Machine Learning
Lecture 2: Linear Models

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Outline

1. Linear models overview
2. Linear Regression under the hood
3. Gauss-Markov theorem
4. Regularization in Linear regression
5. Model validation and evaluation

Previous lecture recap

- Dataset, observation, feature, design matrix, target
- i.i.d. property
- Model, prediction, loss/quality function
- Parameter, Hyperparameter

Supervised learning problem statement

Training set $\mathcal{L} = \{\mathbf{x_i}, y_i\}_{i=1}^{n}$, with **n** objects each having **p** features, where

- $(\mathbf{x_i} \in \mathbb{R}^p, y_i \in \mathbb{R})$ for regression
- $(\mathbf{x_i} \in \mathbb{R}^p, y_i \in \{-1, +1\})$ for binary classification

Model $\hat{y} = f(\mathbf{x})$ predicts some value $\hat{y}$ for every object

Loss function $Q(\mathbf{x}, y, \hat{y}, f)$ that should be minimized

Unsupervised learning problem statement

Training set $\mathcal{L} = \{\mathbf{x_i}\}_{i=1}^{n}$, with **n** objects each having **p** features,

where $\mathbf{x_i} \in \mathbb{R}^p$

Model $\hat{y} = f(\mathbf{x})$ predicts some value $\hat{y}$ for every object

Loss function $Q(\mathbf{x}, \hat{y}, f)$ that should be minimized

Evaluating the quality (simple)

Quality != loss function

Image credit: Joseph Nelson @josephofiowa

Linear Models

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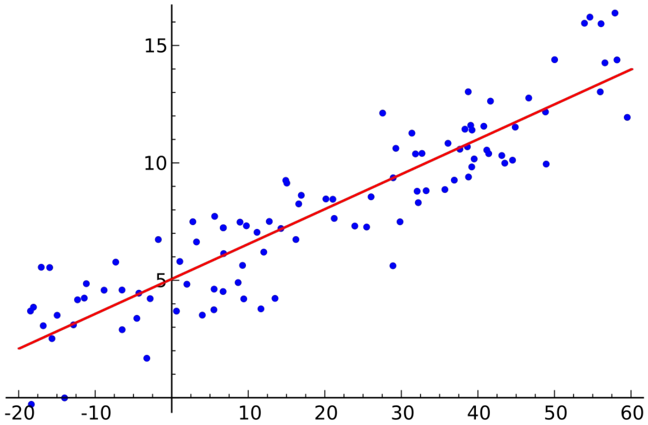
Linear models

