Universidad Zaragoza

Machine Learning (69152)

Machine Learning Fundamentals

Universidad Zaragoza

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- **Classification**
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- **Unsupervised methods**
    - Dimensionality reduction: PCA
    - Clustering: K-means, GMM
- **Evaluation metrics**

Bibliography

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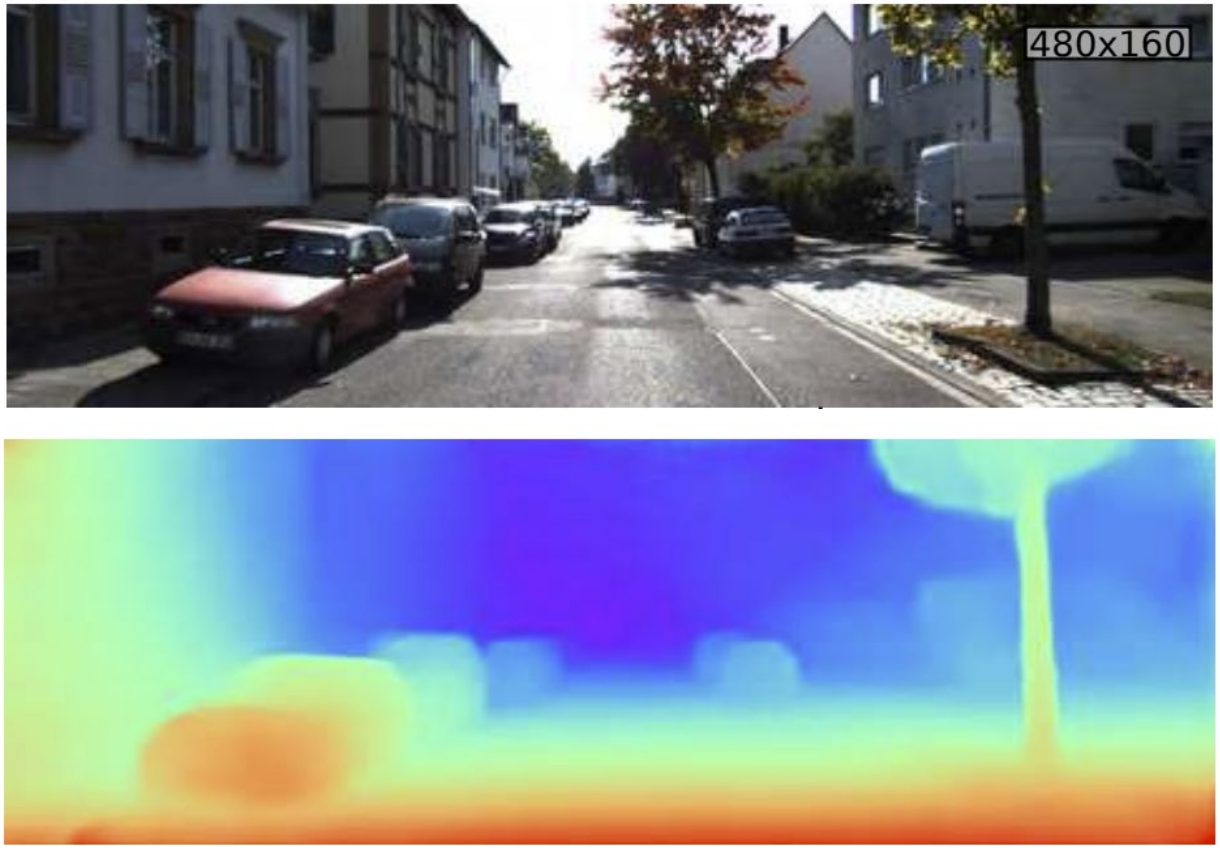
- Aurélien Géron, Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow, O'Reilly, 2019 (2nd edition)
- Online courses
  - Andrew Ng, Stanford CS229: Machine Learning, https://www.youtube.com/playlist?list=PLoROMvodv4rMiGQp3WXShtMGgzqpfVfbU
  - Ayush Singh and @freecodecamp, ML for beginners, https://www.youtube.com/watch?v=NWONeJKn6kc
- Python resources
  - The Python tutorial: https://docs.python.org/3/tutorial/
  - numpy tutorial: https://cs231n.github.io/python-numpy-tutorial/
  - scikit-learn tutorials: https://scikit-learn.org/stable/tutorial/index.html

Regression

- Learns a function that relates an input vector with a **continuous output**.
- Examples: depth prediction, weather forecasting, time-to-destination estimation…



Linear regression

For more details, check Murphy chapter 11, Deisenroth chapter 9

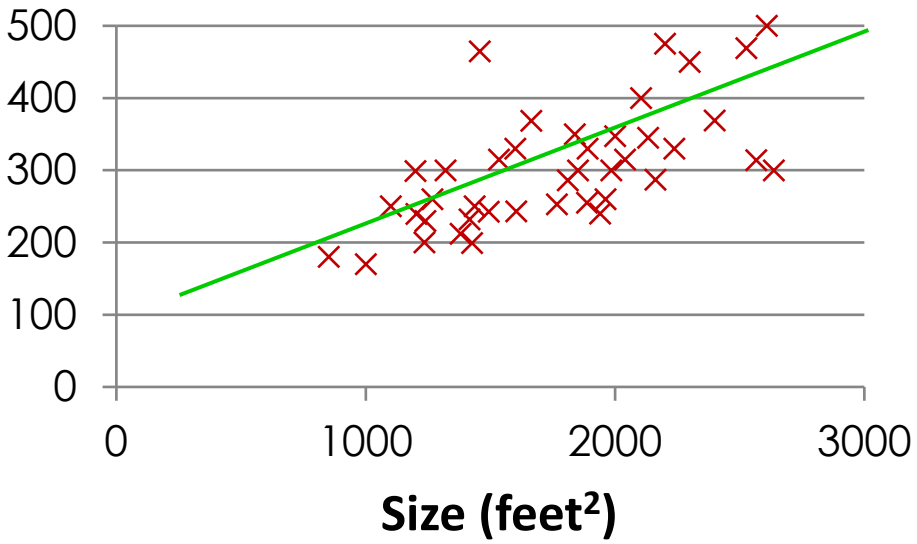
- The input/output relation is linear in the model parameters

$$y = x^T w + \epsilon \quad \epsilon \sim N(0, \sigma^2) \quad \text{one data point}$$

$$\boldsymbol{y} = Xw + \epsilon I_n \quad \epsilon \sim N(0, \sigma^2) \quad \text{dataset (size n)}$$

- Example: Housing prices and size

$y \rightarrow$ output variables



$x \rightarrow$ independent/explanatory variables

Linear regression

- Frequentist approach
  - Assume there is one true model w^*
  - If we had infinite data, we would get the exact model.
  - With finite data, we get an approximation $\hat{w}$.

- How? → By Maximum-likelihood (ML)

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log p(\boldsymbol{y}|X, w)$$

  - If data is independent $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}$ and $\boldsymbol{y} = \{y_1, \dots, y_n\}$

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log \prod_{i=1}^{n} p(y_i|\boldsymbol{x}_i, w) = \underset{w}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(y_i|\boldsymbol{x}_i, w)$$

How do we get w?

- What is the likelihood?

$$p(y_i|\boldsymbol{x}_i, w) = N(y\,|\boldsymbol{x}_i^T w, \sigma^2) \quad \text{one data point}$$

$$p(\boldsymbol{y}|X, w) = N(\boldsymbol{y}\,|\,Xw, \sigma^2 I_n) \quad \text{joint distribution dataset}$$

Ignore all the terms without w

$$\operatorname*{argmax}_w \sum_i \log(p(y_i|\boldsymbol{x}_i, w)) =$$

$$= \operatorname*{argmax}_w \sum_i \log\left(\exp\left(-\frac{1}{2\sigma^2}\left(y_i - \boldsymbol{x}_i^T w\right)^2\right)\right) =$$

$$= \operatorname*{argmin}_w \sum_i \left(y_i - \boldsymbol{x}_i^T w\right)^2 = \operatorname*{argmin}_w \sum_i r_i^2$$

Assume σ^2 is constant

Least squares!

ML = Least squares

How do we get w?

- Minimize Negative Log-Likelihood (NLL).
  - Follow the gradient!

- Rewrite NLL as a function easy to derivate

$$J(w) = \frac{1}{2}(\boldsymbol{y} - Xw)^T(\boldsymbol{y} - Xw)$$

$$\nabla J(w) = X^T Xw - X^T \boldsymbol{y}$$

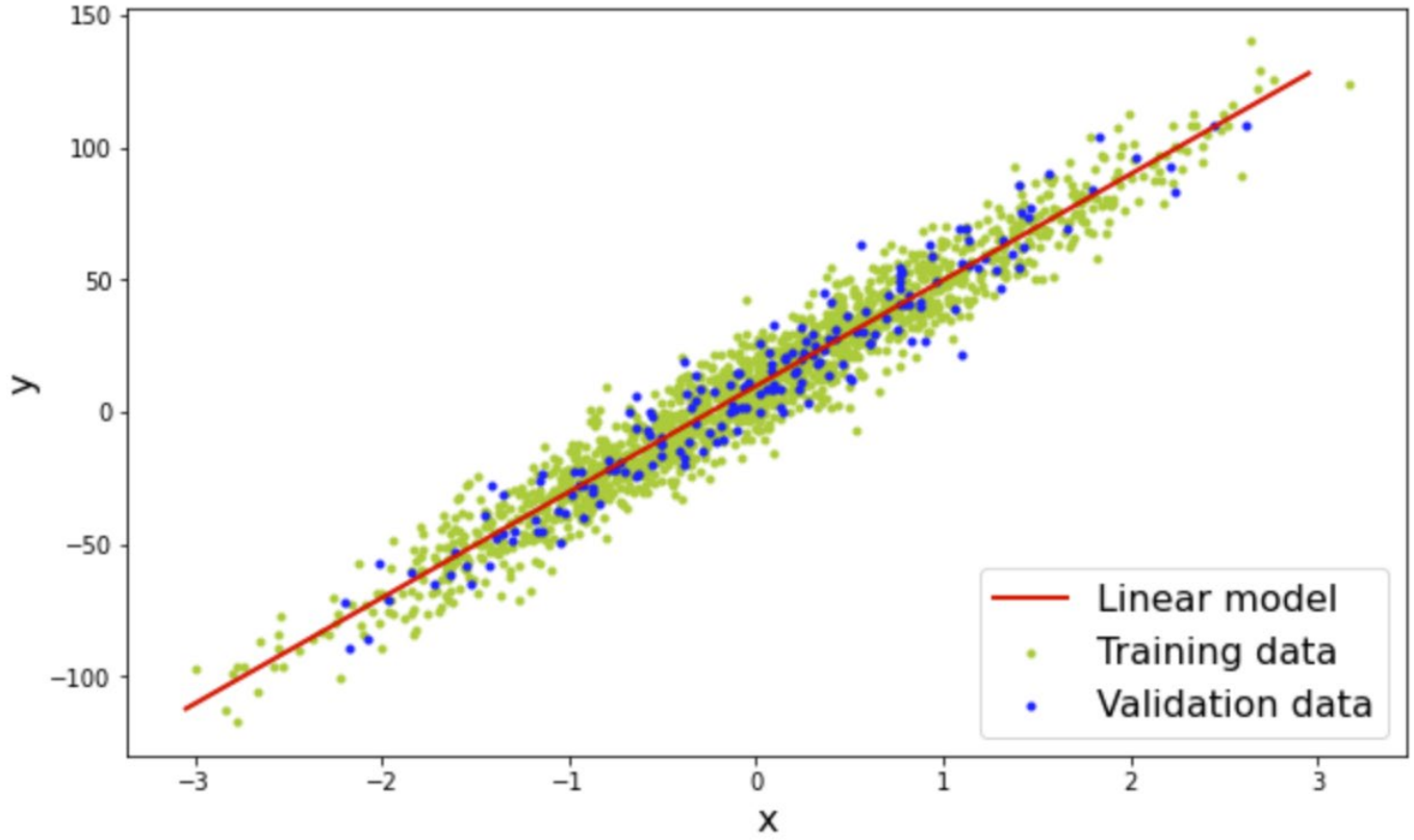
$$\hat{\boldsymbol{w}} = \arg min_w J(w) \Rightarrow \nabla J(\hat{w}) = 0$$

- For the linear-Gaussian case → Analytical solution

$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

Simple linear regression example

- Colab link: https://colab.research.google.com/drive/1EXDJHTIvp4zK3qavGsXO03NMwYRr59JM



Nonlinear Regression (linear in w_i)

- Basis function expansión
  - Linear regression can be made to model non-linear relations by using a feature space $x \rightarrow \phi(x)$

$$y = \phi(x)^T w + \epsilon \quad \epsilon \sim N(0, \sigma^2) \qquad \text{one data point } \{\mathrm{x}, \mathrm{y}\}$$

$$\mathbf{y} = \Phi_X^T w + \epsilon I_n \qquad \text{dataset } \{\mathrm{X}, \mathbf{y}\} \text{ (size n)}$$

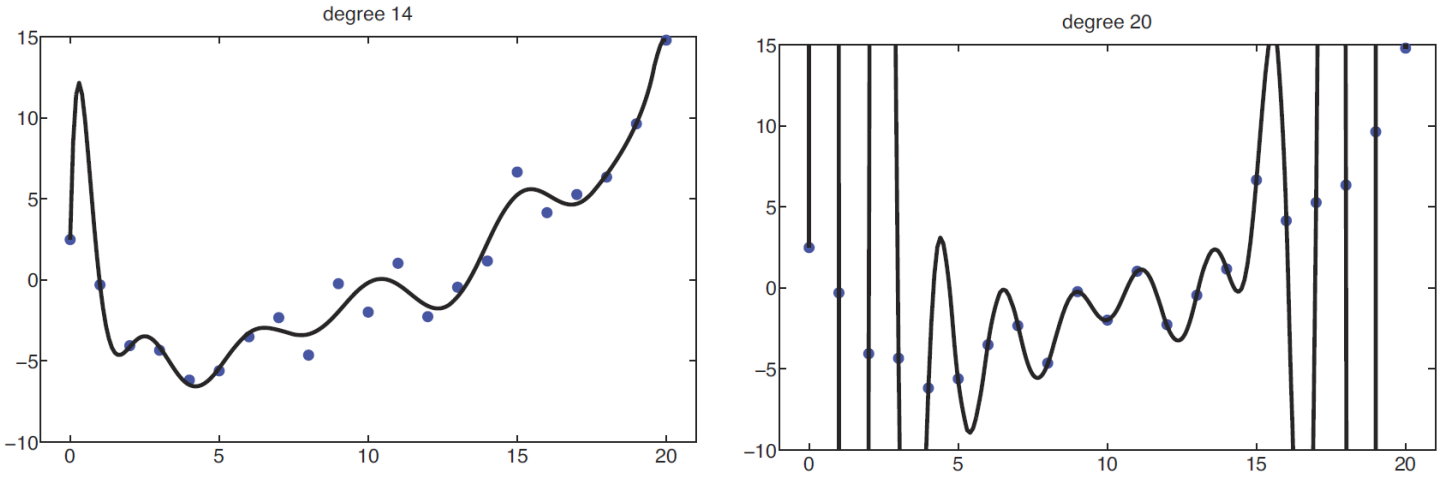
- Example:
  - In the previous example, we were computing the intercept

$$\phi(x) = [1, x]^T$$

$$y = \phi(x)^T w + \epsilon = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n + \epsilon$$

Nonlinear Regression (linear in w_i!)

