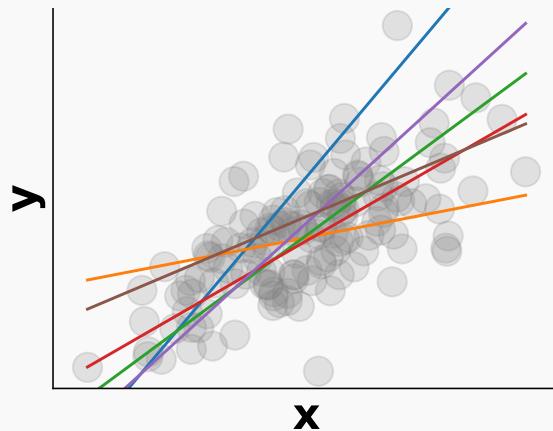
High variance, no bias.



Lasso (regularization): Shrink some coefficients of β .

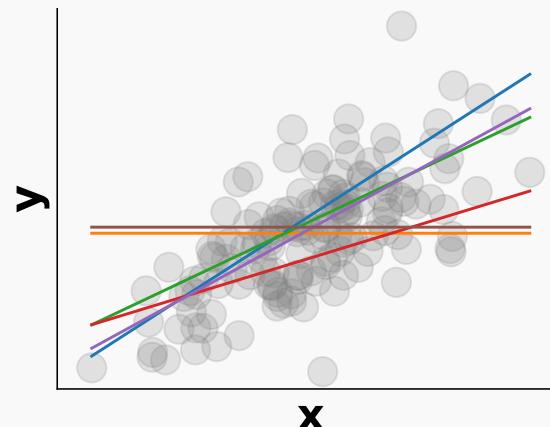
Lower variance, but bias.

Bias variance trade-off with Lasso

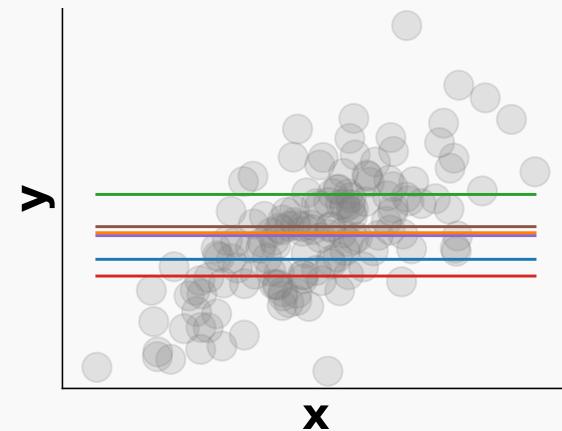


Too much variance

Not enough regularization



Best trade-off



Too much bias

Too much regularization

Objective function of the Lasso

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

$$\min_{\beta} \sum_i^n \left((y_i - \beta^T x_i)^2 \right) \text{ st. } \sum_1^p |\beta_j| \leq t$$

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

$$\min_{\beta} \sum \left((y_i - \beta^T x_i)^2 \right) + \alpha \sum (|\beta_j|)$$

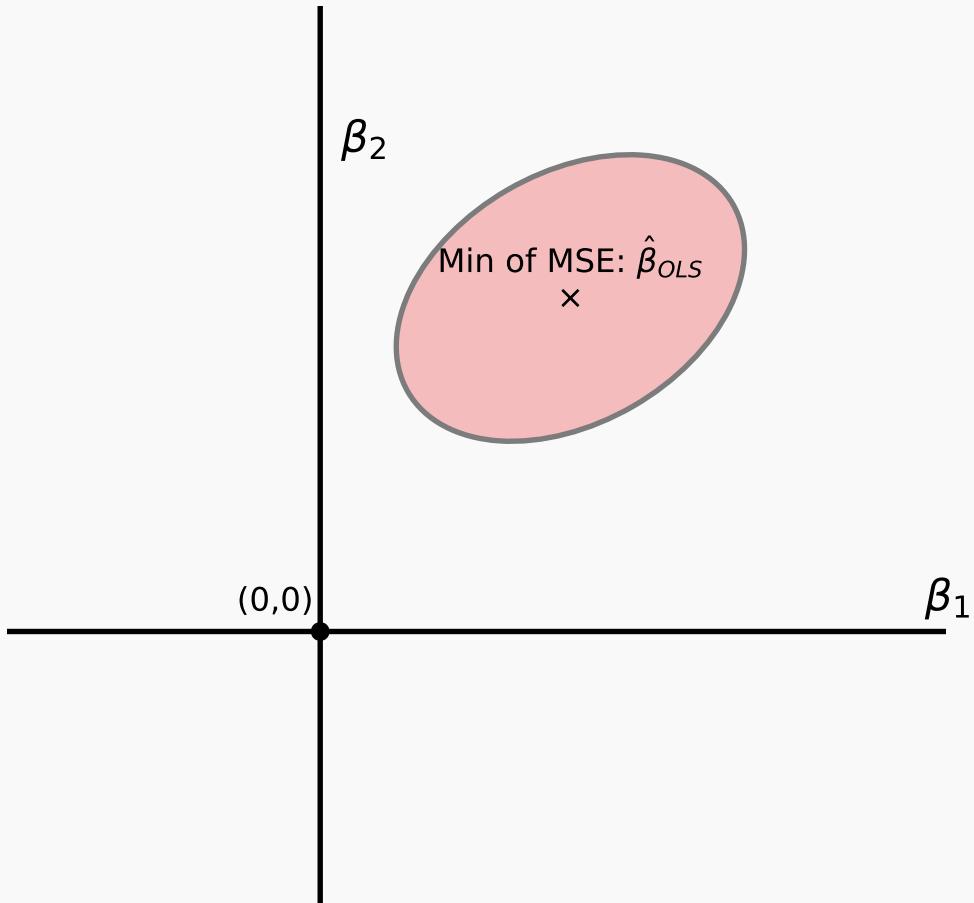
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This penalty discourages large weights and can shrink certain weights to exactly *zero* (not clear yet why).