- Regression models



Estimated (or predicted) Y value for observation i

Estimate of the regression intercept

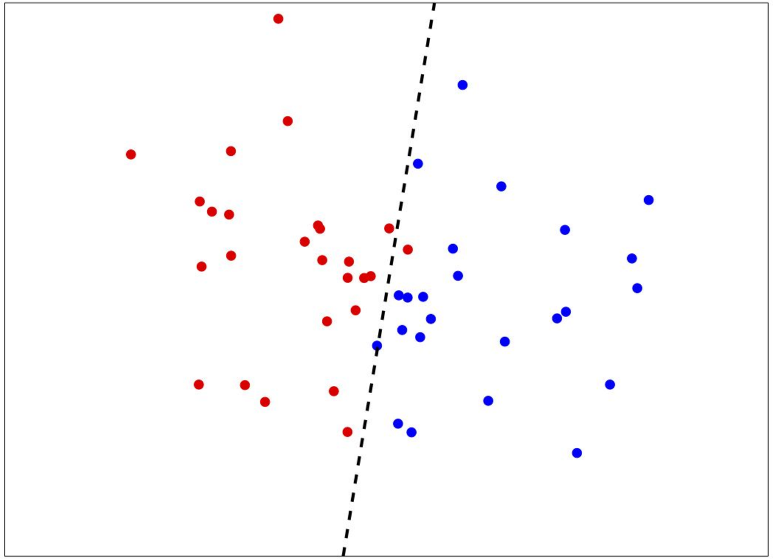
Estimate of the regression slope

Value of X for observation i

$$\hat{Y}_i = b_0 + b_1 X_i$$

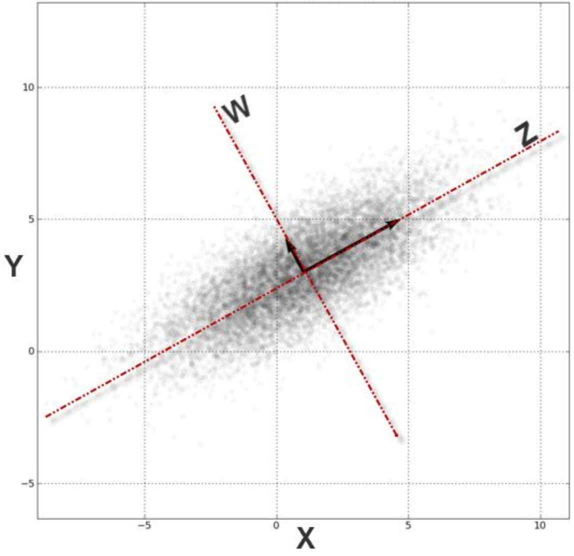
Linear models

- Regression models
- Classification models



Linear models

- Regression models
- Classification models
- Unsupervised models (e.g. PCA analysis):



Linear models

- Regression models
- Classification models
- Unsupervised models (e.g. PCA analysis):
- Building block of other models (ensembles, NNs, etc.):

Linear Regression

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Linear regression

Linear regression problem statement:

- Dataset $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$, where $\mathbf{x}_i \in \mathbb{R}^n, \quad y_i \in \mathbb{R}$.

Linear regression

Linear regression problem statement:

- Dataset $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$, where $\mathbf{x}_i \in \mathbb{R}^n, \quad y_i \in \mathbb{R}$.
- The model is linear:

$$\hat{y} = w_0 + \sum_{k=1}^{p} x_k \cdot w_k = //\mathbf{x} = [1, x_1, x_2, \ldots, x_p]// = \mathbf{x}^T \mathbf{w}$$

Linear regression

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where $\mathbf{w} = (w_0, w_1, \dots, w_n)$, w_0 is bias term.

Linear regression

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we added an additional column of 1's to the design matrix to simplify the formulas

Linear regression

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where $\mathbf{w} = (w_0, w_1, \dots, w_n)$, w_0 is bias term.

- Least squares method (MSE minimization) provides a solution:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|Y - \hat{Y}\|_2^2 = \arg\min_{\mathbf{w}} \|Y - X\mathbf{w}\|_2^2$$

Analytical solution

Denote quadratic loss function:

$$Q(\mathbf{w}) = (Y - X\mathbf{w})^T(Y - X\mathbf{w}) = \|Y - X\mathbf{w}\|_2^2 \, ,$$

where $X = [\mathbf{x}_1, \ldots, \mathbf{x}_n], \quad \mathbf{x}_i \in \mathbb{R}^p$ $Y = [y_1, \ldots, y_n], \quad y_i \in \mathbb{R}$.

To find optimal solution let's equal to zero the derivative of the equation above:

$$\nabla_{\mathbf{w}} Q(\mathbf{w}) = \nabla_{\mathbf{w}}[Y^TY - Y^TX\mathbf{w} - \mathbf{w}^TX^TY + \mathbf{w}^TX^TX\mathbf{w}] =$$
$$= 0 - X^TY - X^TY + (X^TX + X^TX)\mathbf{w} = 0$$

$$\hat{\mathbf{w}} = \boxed{(X^TX)}^{-1}X^TY$$

what if this matrix is singular?

Analytical solution

$$\hat{\mathbf{w}} = \boxed{(X^T X)}^{-1} X^T Y$$

what if this matrix is singular?

Unstable solution

In case of multicollinear features the matrix $X^T X$ is almost singular .

It leads to unstable solution:

```
w_true
```

```
array([ 2.68647887, -0.52184084, -1.12776533])
```

```
w_star = np.linalg.inv(X.T.dot(X)).dot(X.T).dot(Y)
w_star
```

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corresponding features are almost collinear

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```

the coefficients are huge and sum up to almost 0

Regularization

To make the matrix nonsingular, we can add a diagonal matrix:

$$\hat{\mathbf{w}} = (X^T X + \lambda I)^{-1} X^T Y,$$

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Regularization

To make the matrix nonsingular, we can add a diagonal matrix:

$$\hat{\mathbf{w}} = (X^T X + \lambda I)^{-1} X^T Y,$$

where $I = \mathrm{diag}[1_1, \ldots, 1_p]$.