- Example:
  - Polinomial basis function $\phi(x) = [1, x, x^2, \cdots, x^d]^T$ $(x \in \mathbb{R}^1, \phi(x) \in \mathbb{R}^d)$
  - $y = \phi(x)^T w + \epsilon = \sum_{j=1}^{d} w_j x^j + \epsilon = w_0 + w_1 x^1 + w_2 x^2 + \cdots + w_d x^d + \epsilon$
  - Polynomia of degree 14 and 20 fit by LS (which one is better?)

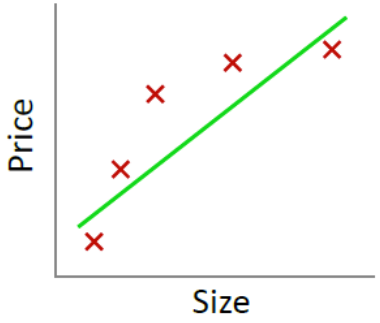


Example and figures taken from Murphy's book

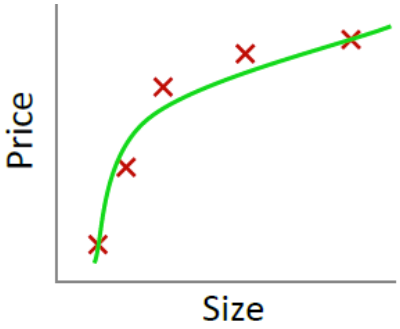
- We can use exponentials, sinusoids, step-functions…
  - We'll see more examples in the Bayesian slides)

Overfitting

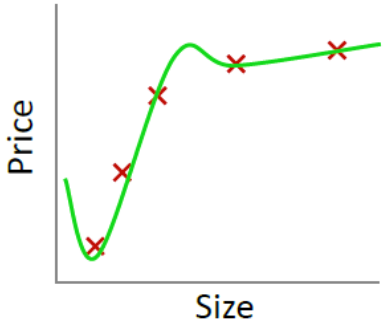
- The function $\phi(x)^T w$ fits the noise in addition to the underlying patterns. It "*memorizes*" the data instead of "*learning to generalize*".
- The function does not capture the structure of the data.
- The predictive capability of an overfitted model is poor.
- Techniques:
  - Cross-validation
  - Regularization



$\theta_0 + \theta_1 x$



$\theta_0 + \theta_1 x + \theta_2 x^2$

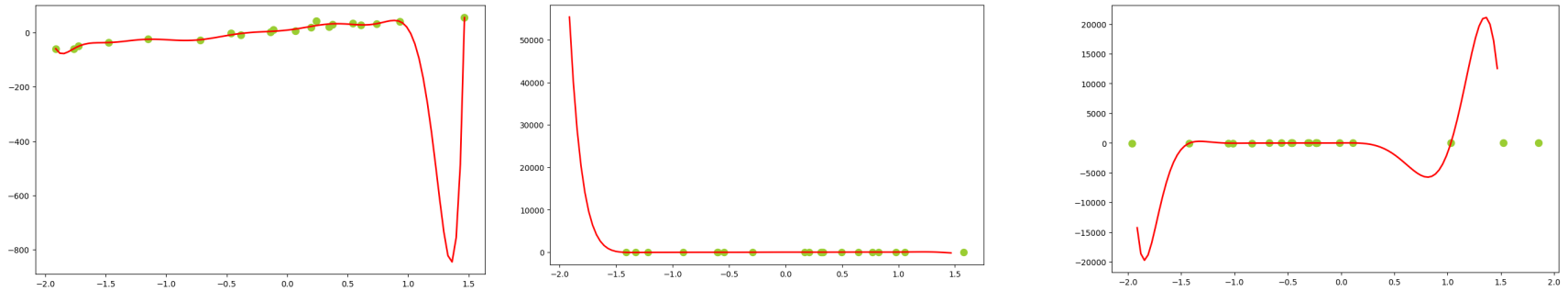


$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{N} (h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$$

Regularization

- Bias-variance trade off.
  - ML is **unbiased** → If data → ∞ then $\mathbb{E}(w^* - \hat{w}) \to 0$
  - Overfitting results in large **variance**
    - If we fit slightly different data, the model is completely different

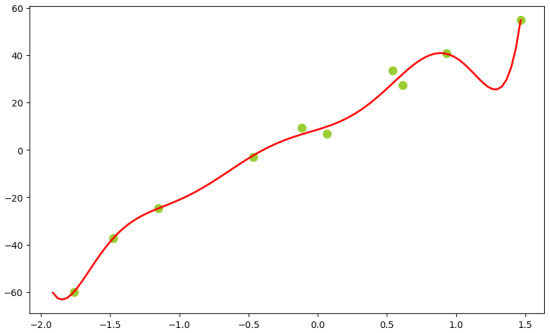
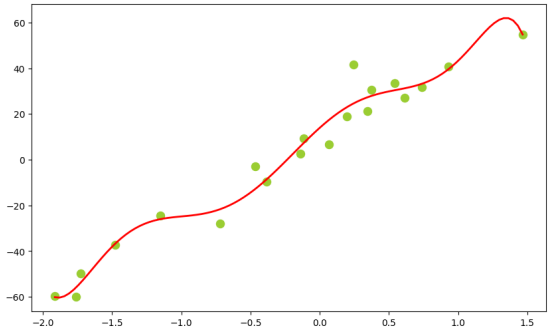
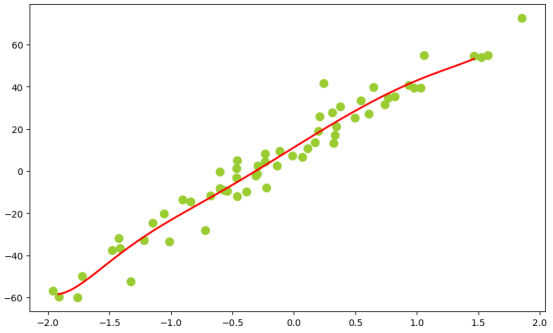


Polynomial regression d=12 for data generated by $y = 33x + 10 + \epsilon$ with $\epsilon \sim N(0,7)$

- Constrain the model while learning.
  - Model restrictions → **Lower variance**
  - ML+restrictions is **biased** → If data → ∞ then $\mathbb{E}(w^* - \hat{w}) \neq 0$

Regularization

- For complex models → Get more data
  - Same polynomial d=8

- If more data is not possible. Many variants:
  - **L2-regularization** (Ridge regression), Weight decay
  - L1 (Lasso)
  - Early stopping
  - Data augmentation
  - Dropout
  - Batch normalization
  - …

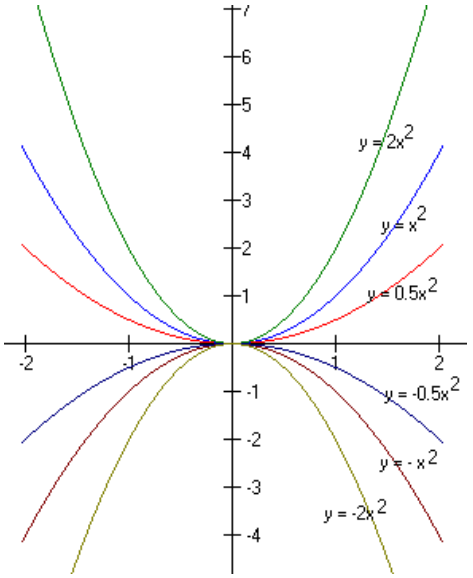
Check deep learning slides

Ridge regression

- Different ways to reach the same idea.
- We want to constraint the weights

$$\underset{w}{\operatorname{argmin}} \frac{1}{N} \sum_i \left(y^{(i)} - w^T x^{(i)} \right)^2$$

$$\text{subject to } \|w\|_2^2 \leq t$$

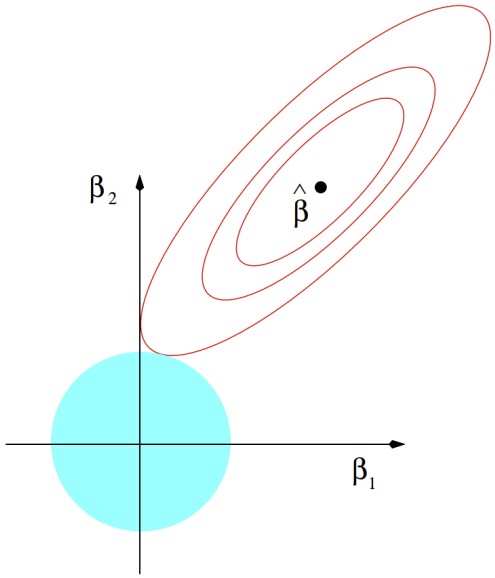


- Equivalent: Lagrange optimizer

$$\underset{w}{\operatorname{argmin}} \frac{1}{N} \sum_i \left(y^{(i)} - w^T x^{(i)} \right)^2 + \lambda \|w\|_2^2;$$

$$\hat{w} = (X^T X + \lambda I_d)^{-1} X^T \boldsymbol{y}$$

- Which is equivalent to assuming a Gaussian prior on **w** and do *maximum a posteriori (MAP)*



Bayesian interpretation

- Remember the Maximum Likelihood

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log p(\boldsymbol{y}|X, w)$$

- We can specify a prior over the model parameters $p(w)$
  - For example, avoid large values $p(w) \sim \mathrm{N}(0, \tau^2 I_d)$
- Use Bayes's rule to compute the posterior

$$p(w|\boldsymbol{y}, X) = \frac{p(\boldsymbol{y}|X, w)p(w)}{p(\boldsymbol{y})} \propto p(\boldsymbol{y}|X, w)p(w)$$

- Maximum a posteri

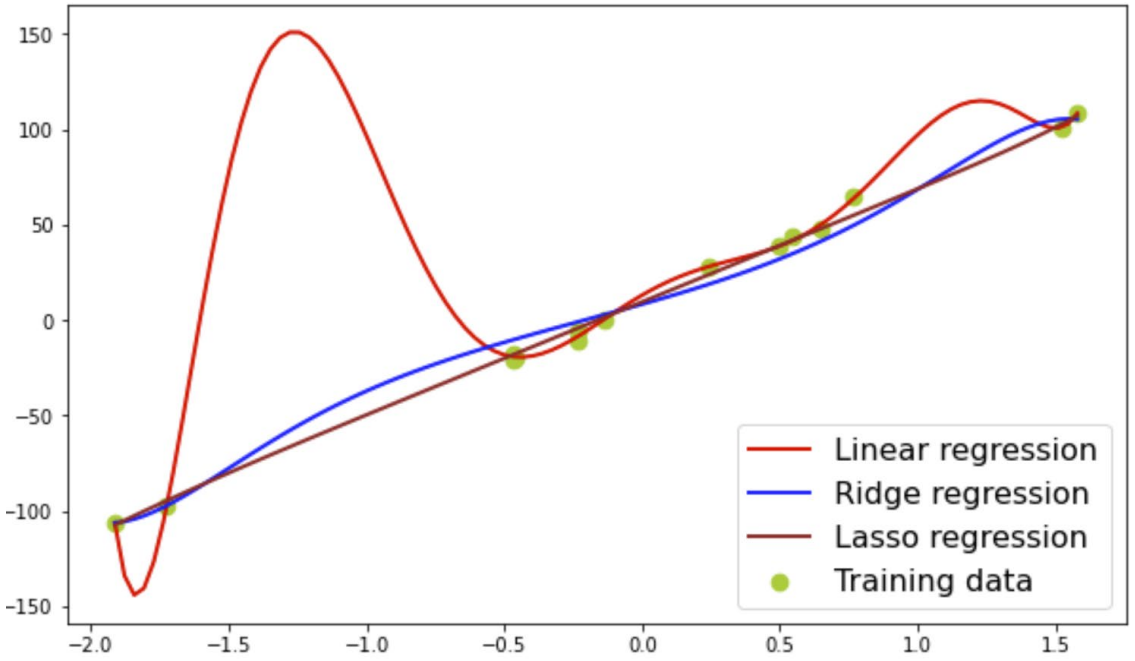
$$\hat{w} = \underset{w}{\operatorname{argmax}} \log p(w|\boldsymbol{y}, X)$$

$$\hat{w} = (X^T X + \lambda I_d)^{-1} X^T \boldsymbol{y} \qquad \text{with: } \lambda = \frac{\sigma^2}{\tau^2}$$

Ridge Regression

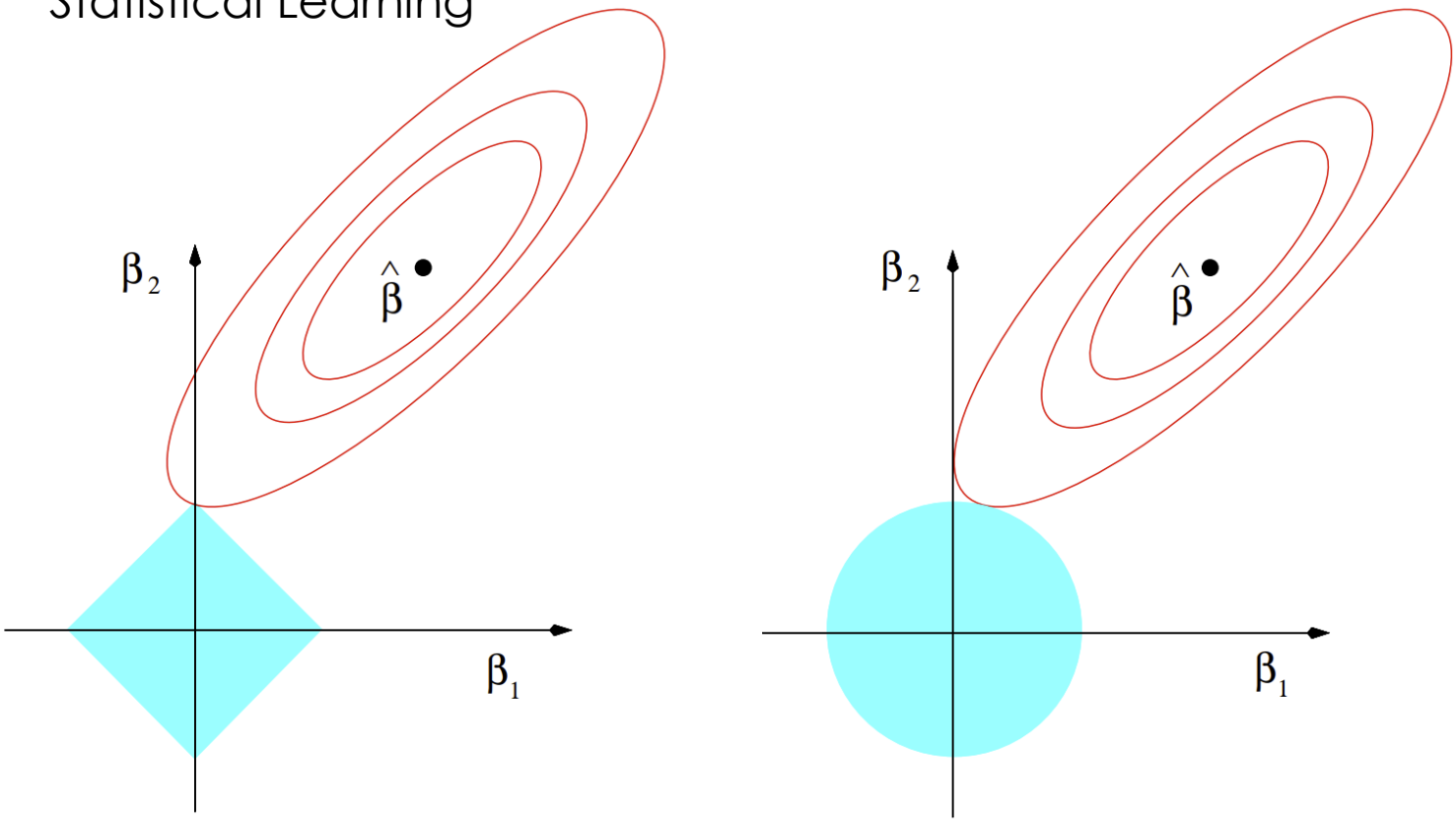
Colab link:
https://drive.google.com/file/d/1EnrFqx8Ks0L3-Uy99IB6DJ4DdEHyP5pl