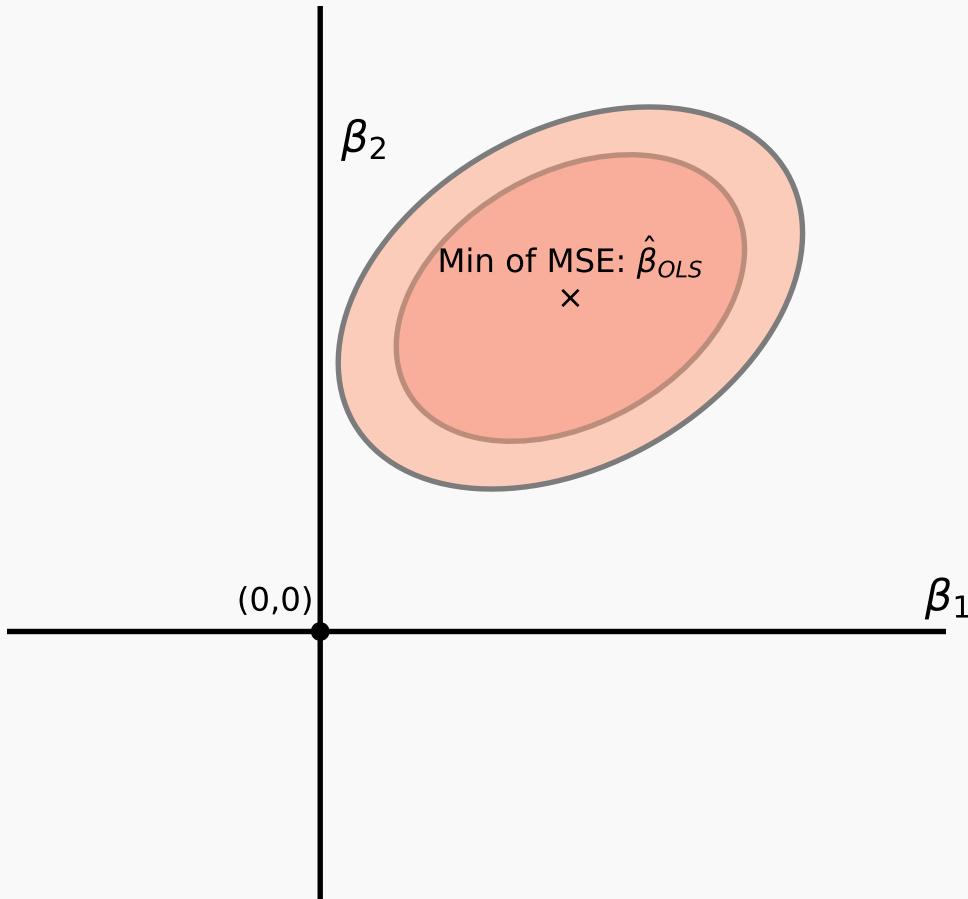
Why does Lasso shrink some coefficients to zero?



- Plot the MSE of the model as a function of the coefficients.