Actually, it's a solution for the following loss function:

$$Q(\mathbf{w}) = \|Y - X\mathbf{w}\|_2^2 + \lambda^2 \|\mathbf{w}\|_2^2$$

exercise: derive it by yourself

Gauss-Markov theorem

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Gauss-Markov theorem

Suppose target values are expressed in following form:

$Y = X\mathbf{w} + \boldsymbol{\varepsilon}$, where $\boldsymbol{\varepsilon} = [\varepsilon_1, \ldots, \varepsilon_N]$ are random variables

Gauss–Markov assumptions:

- $\mathbb{E}(\varepsilon_i) = 0 \quad \forall i$
- $\mathrm{Var}(\varepsilon_i) = \sigma^2 < \inf \quad \forall i$
- $\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0 \quad \forall i \neq j$

Gauss-Markov theorem

- $\mathbb{E}(\varepsilon_i) = 0 \quad \forall i$
- $\mathrm{Var}(\varepsilon_i) = \sigma^2 < \inf \quad \forall i$
- $\mathrm{Cov}(\varepsilon_i, \varepsilon_j) = 0 \quad \forall i \neq j$

$$\boxed{\hat{\mathbf{w}} = (X^T X)^{-1} X^T Y}$$

delivers **B**est **L**inear **U**nbiased **E**stimator

Different norms

Once more: loss functions:

$$\boxed{MSE = \frac{1}{n}\|\mathbf{x}^T\mathbf{w} - \mathbf{y}\|_2^2}$$

only works for Gauss-Markov theorem

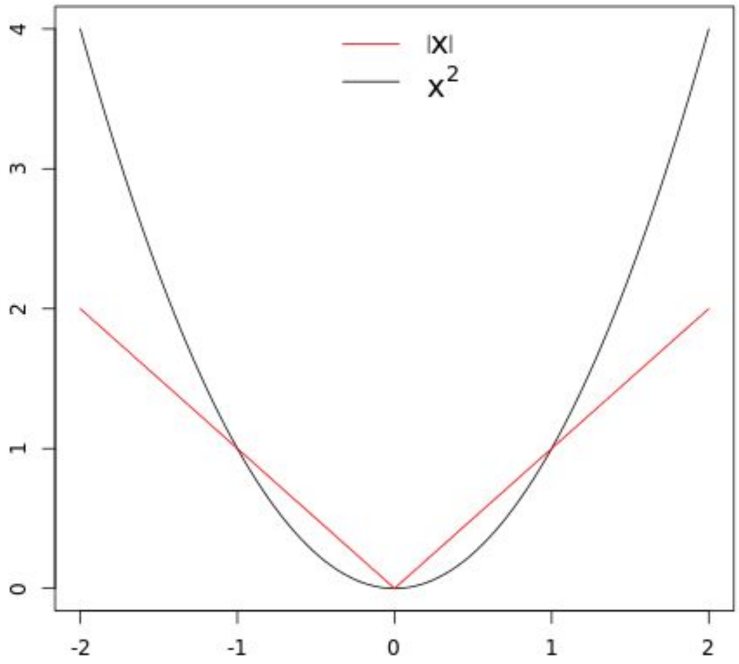
$$MAE = \frac{1}{n}\|\mathbf{x}^T\mathbf{w} - \mathbf{y}\|_1$$

Regularization terms:

- L2 $\|\mathbf{w}\|_2^2$
- L1 $\|\mathbf{w}\|_1$

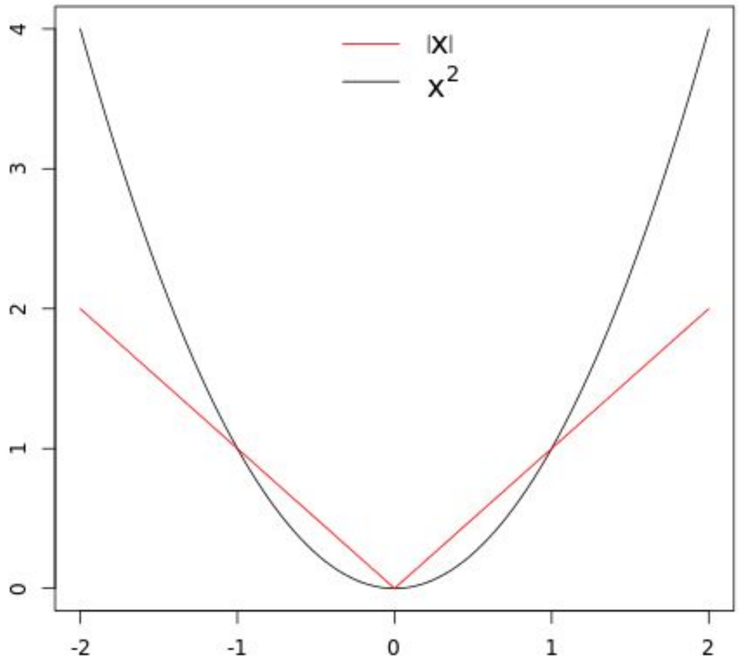
What’s the difference?

- MSE (L_2)
  - delivers BLUE according to Gauss-Markov theorem
  - differentiable
  - sensitive to noise
- MAE (L_1)
  - non-differentiable
    - not a problem
  - much more prone to noise