- Avoids overfitting
- $\lambda w^T w = \lambda \|w\|_2$ similar to "weight decay" in deep learning
- $\lambda \|w\|_1$ LASSO (Least Absolute Shrinkage and Selection Operator)
  - Assumes a Laplacian distribution prior for the weights (then $\lambda = \frac{2\sigma^2}{b^2}$)
  - Can assign zero values to some coefficients (feature selection)



L1 norm leads to sparse models

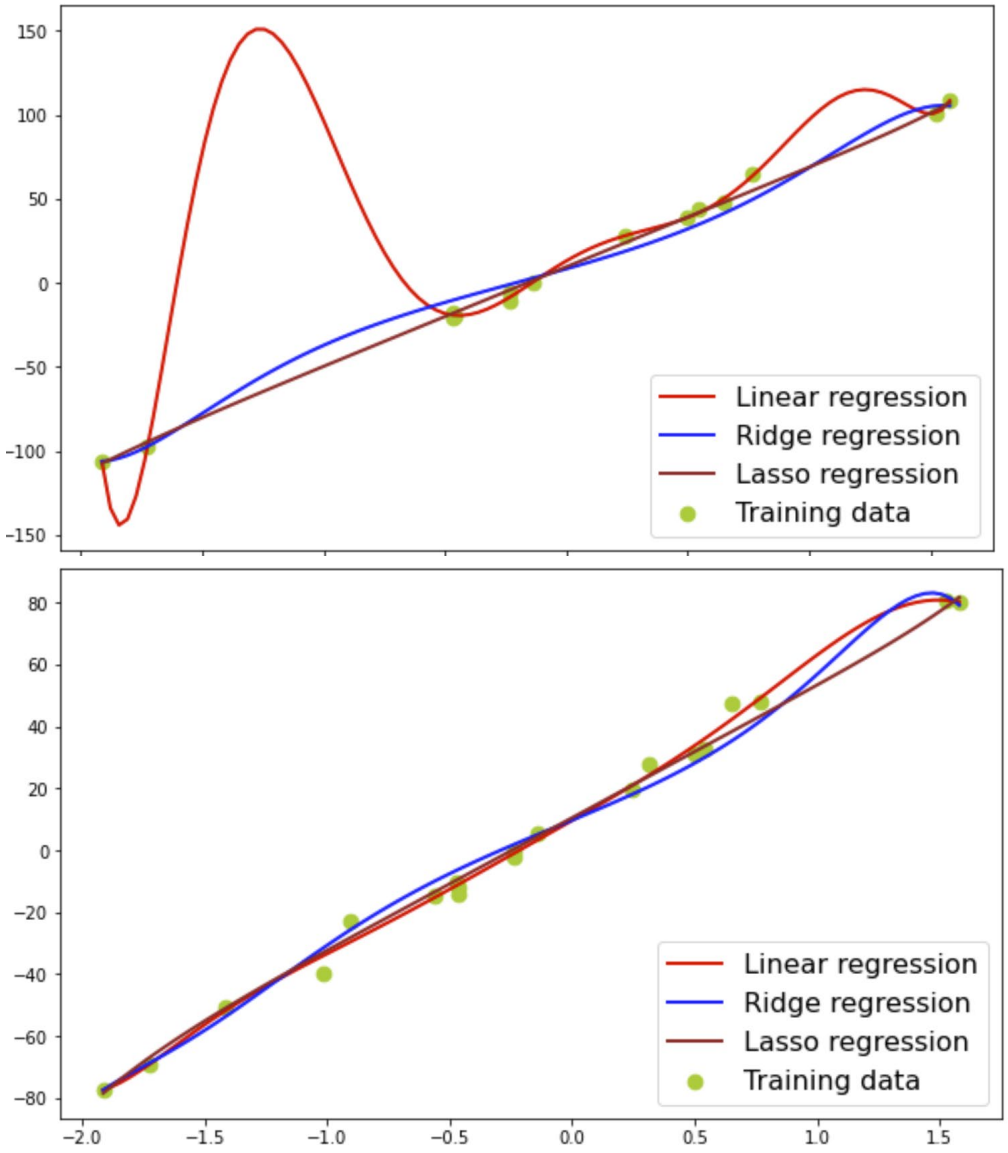
- Sparse models
  - Some coefficients are equal to zero
  - Feature selection → uninformative features are given zero weight
  - Geometrical interpretation: Fig. 3.11, Hastie et al., The Elements of Statistical Learning



Data regularization

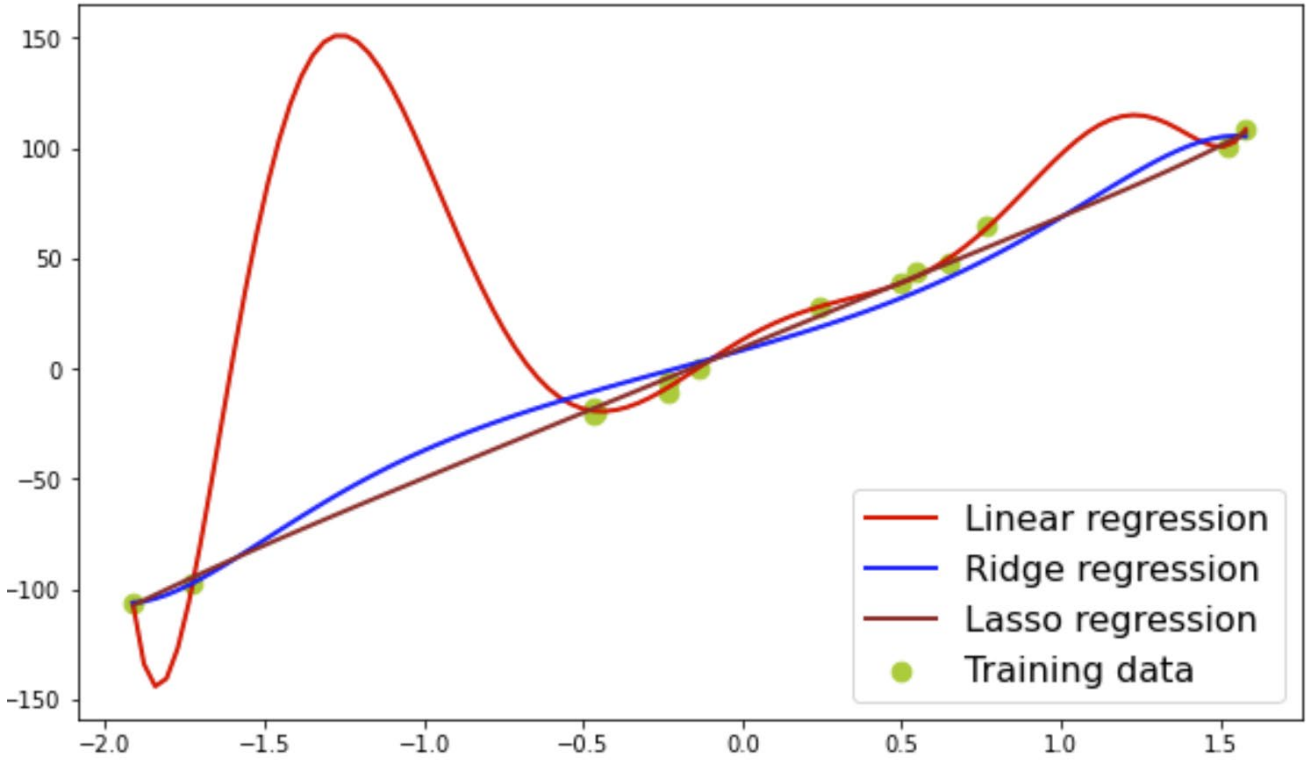
Colab link:
https://colab.research.google.com/drive/1j3kYQAHeGSbEFf66U_f2P9wlSatT1Erl

- BTW, in this example, check the regularization effect of adding more data
  - 15 data samples
  - 20 data samples



Summary: avoiding overfitting

- Do cross-validation to select the best model
- Add constraints that do not involve training data (e.g., weight decay)
- Add more training data!

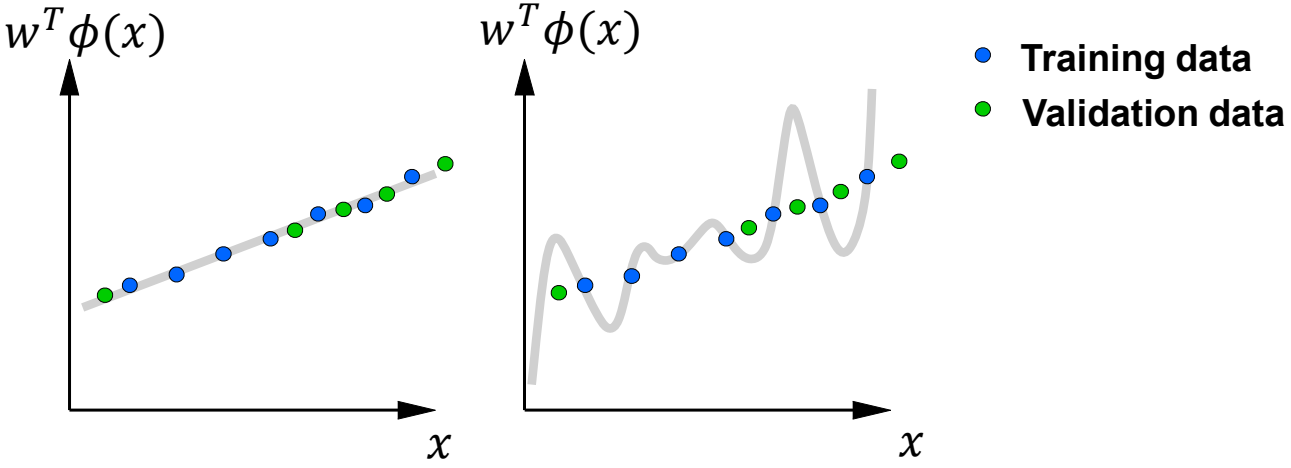


Hyperparameter and model selection

- How do we select λ regularizer?
  - … or the model complexity?
  - … or other hyperparameters* of the learning process?

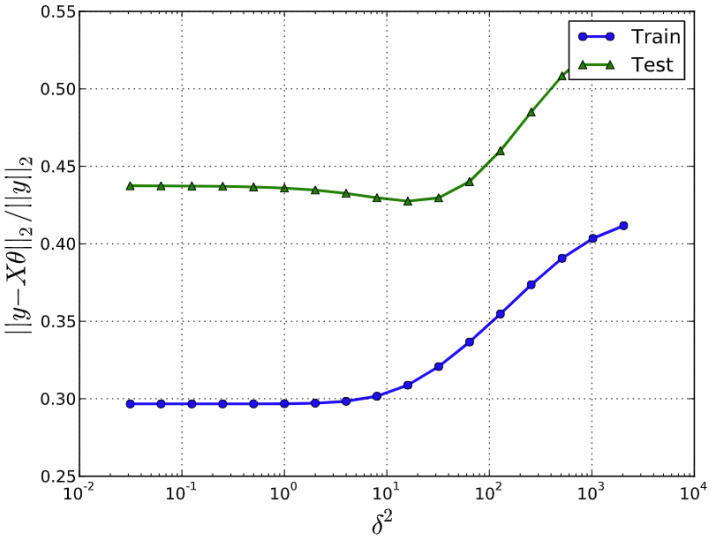
* Hyperparameters are all the model/algorithm numbers that we select that are not part of the trainable parameters w

- Remember to partition the data: train/validation/test!
  - The **training set** is used to estimate the model parameters w
  - The **validation set** is used to decide among a set of hyperparameters (models)
  - What we care about is generalization! → Final performance metrics should be given for a **test set**



Cross-validation

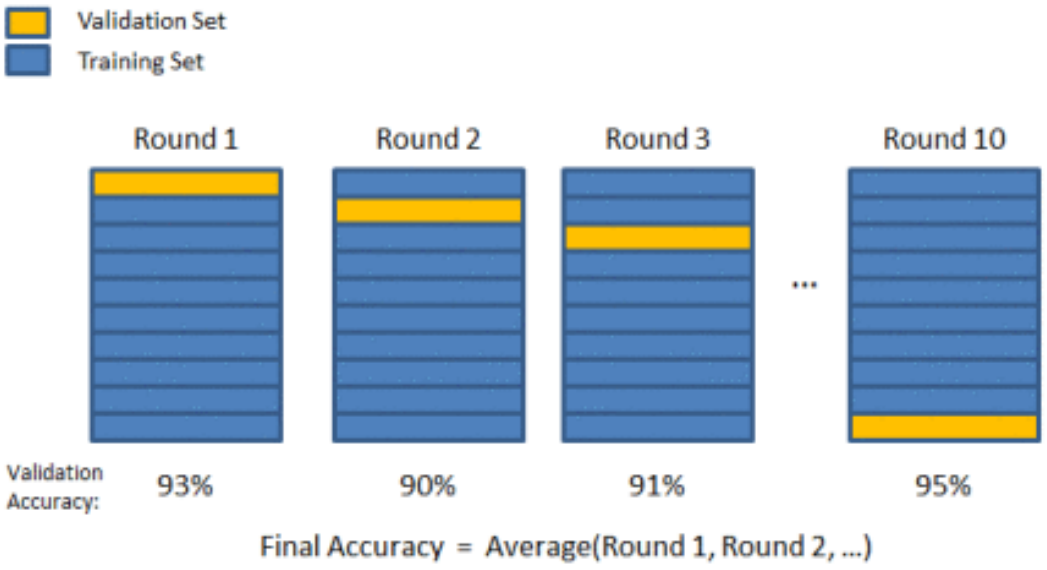
- Compute evaluation metrics (e.g. : prediction error) on the validation data for different hyperparameters/models



- How do we explore the hyperparameter space?
  - Randomly
  - Exhaustively
  - Intelligently ← Check Bayesian optimization slides!