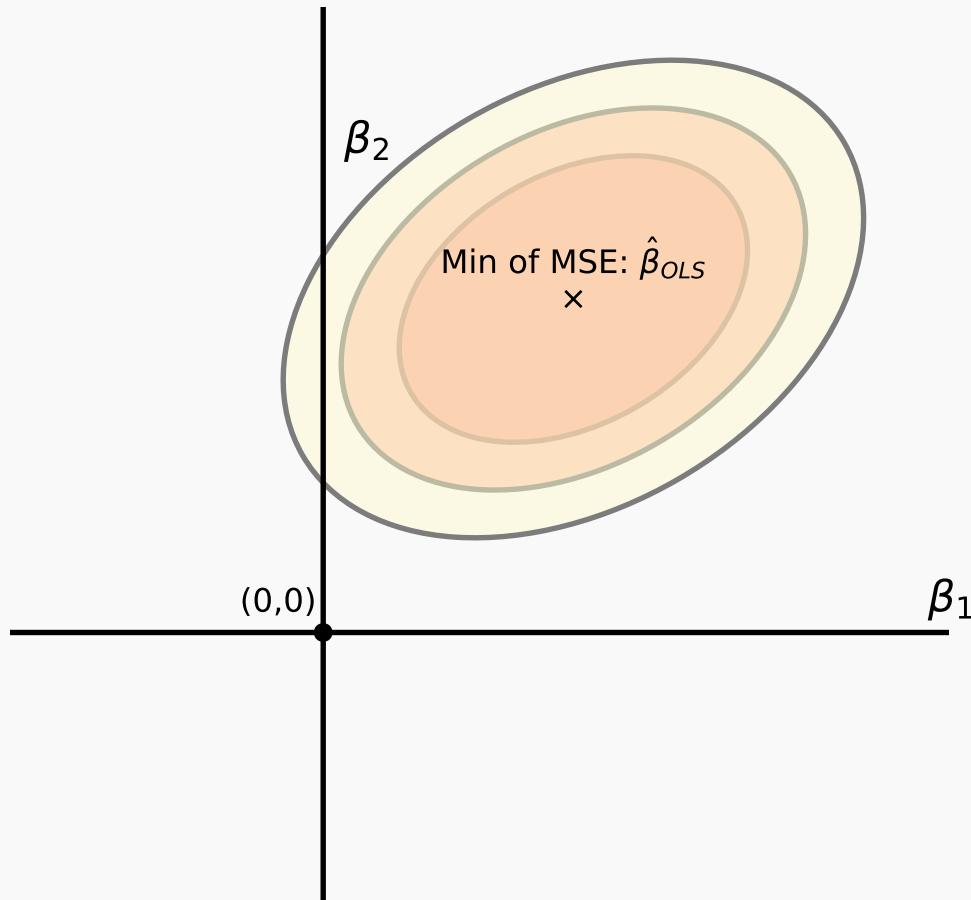
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Why does Lasso shrink some coefficients to zero?



- Plot the MSE of the model as a function of the coefficients.
- The MSE surface is an ellipsoid in β .
-

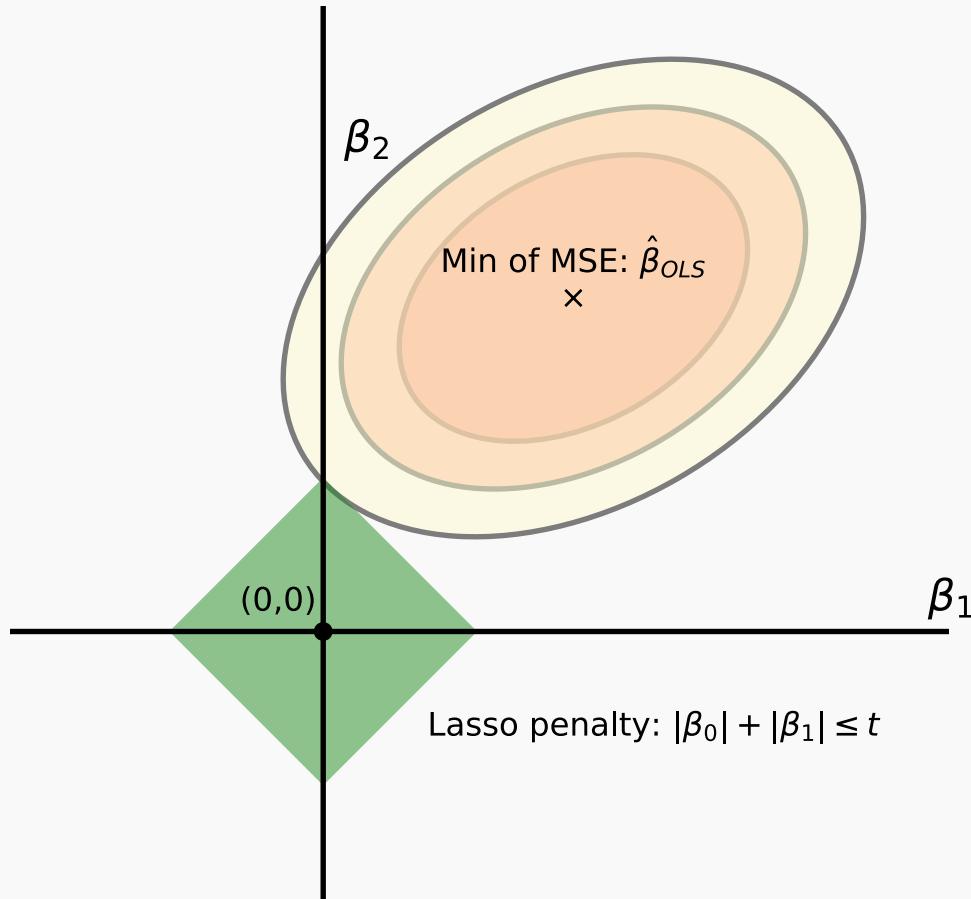
Why does Lasso shrink some coefficients to zero?