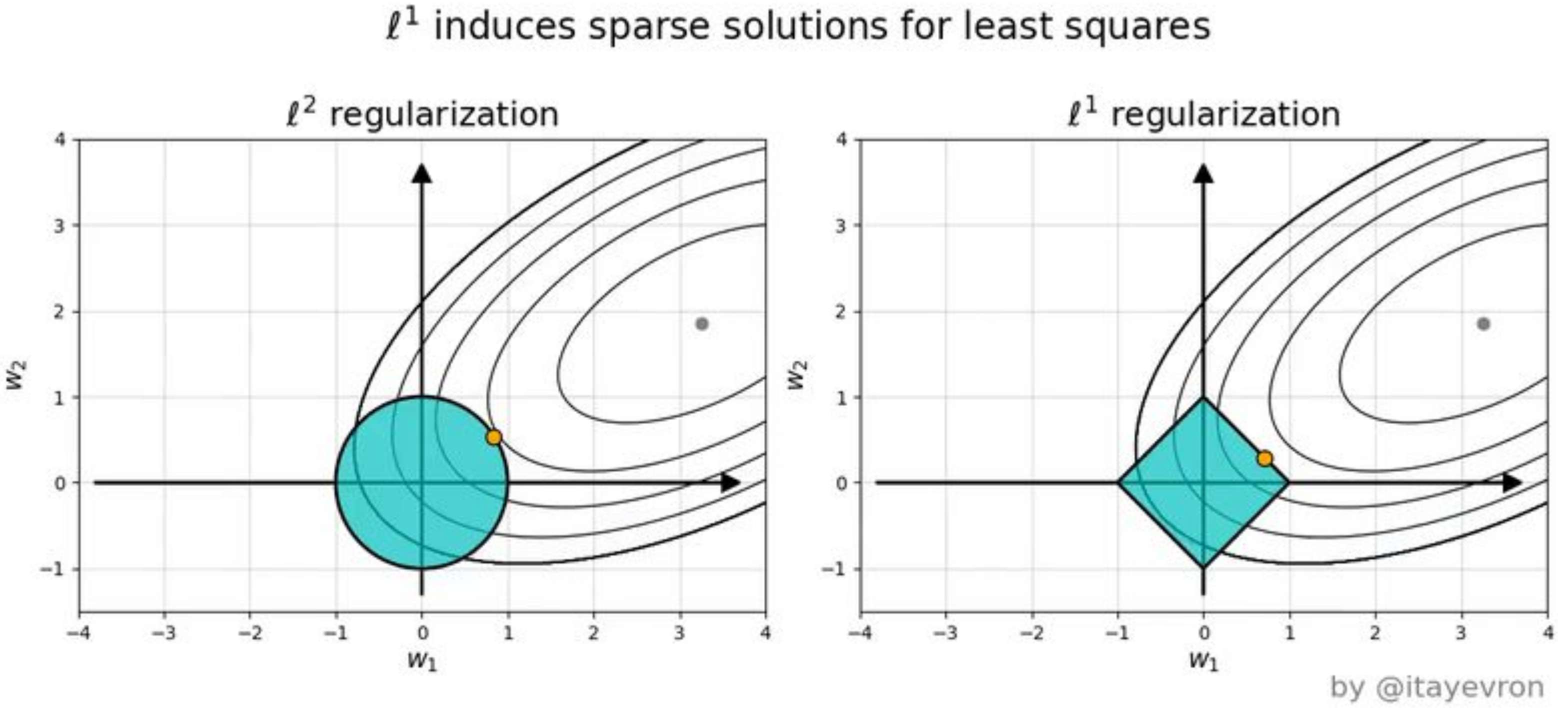


What’s the difference?

- L_2 regularization
  - constraints weights
  - delivers more stable solution
  - differentiable
- L_1 regularization
  - non-differentiable
  - not a problem
  - selects features



What's the difference?



source: https://people.eecs.berkeley.edu/~jrs/189/

Loss functions in regression

Other functions to measure the quality in regression:

- R2 score

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - f(\mathbf{x_i}))}{\sum_{i=1}^{n}(y_i - \mathbf{\overline{y}})}$$

Loss functions in regression

Other functions to measure the quality in regression:

- MAPE

$$MAPE = \frac{1}{n} \sum \frac{|y_i - f(\mathbf{x_i})|}{y_i}$$

Loss functions in regression

Other functions to measure the quality in regression:

- SMAPE (=Symmetric MAPE)

$$SMAPE = \frac{1}{n} \sum \frac{|y_i - f(\mathbf{x_i})|}{C}$$

$$C = \frac{(|y_i| + |f(\mathbf{x_i})|)}{2}$$

Loss functions in regression

Other functions to measure the quality in regression:

- R2 score
- MAPE
- SMAPE
- ...

Model validation and evaluation

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Supervised learning problem statement