K-fold cross-validation

- Common practice to have a higher degree of invariance to the validation/test split.
  - Separate the data into k folds
  - Do k training-validation rounds. A usual value for k is 10.
  - The validation/training sets are changed each round.
  - Metrics are averaged over all folds.
  - If k=N, the we have **leave-one-out cross-validation** or LOOCV



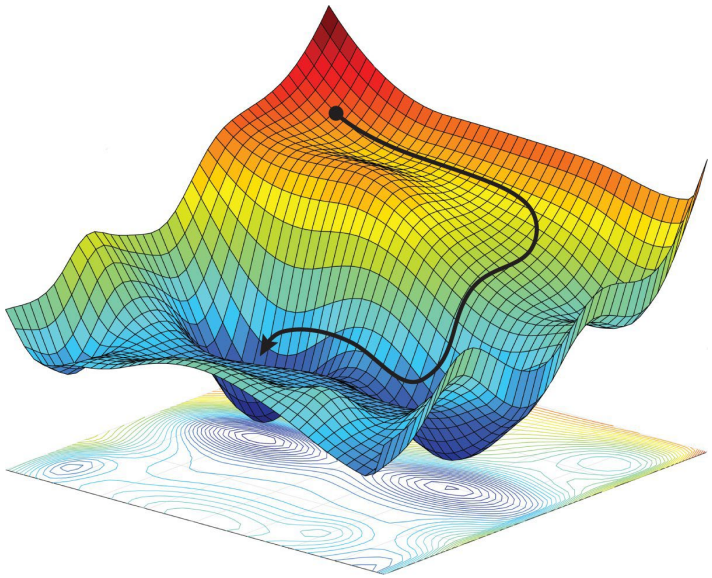
Remainder: data splits

- Training data (~80% of the data)
  - Used to learn the model parameters
- Validation (~10% of the data)
  - Used to select the hyper-parameters
  - After used, can be added to the training data to train the final model
  - Training/validation splits can change during training (k-fold cross-validation)
- Test (~10% of the data)
  - Never used at the training stage!
  - Used to obtain the final specs of our model
  - After used, can be added to the training data to train the final model

Analytical solution may not work…

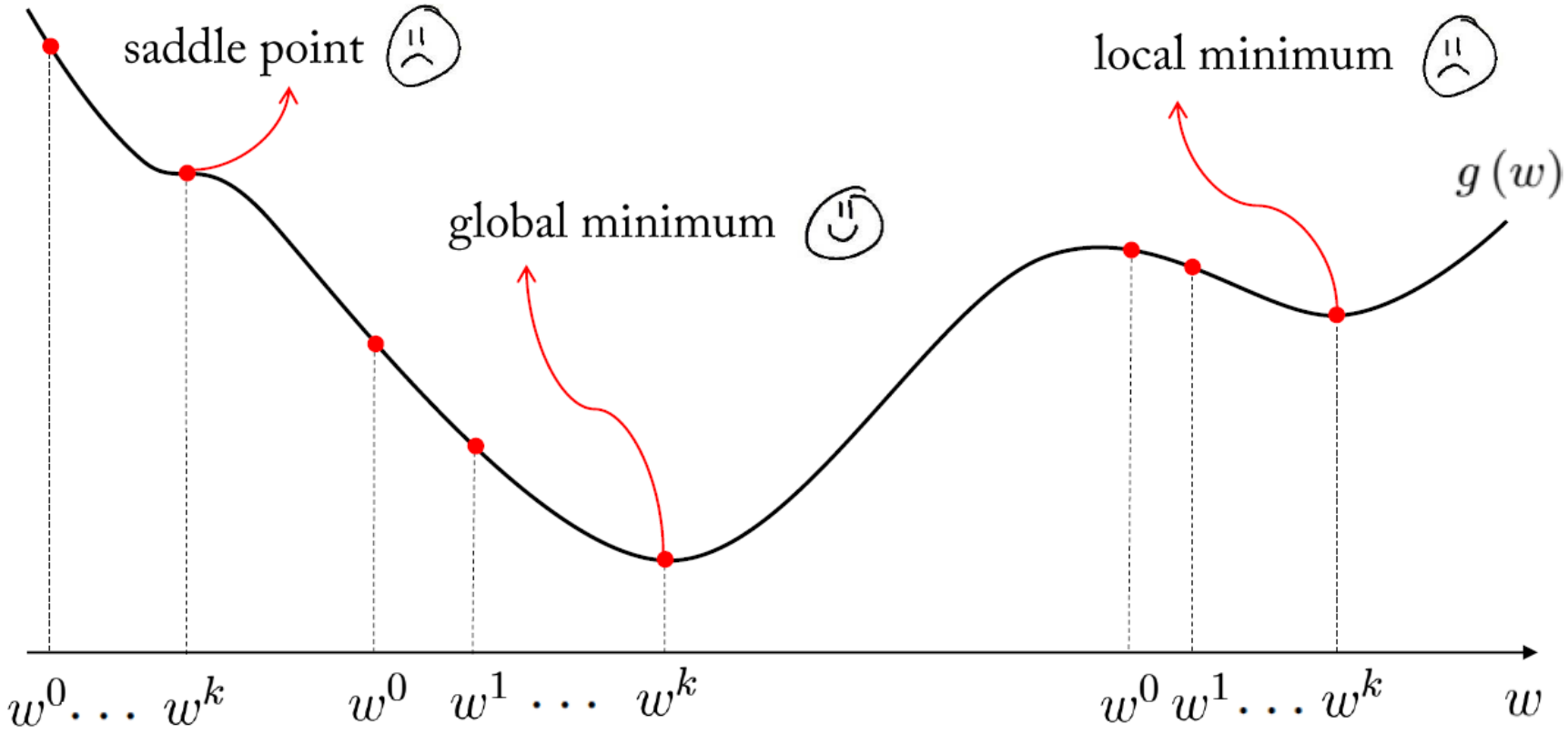
- Most algorithms in Machine Learning do not have an analytical solution.

- Large datasets → Huge $X^T X$ matrix
  - Minimization avoids computing inverse $(X^T X)^{-1}$
  - Follow the gradient $\nabla J(w)$
  - We can even optimize one data point at a time



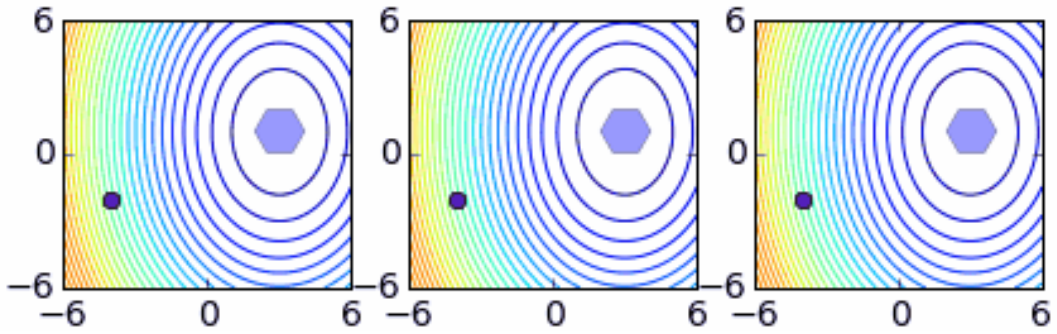
Gradient descent

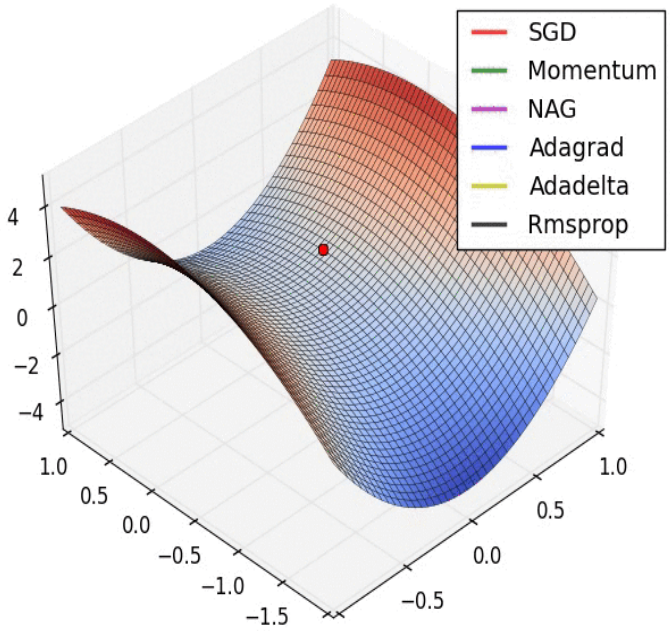
- Gradient descent → Iterative weight updates in the downward direction, $w_{k+1} = w_k - \eta_k \nabla J(w)$
- In general, it converges to a local minimum



Gradient descent

- Issues:
  - Select the initial seed w_0
  - Select the learning rate η_k
    - Small $\eta_k \rightarrow$ slow convergence, large $\eta_k \rightarrow$ fail to converge





Stochastic gradient descent

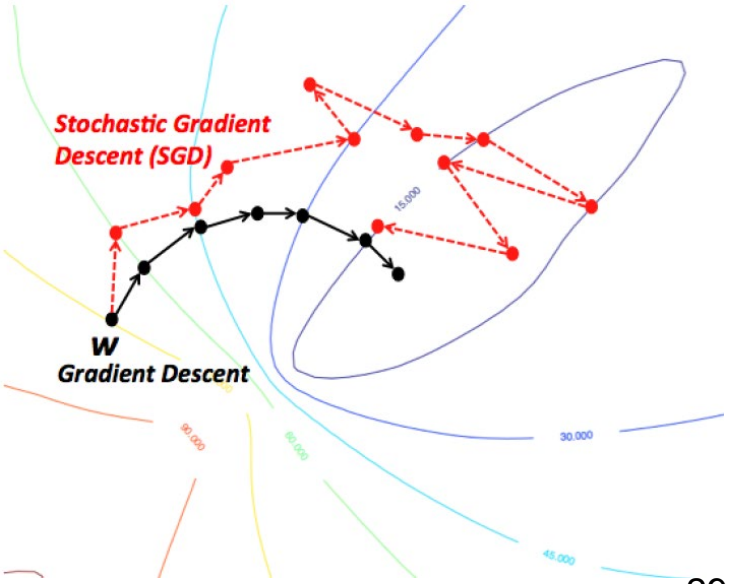
- Remember:

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log \prod_{i=1}^{n} p(y_i|\boldsymbol{x}_i, w) = \underset{w}{\operatorname{argmax}} \sum_{i=1}^{n} \log p(y_i|\boldsymbol{x}_i, w)$$

- We are computing a loss based on an expectation

$$\hat{w} = \underset{w}{\operatorname{argmax}} \mathbb{E}[\log p(y_i|\boldsymbol{x}_i, w)]$$

- Then, we can optimize one data at a time and still find the optimum.
- One of the most important algorithms in the last decades!

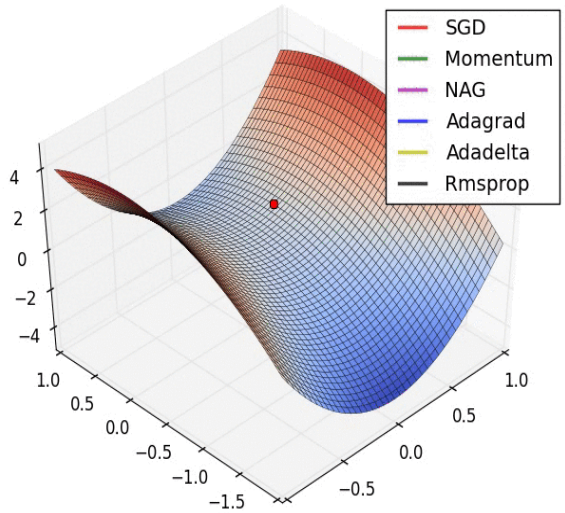


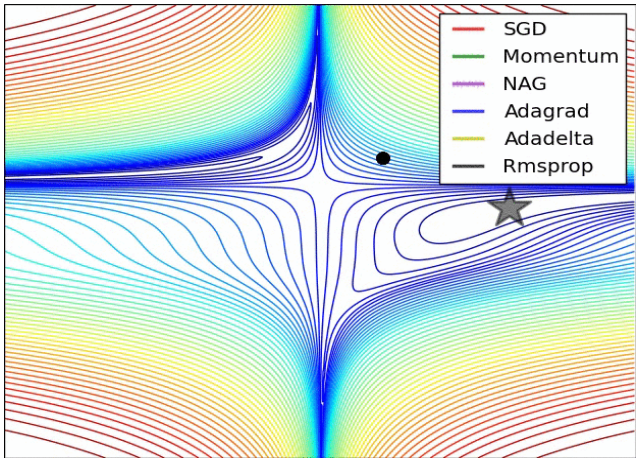
Stochastic gradient descent

- In our linear-Gausssian case

$$\nabla J_i(w) = -2\boldsymbol{x}_i(\boldsymbol{x}_i^T\boldsymbol{w} - y_i)$$

- Highly efficient for large datasets.
- **WARNING!**
  - At each iteration, we must use data **independent** from previous iterations.
  - For example, select data **randomly** from training set.
- Random → Might avoid local minima and saddle points!
- Every time we go over all data points is called an **epoch**.





GD vs SGD

- Batch gradient descent
  - Expensive for large datasets
  - N → whole dataset
  - Low variance

$$w_{k+1} = w_k - \eta_k \sum_{i=1}^{N} \nabla J_i(w)$$

- Stochastic gradient descent
  - Cheap but more grad steps
  - Might avoid local optima
  - High variance/fluctuations

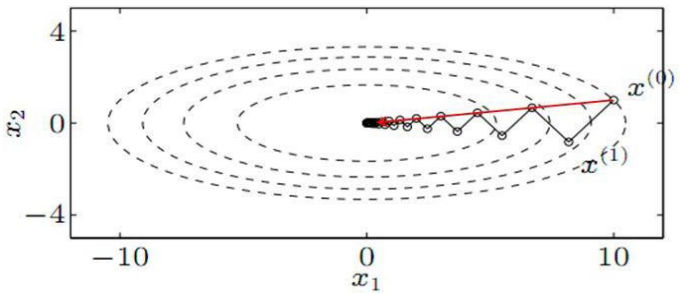
$$w_{k+1} = w_k - \eta_k \nabla J_i(w)$$

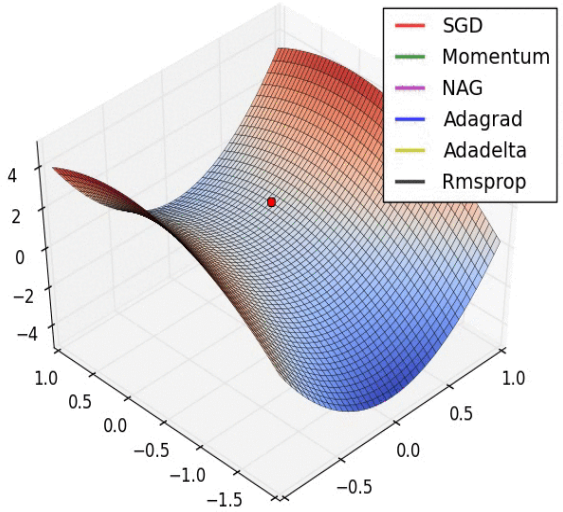
- SGD with mini-batch
  - Best of both worlds
  - Choose a small batch size ($n = 2, 4, 8, \dots, 128, 256, \dots$)

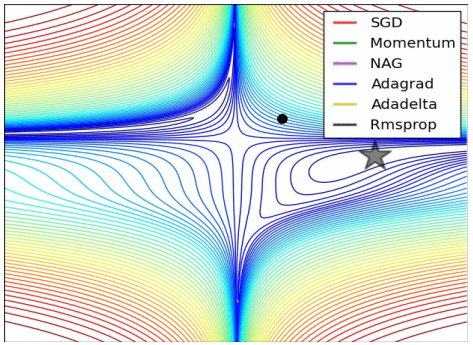
$$w_{k+1} = w_k - \eta_k \sum_{i=1}^{n} \nabla J_i(w)$$