- Plot the MSE of the model as a function of the coefficients.

-
-

Why does Lasso shrink some coefficients to zero?



- Plot the MSE of the model as a function of the coefficients.
-
- The lasso objective function is a diamond.

Another regularized linear model: Ridge

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

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This penalty shrinks the coefficients towards zero and each other.

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.

How to rescale?

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

Importance of rescaling: illustration

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.

Regularized linear models for classification

Log likelihood for Lasso classification



Log likelihood for vanilla logistic regression

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

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

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

Regularized linear models for classification

Log likelihood for Lasso classification

$$L(\beta) = \frac{1}{N} \sum_{i=1}^N \left[(y_i \beta^T X_i - \log[1 + \exp(\beta^T X_i)]) - \lambda \sum_{j=1}^p |\beta_j| \right]$$



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Post lasso

TODO

How to choose lambda?

Theoretical guarantees

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

How to choose lambda?

Theoretical guarantees

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

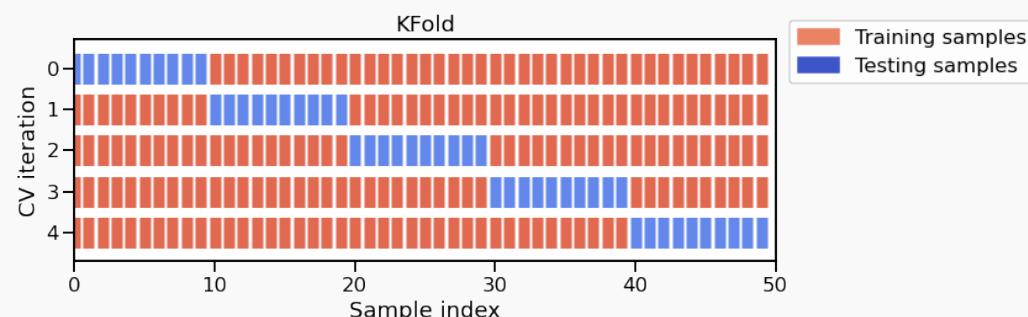
How to choose lambda?

Theoretical guarantees

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

In practice

Use cross-validation: repeated train/test splits.



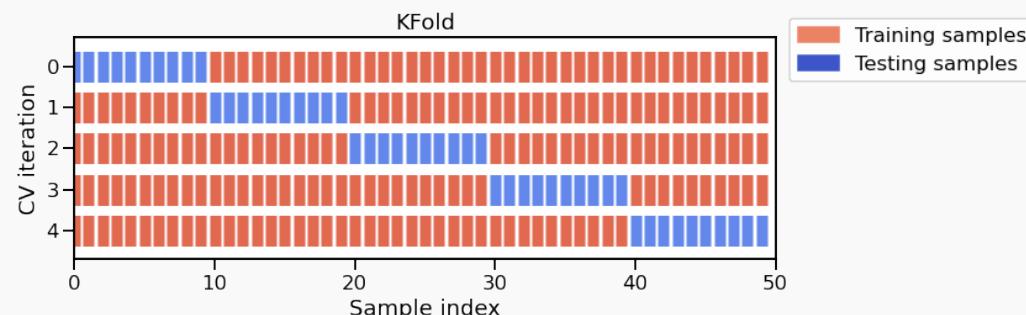
How to choose lambda?

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In practice

Use cross-validation: repeated train/test splits.



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

Short introduction to scikit-learn

- url: <https://github.com/strayMat/causal-ml-course/tree/main/notebooks>

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

To your notebooks !



- url: <https://github.com/strayMat/causal-ml-course/tree/main/notebooks>

Take home messages: Bias-variance trade-off

High bias == underfitting

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

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