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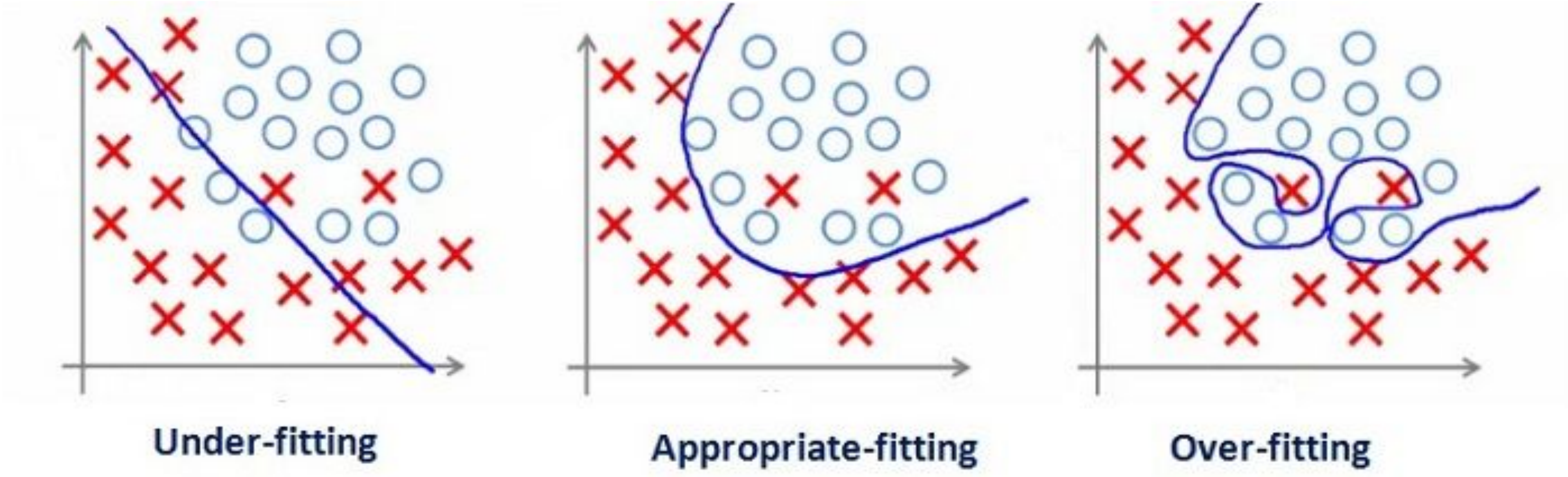
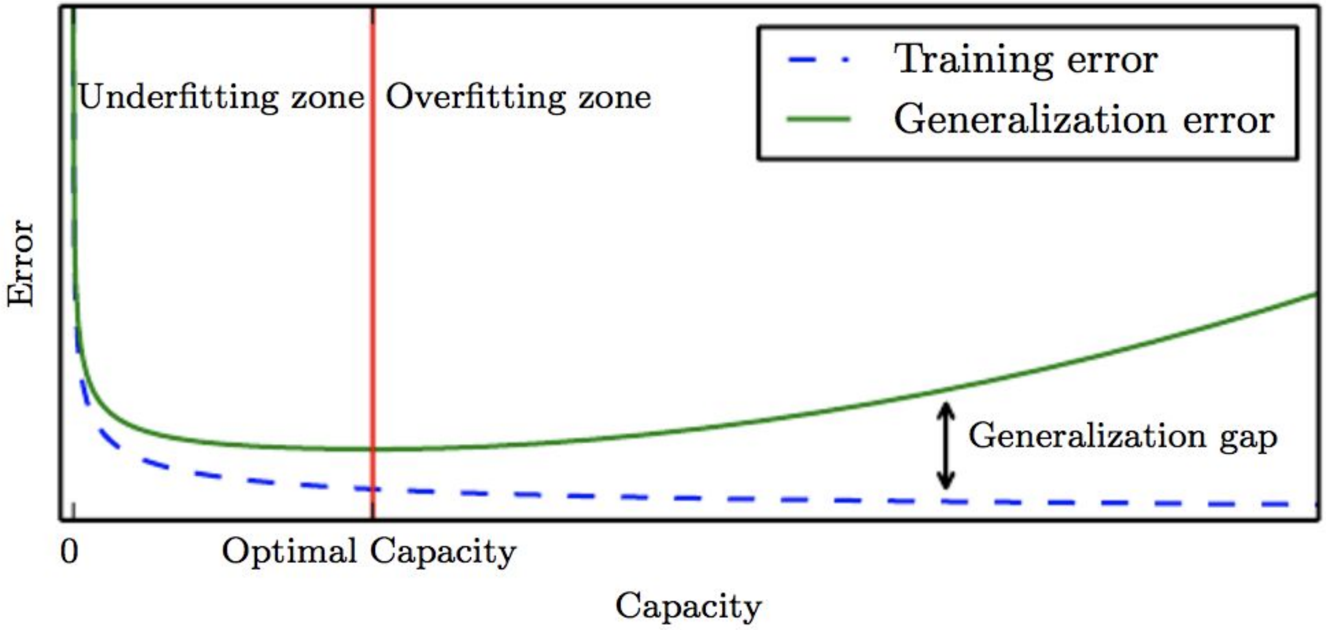
Overfitting vs. underfitting



(too simple to explain the variance)

(forcefitting -- too good to be true)

Overfitting vs. underfitting



Overfitting vs. underfitting

- We can control overfitting / underfitting by altering model's capacity (ability to fit a wide variety of functions):
- select appropriate hypothesis space
- learning algorithm's effective capacity may be less than the representational capacity of the model family

Evaluating the quality

Image credit: Joseph Nelson [@josephofiowa]

Evaluating the quality

Is it good enough?