SGD variants

- Momentum can stabilize/smooth SGD variance
- Adaptive methods adapt the learning rate for each feature depending on the estimated geometry of the problem.
- Many in ML libraries: AdaGrad, AdaDelta, RMSProm, Adam,…







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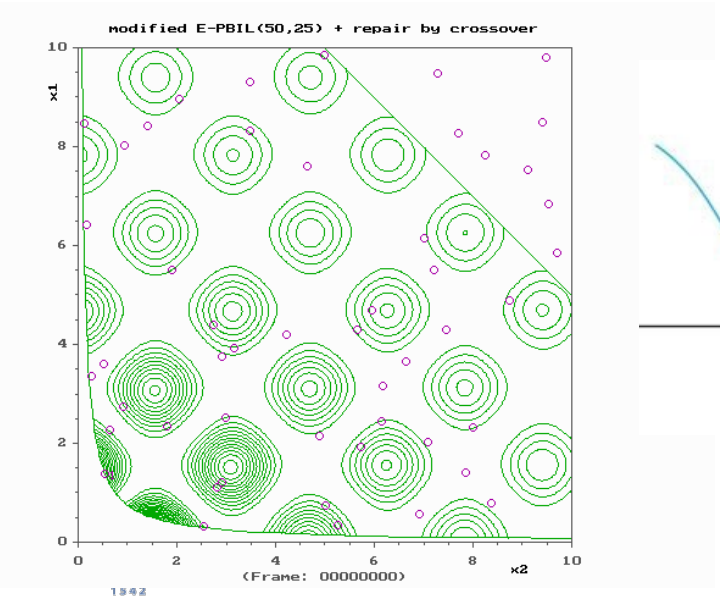
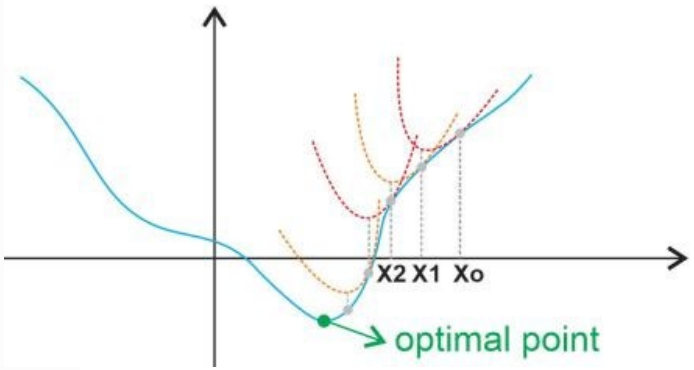
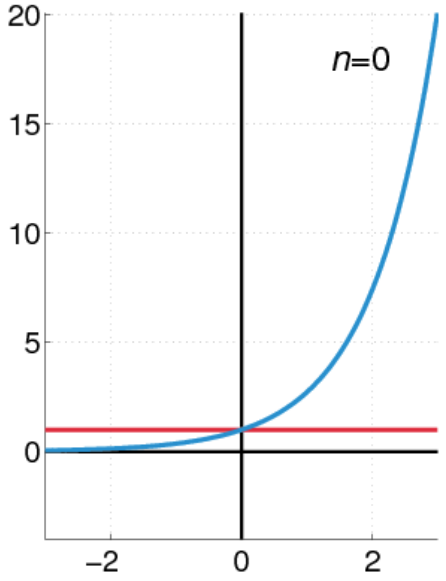
Other optimization algorithms

- They are ALL very computationally intensive for large models/data.
- Bayesian optimization → Later in the course. ☺
- Evolutionary algorithms
  - No need for gradient. Global optimization. Poor dimensional scaling.
- Second order methods:
  - Newton, Conjugate Gradient, BFGS, L-BFGS,...
  - They approximate the Hessian (second derivative of cost)

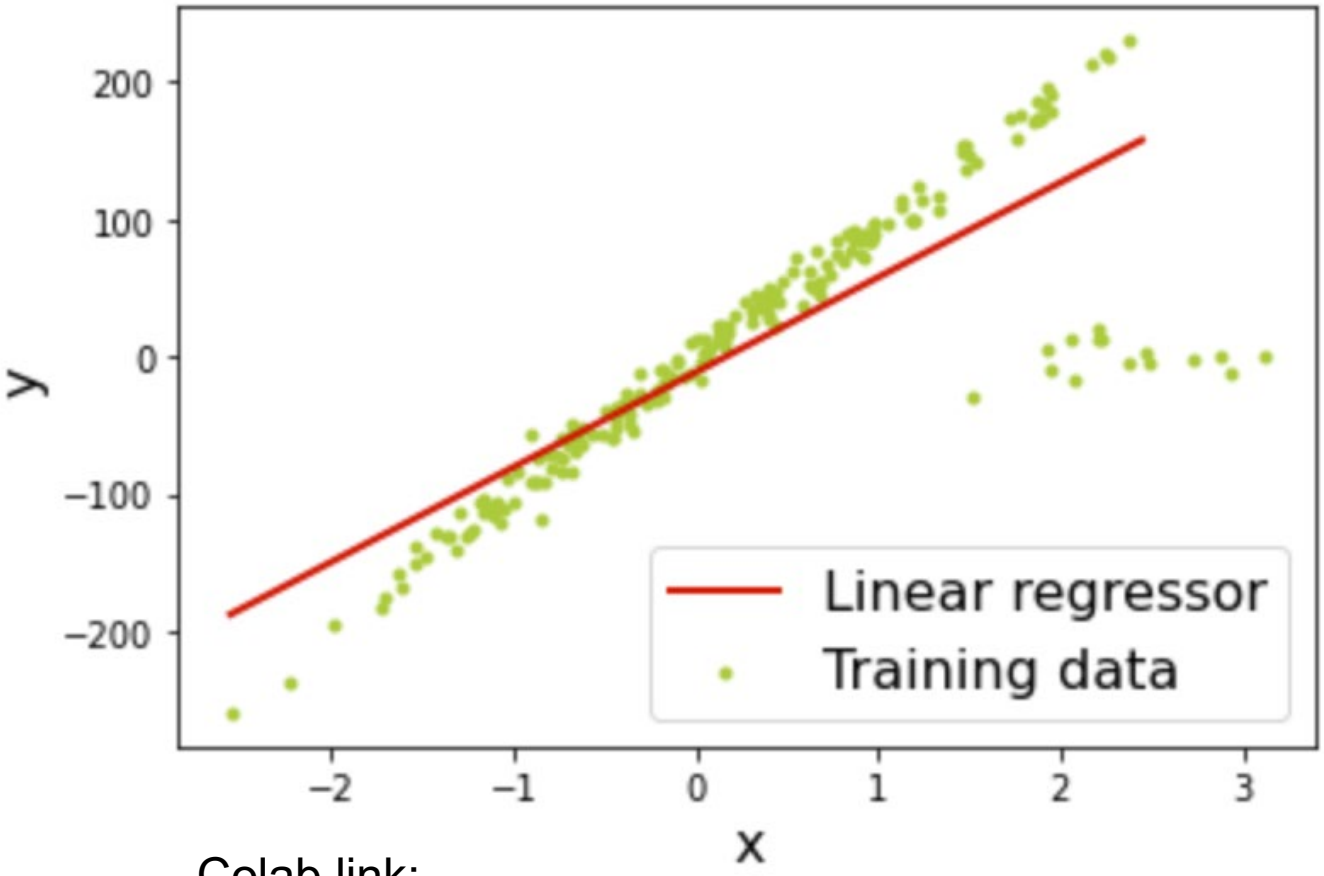






Robust Regression

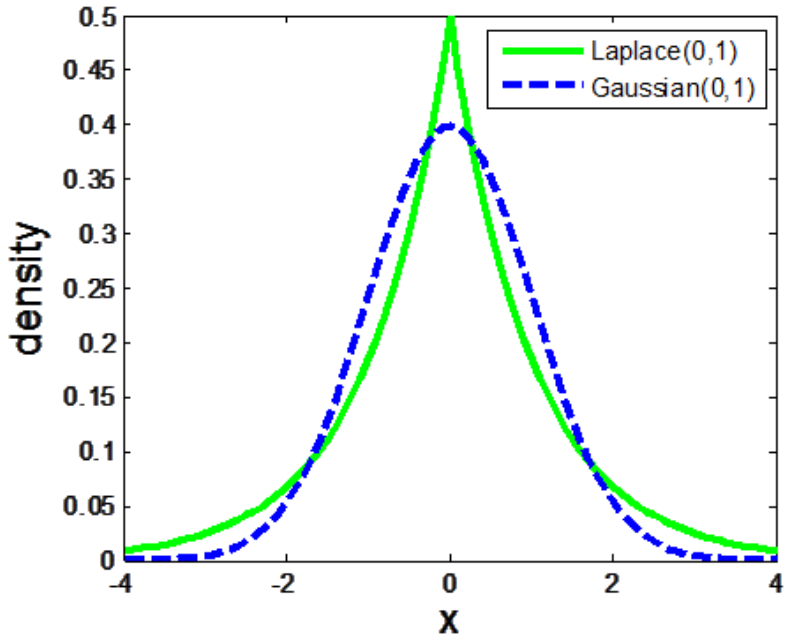
- The quadratic error penalty from the Gaussian noise gives a high weight to outliers



Colab link:
https://drive.google.com/file/d/1G5E6QHihfK1TyaYe6dxlF2FF5XC1kXn-

Robust Regression

- Probabilistic view: The low tolerance of Gaussian pdfs for high-noise data samples causes problems with outliers
- One possible solution: assume longer-tailed distributions, e.g., Laplace, Student's t, etc.
- Other: detect outliers and remove them
  - You will learn about RANSAC in the computer vision course



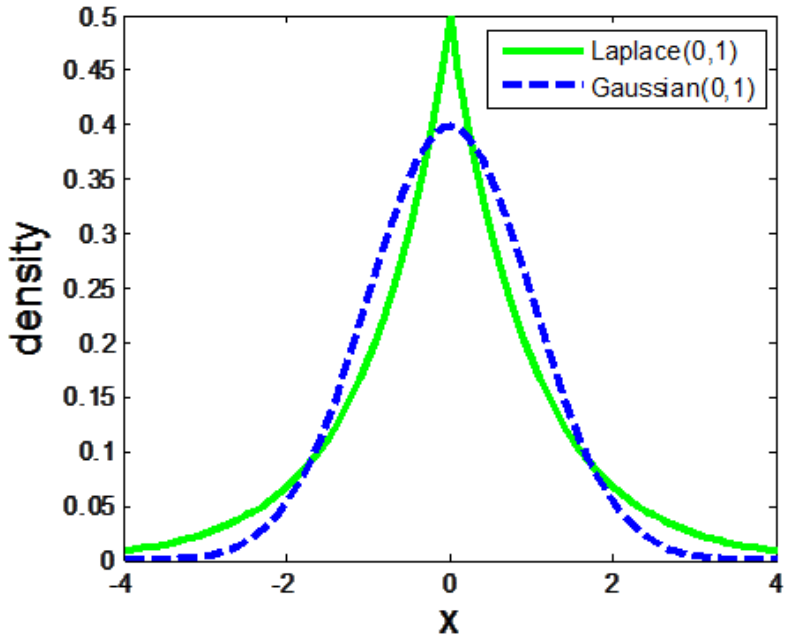
Robust Regression

- Laplace distribution:

$$p\left(y^{(i)}\middle|x^{(i)},w\right)=\exp\left(-\frac{1}{2b^2}\left|y^{(i)}-w^Tx^{(i)}\right|\right)\rightarrow\cdots\rightarrow$$

$$J(w)=\frac{1}{2}\sum_i\left|y^{(i)}-w^Tx^{(i)}\right|=\sum_i\left|r^{(i)}\right|$$

- Non-linear, hard to optimize!



Robust Regression: Huber loss function

- Equivalent to L2 near zero, to L1 for large errors

$$r^{(i)} = \begin{cases} \frac{r^{(i)^2}}{2} & if\ |r| \leq \delta \\ \delta|r| - \frac{\delta^2}{2} & if\ |r| > \delta \end{cases}$$

- Differentiable!

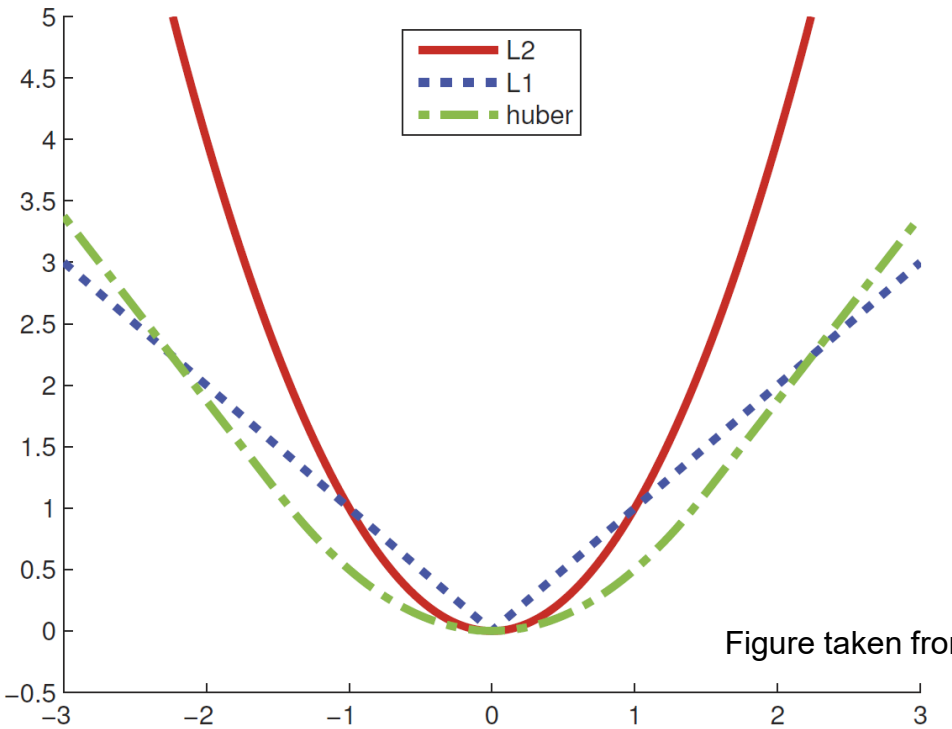
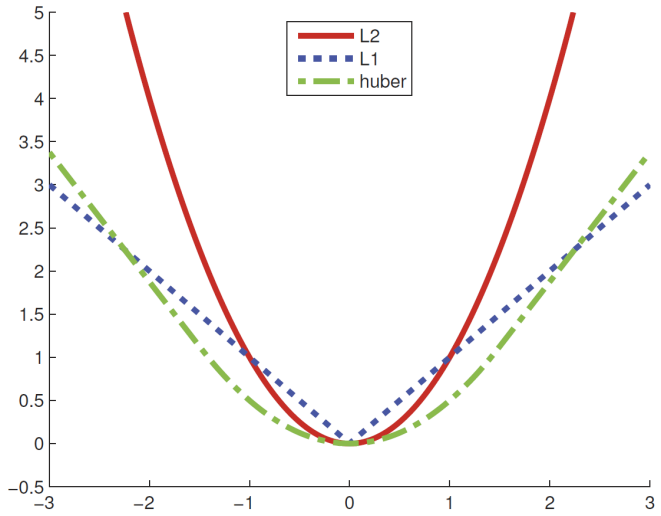


Figure taken from Murphy's book

Huber loss function

- How do we tune the parameter δ?