Image credit: Joseph Nelson @josephofiowa

Evaluating the quality

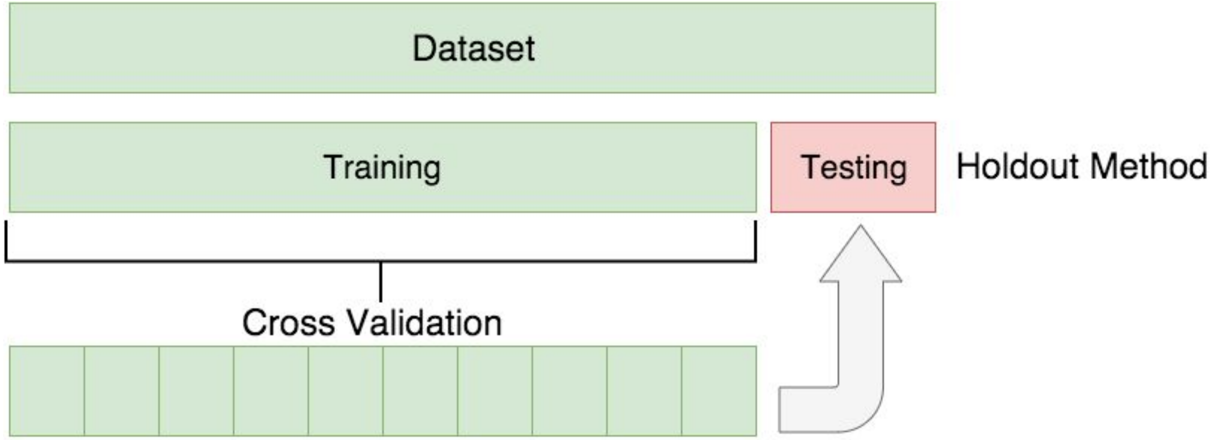


Image credit: Joseph Nelson [@josephofiowa]