$$r^{(i)} = \begin{cases} \dfrac{{r^{(i)}}^2}{2} & if\ |r| \le \delta \\ \delta|r| - \dfrac{\delta^2}{2} & if\ |r| > \delta \end{cases}$$



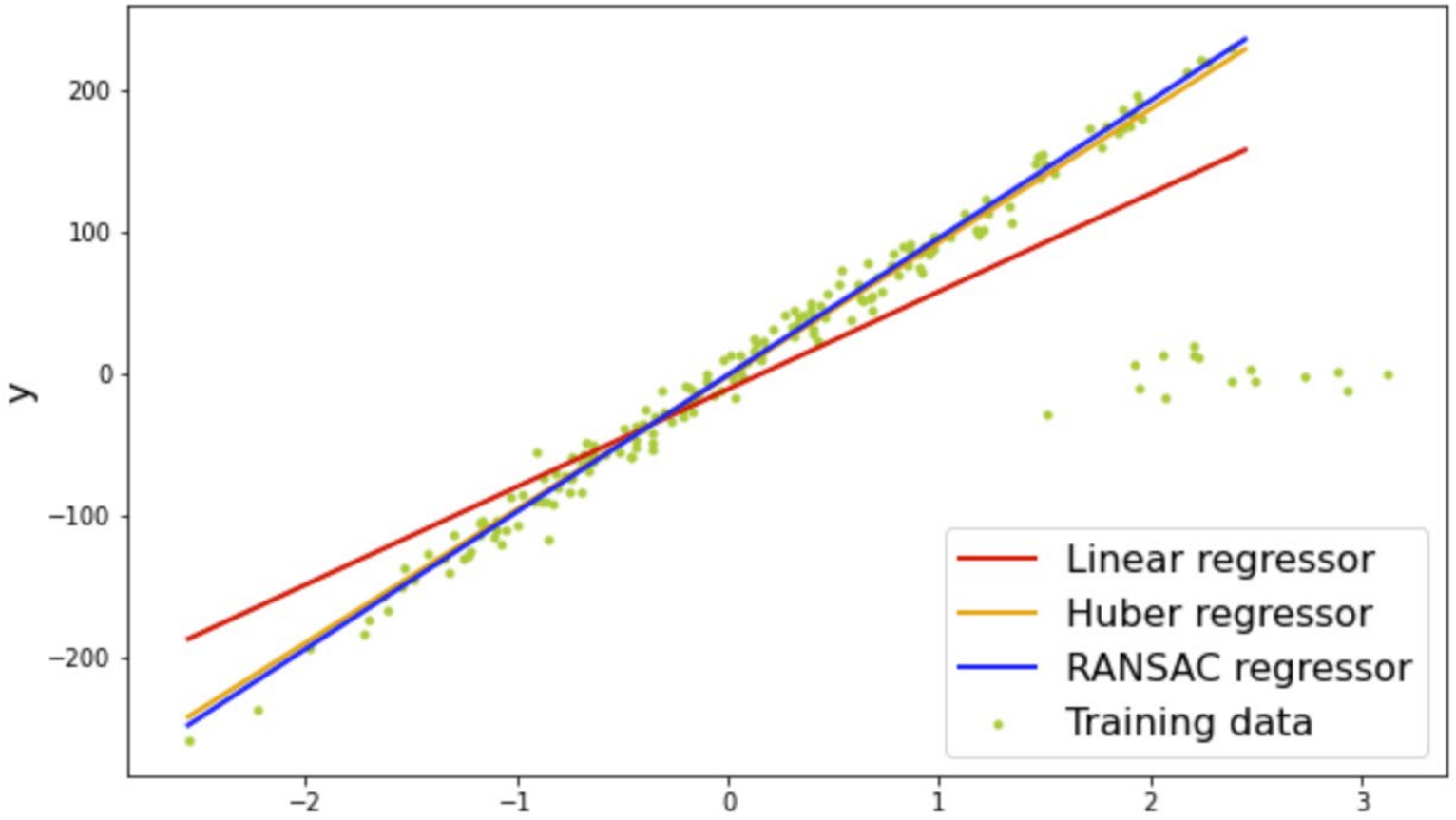
- δ is the "boundary" between inliers (Gaussian pdf assumed) and the outliers (Laplacian pdf assumed). So:

1. [Huber 1981], says: "good choices are between σ and 2σ"
   - σ is the standard deviation of the residuals $r^{(i)}$ of the inliers
2. If you do not know σ, you estimate it from the training data residuals $r^{(i)}$.
   - IMPORTANT! You have outliers, so use a robust estimator for σ. MAD (Median Absolute Deviation) is common:

$$\hat{\sigma} = 1.4826 \cdot \mathrm{MAD}, \mathrm{MAD} = \mathrm{median}\left(\left|r^{(1)} - \tilde{r}\right|, \dots, \left|r^{(N)} - \tilde{r}\right|\right), \tilde{r} = \mathrm{median}\left(r^{(1)}, \dots, r^{(N)}\right)$$

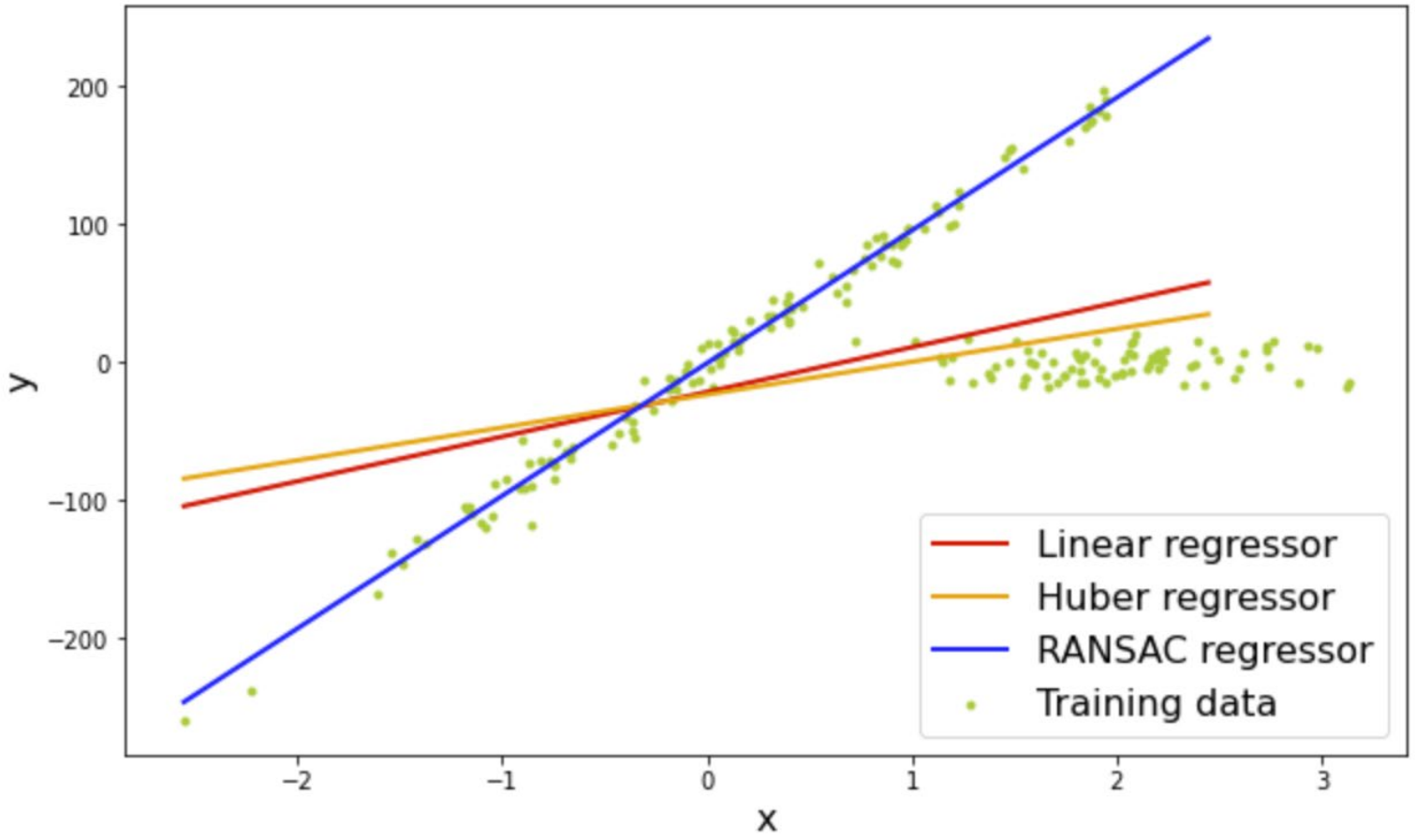
Robust regression example

- The Huber loss and RANSAC are robust to outliers



Robust regression example

- But RANSAC can tolerate a higher outlier ratio!



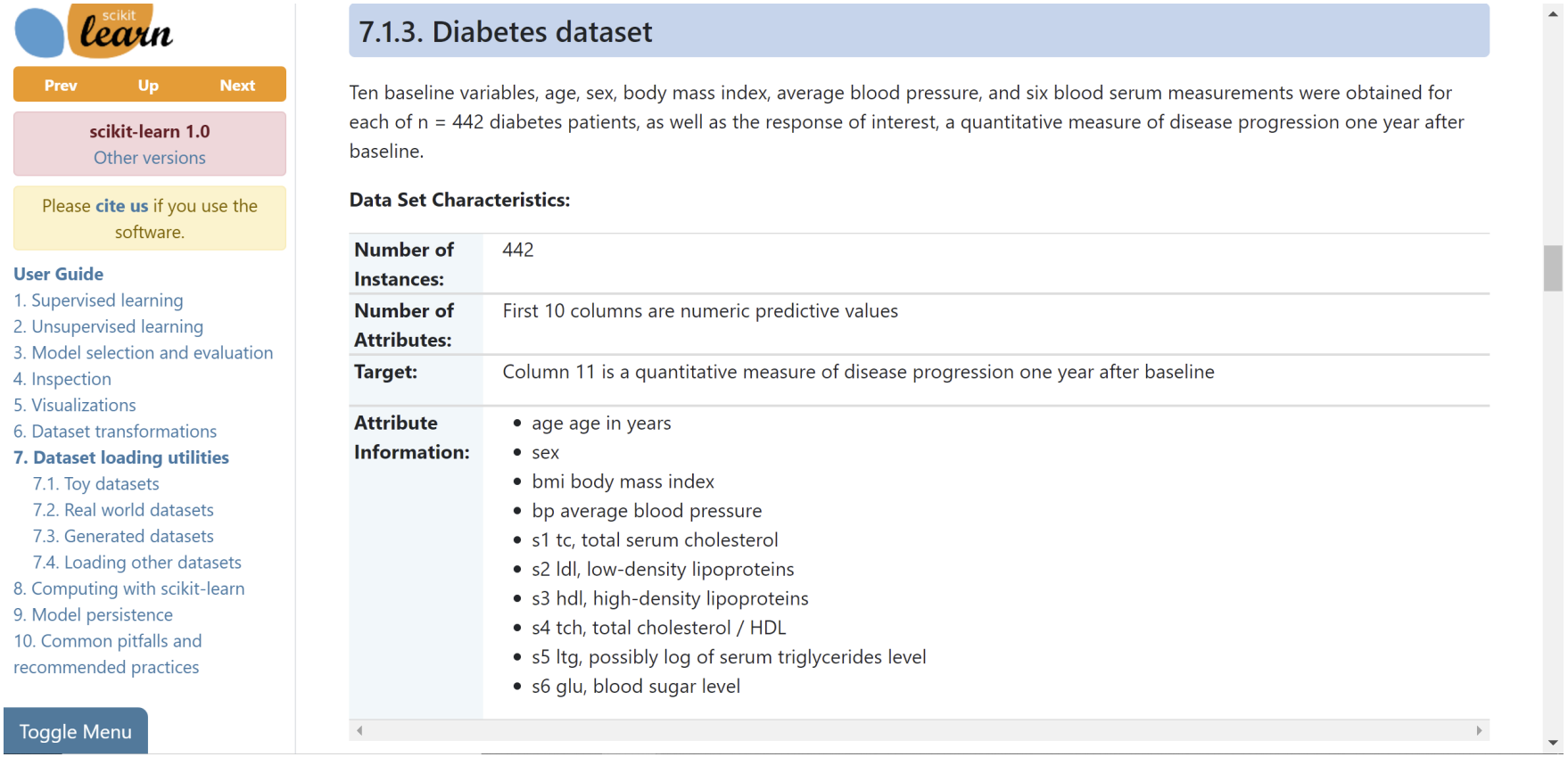
Regression metrics

- **Mean absolute error** $\rightarrow \frac{1}{N}\sum_{i=1}^{N}\left|y^{(i)} - w^T x^{(i)}\right|$
  - Small influence of large errors
- **Mean squared error** $\rightarrow \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T x^{(i)}\right)^2$
  - Highly influenced by large errors
- **Root mean squared error** $\rightarrow \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y^{(i)} - w^T x^{(i)})^2}$
- **Median absolute error** $\rightarrow \text{median}\left(\left|y^{(1)} - w^T x^{(1)}\right|, \ldots, \left|y^{(N)} - w^T x^{(N)}\right|\right)$
  - Robust to outliers!
- **R^2 score** $\rightarrow 1 - \frac{\sum_{i=1}^{N}\left(y^{(i)} - w^T x^{(i)}\right)^2}{\sum_{i=1}^{N}\left(y^{(i)} - \bar{y}\right)^2} \in [-\infty, 1], \bar{y} = \frac{1}{N}\sum_{i=1}^{N} y^{(i)}$
  - Proportion of variance in y explained by the variables of the model
- Many others! Maximum error, Mean absolute percentage error, explained variance score, etc.
- Compare against dumb baseline (mean of the training predictions?)

Regression example: The diabetes dataset

- Colab links:

Simple:
https://drive.google.com/file/d/1EIKbBCWetqEVKumrTX4GEpxdbRSFXwVw
With cross_validation, grid search and pipelines:
https://colab.research.google.com/drive/1xAhcsXMqoJD-sFRfGfMk-pB4FBuZE2Gf



scikit learn

Prev Up Next

scikit-learn 1.0
Other versions

Please cite us if you use the software.

User Guide
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2. Unsupervised learning
3. Model selection and evaluation
4. Inspection
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   7.4. Loading other datasets
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Toggle Menu

7.1.3. Diabetes dataset

Ten baseline variables, age, sex, body mass index, average blood pressure, and six blood serum measurements were obtained for each of n = 442 diabetes patients, as well as the response of interest, a quantitative measure of disease progression one year after baseline.

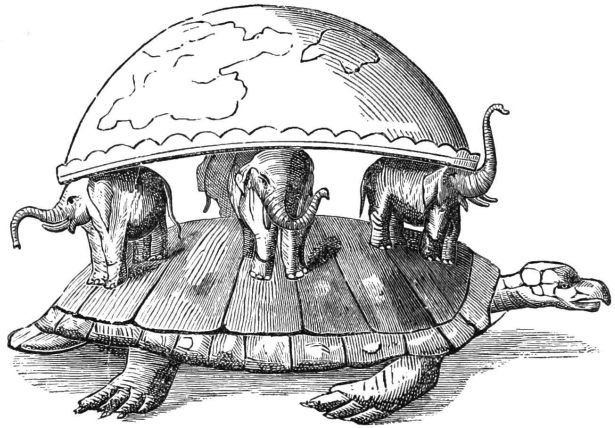
Data Set Characteristics:

Number of Instances:	442
Number of Attributes:	First 10 columns are numeric predictive values
Target:	Column 11 is a quantitative measure of disease progression one year after baseline
Attribute Information:	• age age in years • sex • bmi body mass index • bp average blood pressure • s1 tc, total serum cholesterol • s2 ldl, low-density lipoproteins • s3 hdl, high-density lipoproteins • s4 tch, total cholesterol / HDL • s5 ltg, possibly log of serum triglycerides level • s6 glu, blood sugar level

Bayesian Ridge Regression and ADR?

- They show the best performance in the Diabetes dataset!
- In the MAP estimate, we have a prior and likelihood with some parameters (noise, prior variance, etc.)
- Can we set up a prior on those parameters?

- Yes! That is called **hierarchical Bayesian model**!
  - *Turtles all the way down…*
  - We'll come back in the Bayesian learning, part



Data standardization

- Many ML algorithms (SVM, L2/L1 regularization) assume all dimensions of x has zero-mean and similar covariance.
- It also helps numerically.
- Most usual standardization:

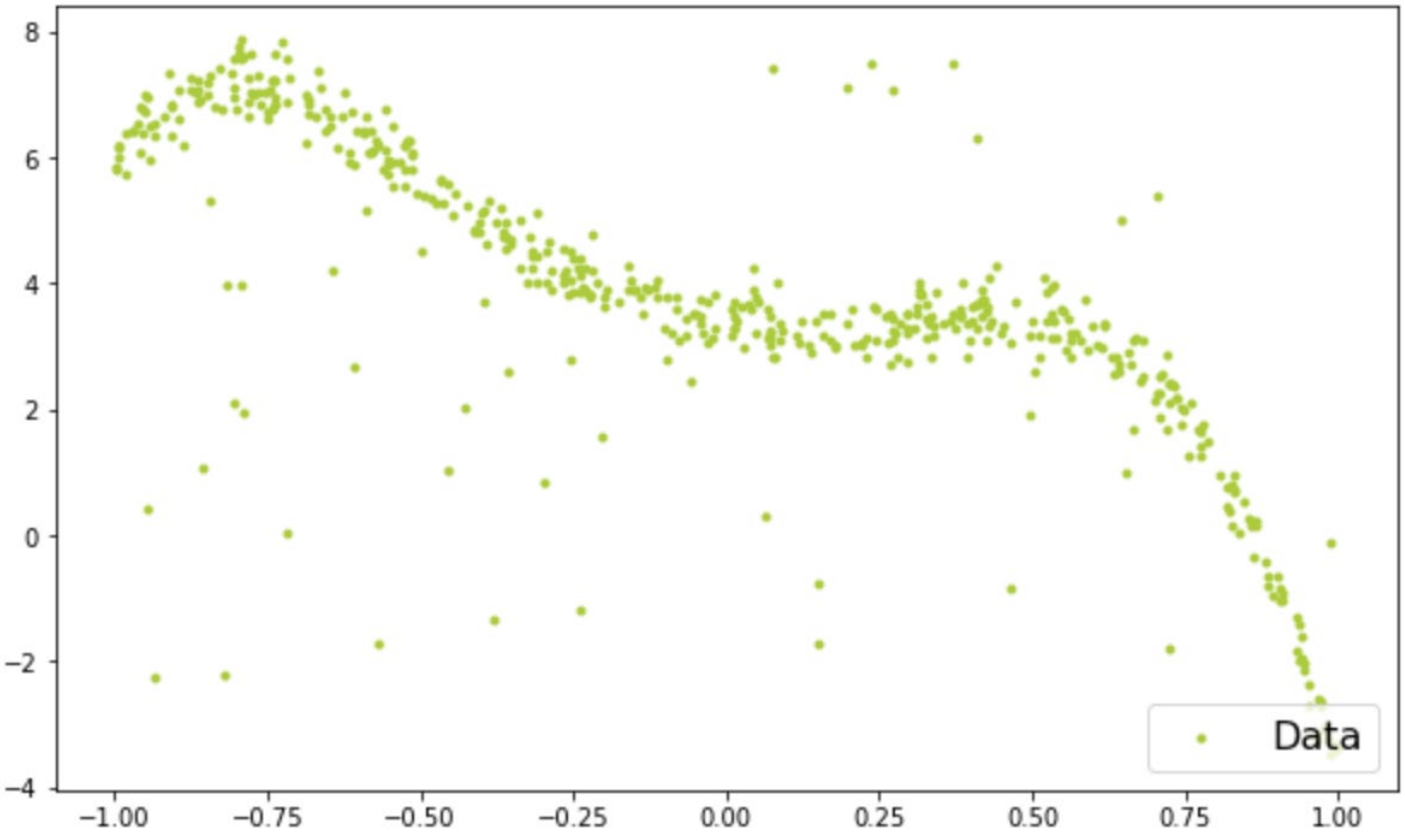
$$x = (1, x_1, \cdots, x_d)^T \rightarrow x' = (1, x'_1, \cdots, x'_d)^T$$

$$x'_j = \frac{x_j - \mu_j}{\sigma_j}$$

- For more details, you can check https://scikit-learn.org/stable/modules/preprocessing.html
  - For example, for data with outliers, you should use robust estimates for mean and covariance

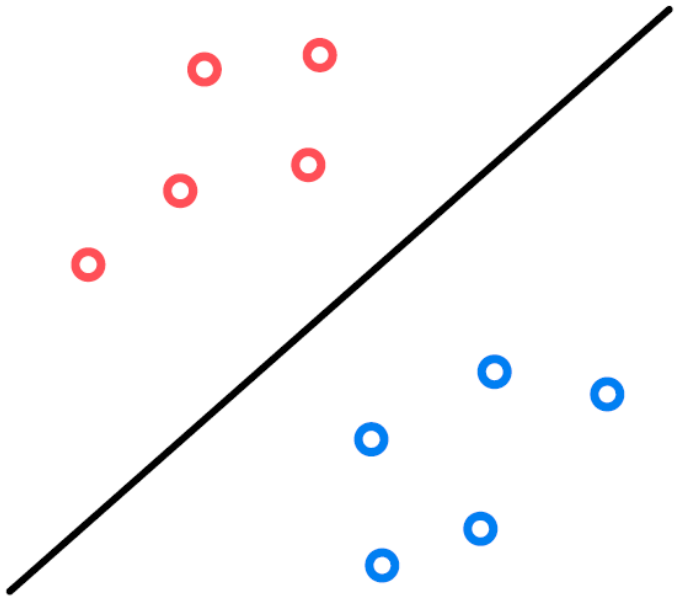
Exercise: Fit a polynomial model

- Link to Colab: https://drive.google.com/file/d/1G1N9C9Yry-3Lc9A1mL5yawM1rDB6TnKM
- Link to data: https://drive.google.com/file/d/1G_XseoB0lhII21jGdEkSYQyaEtMoSfQy



Linear Classification

- Classification: The output of the learned model is discrete
- Linear classification: The model is based on a linear combination of the input features
- Intuition: there is an hyperplane $\pi \in \mathbb{R}^{d-1}$ (e.g., a line for a 2D space) that separates the two classes/categories.

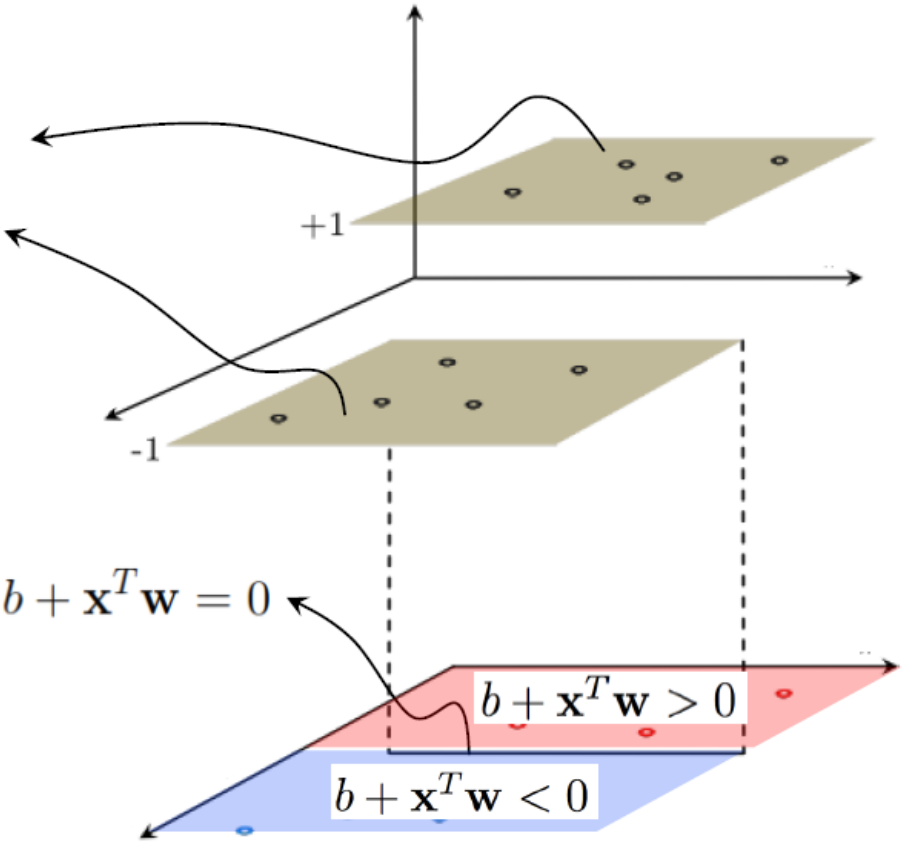


Binary Classification (intuition)

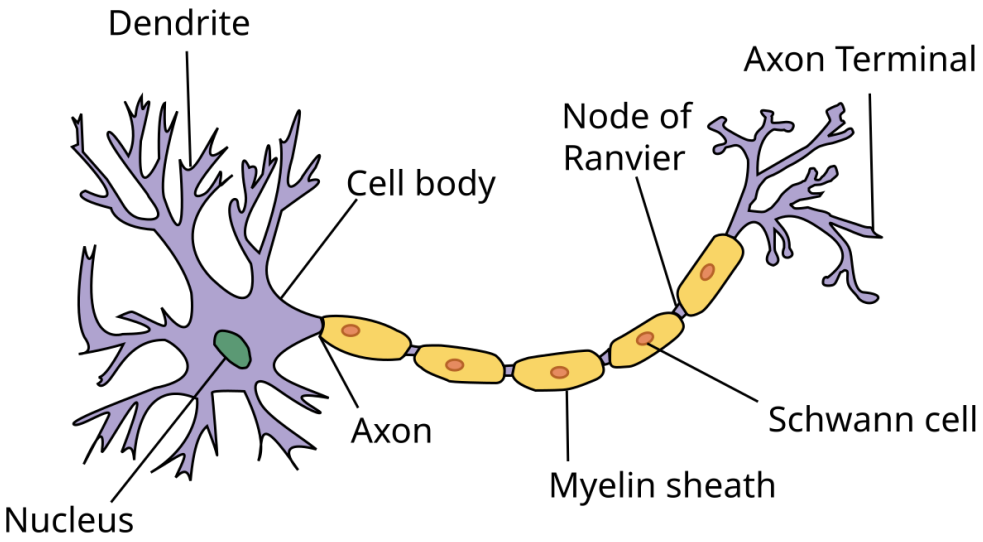
- We can get a discrete output $y \in \{-1, +1\}$ by taking the sign of the signed point-to-hyperplane distance
- The linear decision boundary is perpendicular to w
- The formulation can be extended easily to multi-class

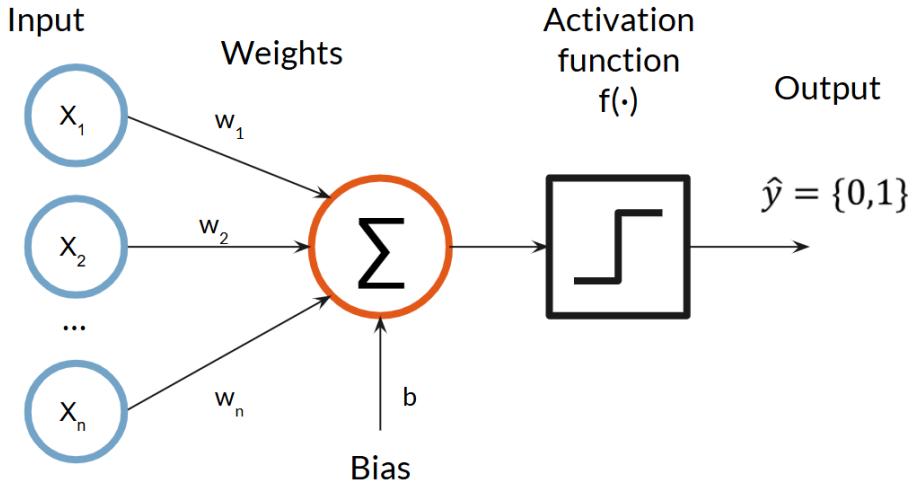
$$y(\mathbf{x}) = \text{sign}\left(b + \mathbf{x}^T\mathbf{w}\right)$$

Heaviside (step) function if $y \in \{0,1\}$



Perceptron (McCulloch-Pitts, 1943)

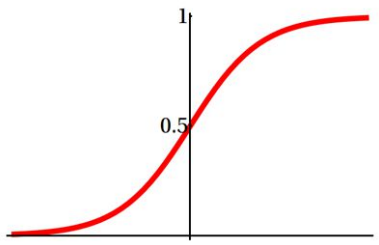




Activation functions

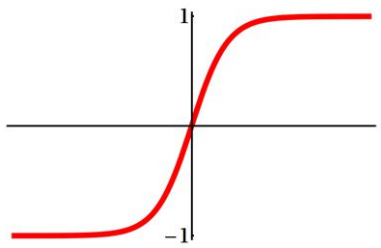
- Heaviside and sign() functions are not continuous.
  - Not differentiable!
- We can use continuous functions that approximate the sign function.
  - The sigmoid function
  - The tanh function
  - …

$$\sigma(\Sigma) = \frac{1}{1+e^{-\Sigma}}$$

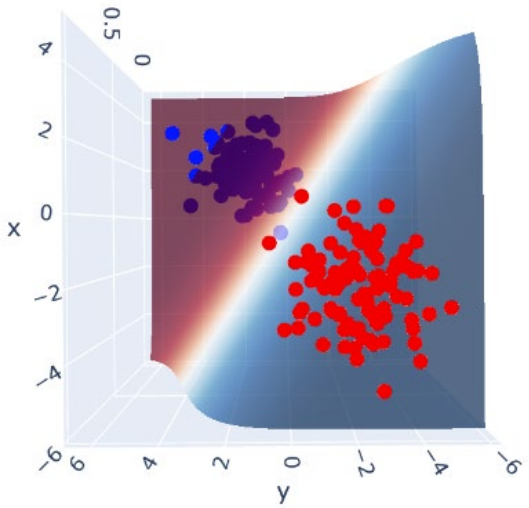


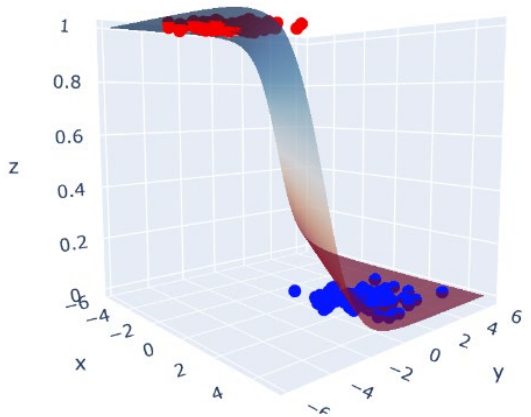
logistic (sigmoid, unipolar)

$$\tanh(\Sigma) = \frac{e^{\Sigma} - e^{-\Sigma}}{e^{\Sigma} + e^{-\Sigma}}$$



tanh (bipolar)