Evaluating the quality

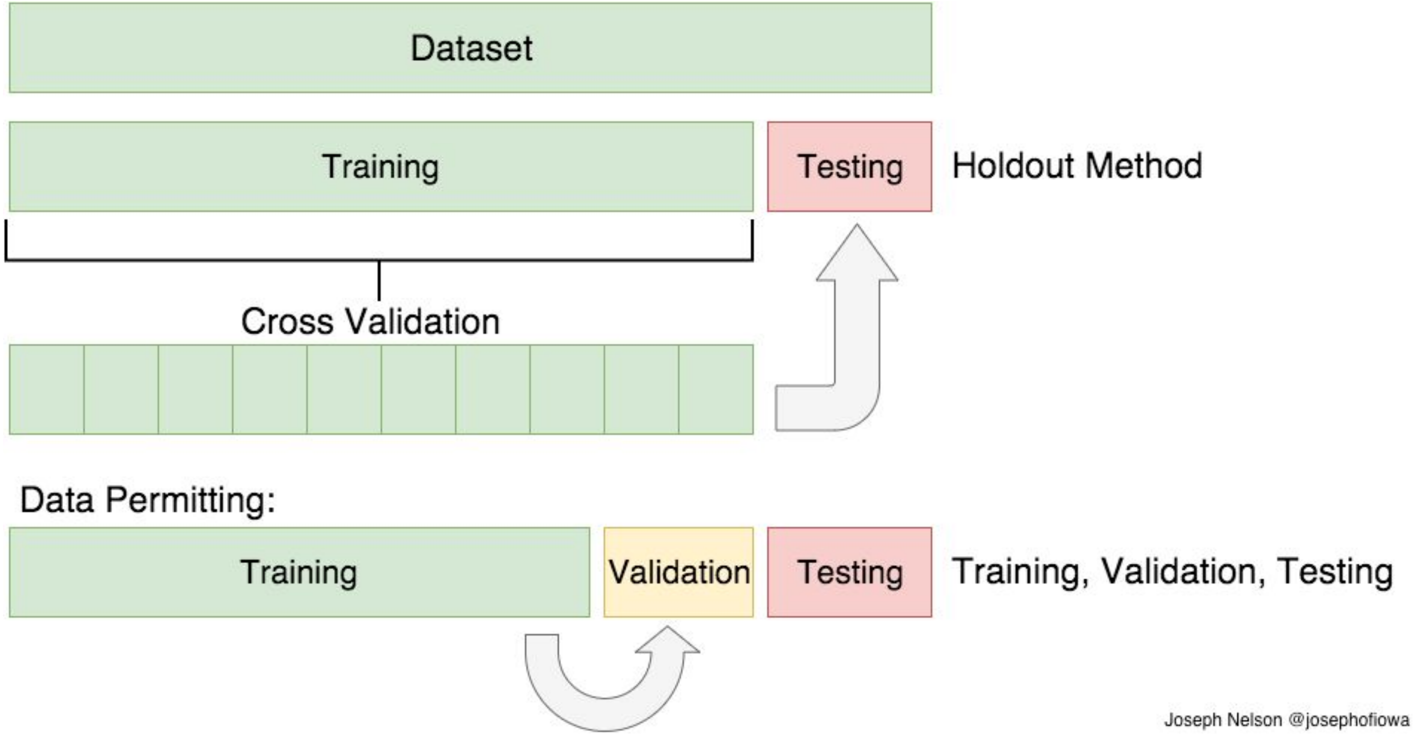
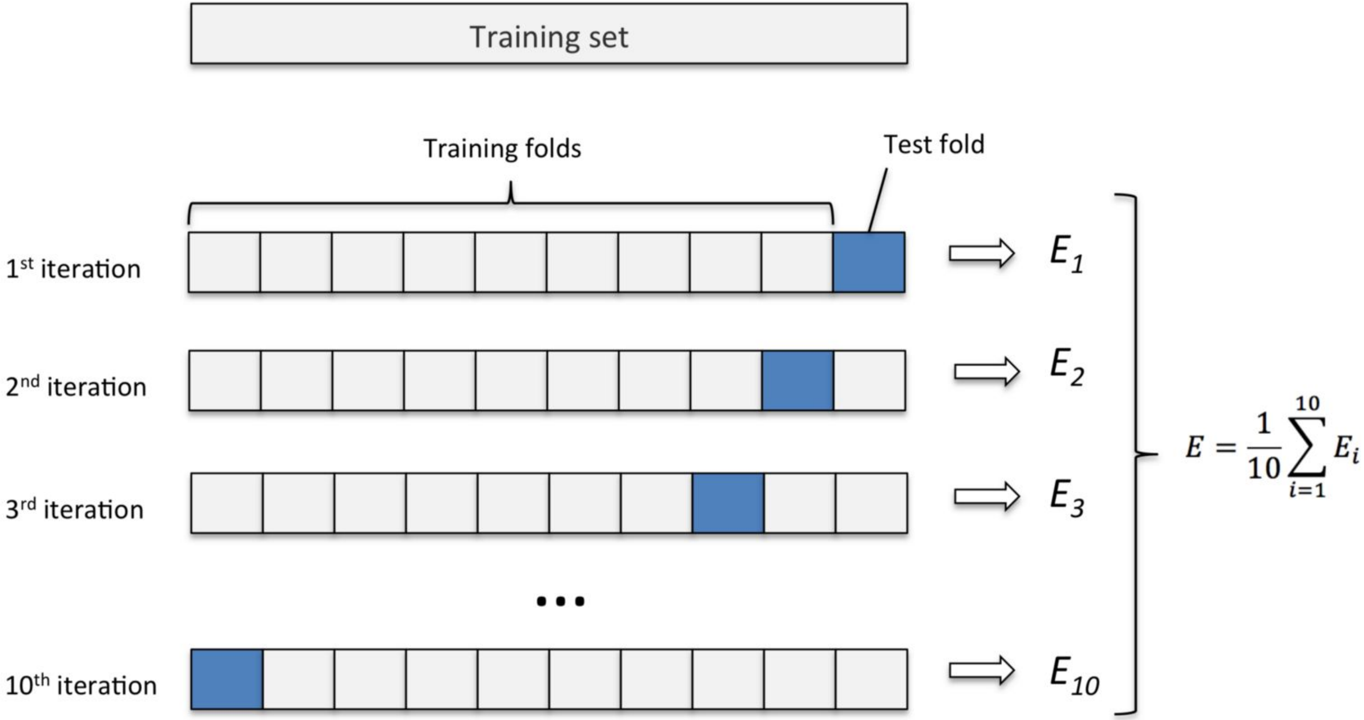


Image credit: Joseph Nelson [@josephofiowa]

Cross-validation



Outro

- Linear models are simple yet quite effective models
- Regularization incorporates some prior assumptions/additional constraints
- Trust your validation

Revise

1. Linear models overview
2. Linear Regression under the hood
3. Gauss-Markov theorem
4. Regularization in Linear regression
5. Model validation and evaluation

Thanks for attention!

Questions?

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