Logistic Regression (probabilistic interpretation)

- We can write the likelihood function as (see Math notes):

$$p(y|\boldsymbol{x}, w) = \text{Ber}(y|\lambda(\boldsymbol{x}))$$

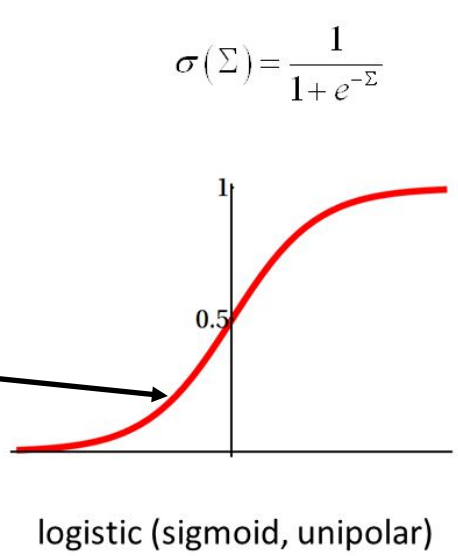
where $p(y = 1|\boldsymbol{x}) = \lambda(\boldsymbol{x})$ and $p(y = 0|\boldsymbol{x}) = 1 - \lambda(\boldsymbol{x})$

- The probability of the positive class is output of the sigmoid.

$$\lambda(\boldsymbol{x}) = \sigma(\boldsymbol{x}^\top w) = \frac{1}{1 + e^{-\boldsymbol{x}^\top w}}$$

Remember the trick to add a bias term $\phi(x) = [1, x]^T$

Probability of being class 1



logistic (sigmoid, unipolar)

Logistic Regression (probabilistic interpretation)

- We can write the likelihood function as (see Math notes):

$$p(y_i|\boldsymbol{x_i}, w) = \left[\frac{1}{1+e^{-\boldsymbol{x}_i^\top w}}\right]^{y_i}\left[1-\frac{1}{1+e^{-\boldsymbol{x}_i^\top w}}\right]^{1-y_i} = \lambda(\boldsymbol{x})^{y_i} + (1-\lambda(\boldsymbol{x}))^{1-y_i}$$

$$p(\boldsymbol{y}|X, w) = \prod_{i=1}^{N} p(y_i|\boldsymbol{x_i}, w)$$

assuming **iid data**.

- Then, we can compute logs:

$$\log p(y_i|\boldsymbol{x_i}, w) = y_i \log \lambda(\boldsymbol{x}) + (1-y_i)\log(1-\lambda(\boldsymbol{x}))$$

$$\log p(\boldsymbol{y}|X, w) = \sum_{i=1}^{N} \log p(y_i|\boldsymbol{x_i}, w)$$

Learning the parameters

- Remember maximum likelihood:

$$\hat{w} = \underset{w}{\operatorname{argmax}} \log p(\boldsymbol{y}|X, w) = \underset{w}{\operatorname{argmax}} \frac{1}{N} \sum_{i=1}^{N} \log p(y_i|\boldsymbol{x}_i, w)$$

- It is the same as minimize NLL:

$$\hat{w} = \underset{w}{\operatorname{argmin}} - \log p(\boldsymbol{y}|X, w) = \underset{w}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} -\log p(y_i|\boldsymbol{x}_i, w)$$

- What is $-\log p(y_i|\boldsymbol{x}_i, w)$? Cross-entropy! (Check Math notes)

$$-\log p(y_i|\boldsymbol{x}_i, w) = -y_i \log \lambda(\boldsymbol{x}) - (1 - y_i) \log(1 - \lambda(\boldsymbol{x}))$$

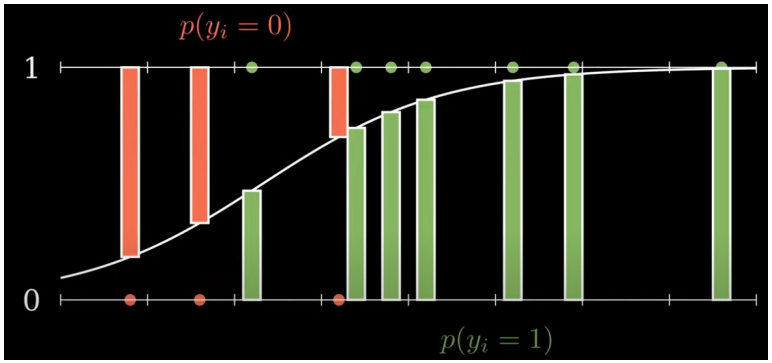
  - y_i is the **true** value (probability) of the class 1 $p(y_i = 1) = 1$
  - $\lambda(\boldsymbol{x})$ is **our model** probability of class 1
  - $\log \lambda(\boldsymbol{x})$ is **the information** of our model for class 1

Cross entropy vs ML

- Maximize likelihood = minimize cross-entropy
  - We want to find the model that minimizes the uncertainty of our predictions with respect to the *true world*.

$$\mathcal{L}(w) = -\frac{1}{N}\sum_{i=1}^{N} \log p(y_i|x_i, w) = -\left[\sum_{i=1}^{N} \underbrace{\frac{1}{N} y_i}_{\substack{true\ prob \\ class=1}} \log \lambda(x) + \sum_{i=1}^{N} \underbrace{\frac{1}{N}(1-y_i)}_{\substack{true\ prob \\ class=0}} \log(1-\lambda(x))\right]$$

- Intuition (check math notes):
  - Cross-entropy is the *expected surprise* of our model predictions averaged over the true probabilities of the elements *in the world*.
    - $-\log p(x)$ is the *surprise* of an event/observation.



Cross-entropy optimization

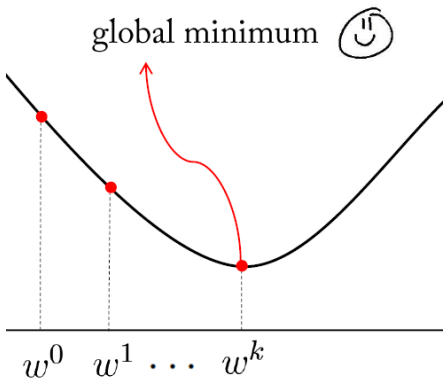
- To find the optimal model, we can use the same strategy as linear regression

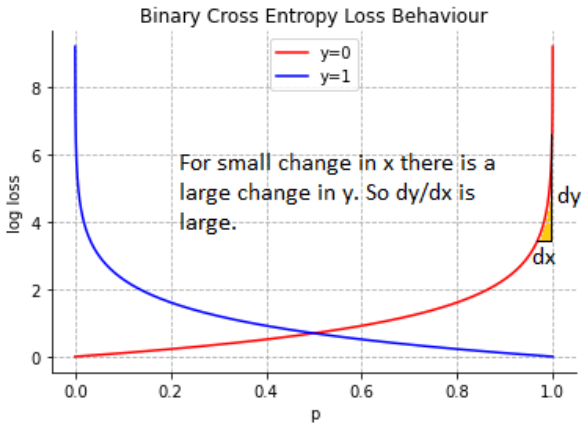
$$\mathcal{L}(w) = -\frac{1}{N}\sum_{i=1}^{N} y_i \log \lambda(\boldsymbol{x_i}) + (1 - y_i)\log(1 - \lambda(\boldsymbol{x_i}))$$

$$\nabla\mathcal{L}(w) = -\frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x_i}^{\top}(\lambda(\boldsymbol{x_i}) - y_i) = -\frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x_i}^{\top}(\sigma(\boldsymbol{x}^{\top}w) - y_i)$$

- Unfortunately, there is **no closed form** solution!
  - … but, the loss is **convex** and has a **single minimum**!
  - (Stochastic) Gradient Descent will take us to it.

Hessian has a quadratic form (positive definite)





Generalize to multi-class problems

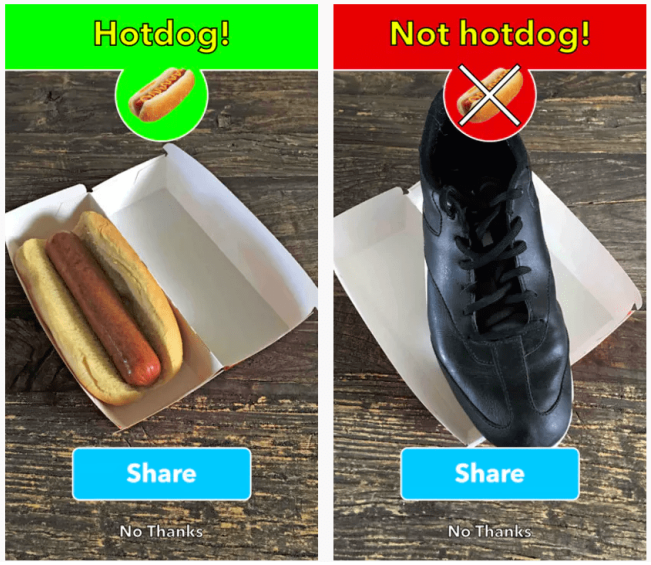
- Logistic regression works for binary classification problems

$$y = \{0,1\}$$

- What if we had multiple classes?

$$y = \{dog, cat, person, bed, \dots\}$$

- Solutions:
  - OVR: One-vs-Rest
    - Perform logistic regression for class 1 vs not class 1 (*hotdog/not hotdog*)
    - Repeat for all classes.
  - Replace Bernouilli → **Multinomial**
    - Distribution for ***k* categories** and *n* trials
    - It models throwing a k-sided dice n-times.
    - Multinomial(k=2, n=1) = Bernouilli
    - Bernouilli distribution models a coin flip.

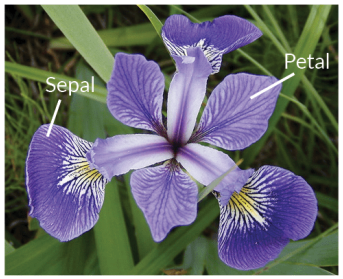


Multinomial logistic regression

Logistic regression in the Iris dataset

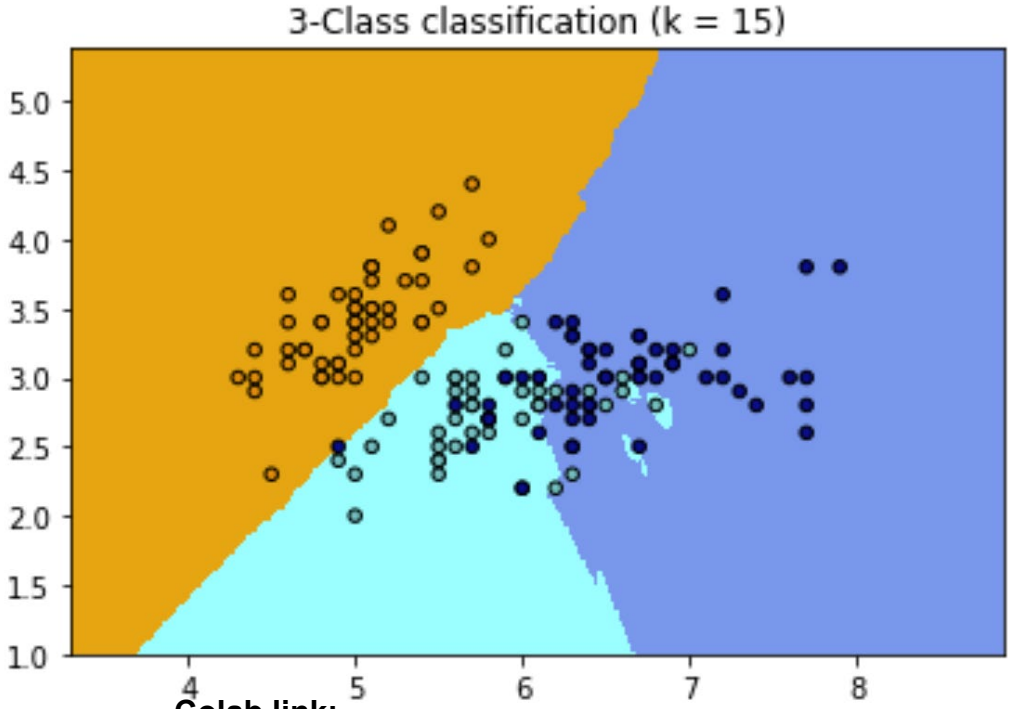
- Take-home messages:
  - Slightly outperforms k-nn (remember from our plots in slide 18, class boundaries are quite linear)
  - More sophisticated methods (SVM) do not improve, again class boundaries are quite linear
  - k-fold cross-validation IS relevant in this case!

Iris Setosa



Iris Versicolor

Iris Virginica



Colab link:
https://drive.google.com/file/d/1GftP9OQDIe6_7dP-AhIe_QgIZGiGPOjm

Welcome to deep learning

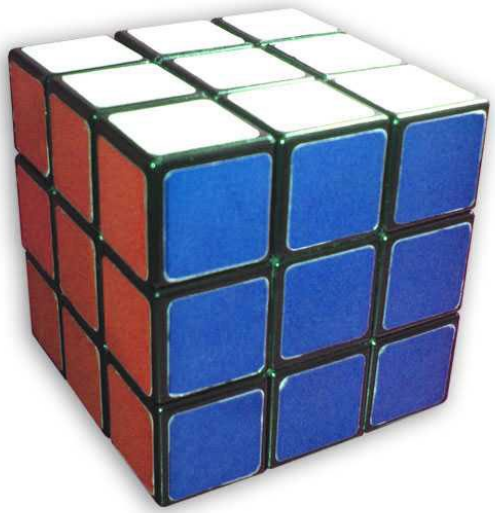
- Multilayer perceptron
  - Feedforward neural network
  - Trained using SGD
  - Forward *inference*, backward loss/gradient

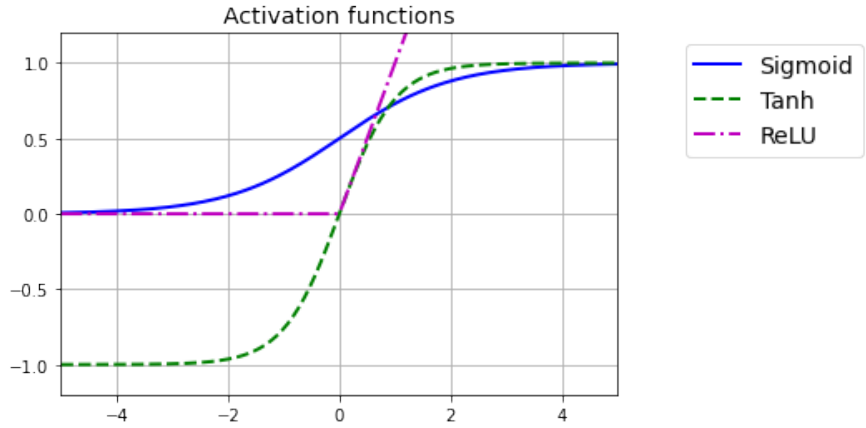
Welcome to deep learning

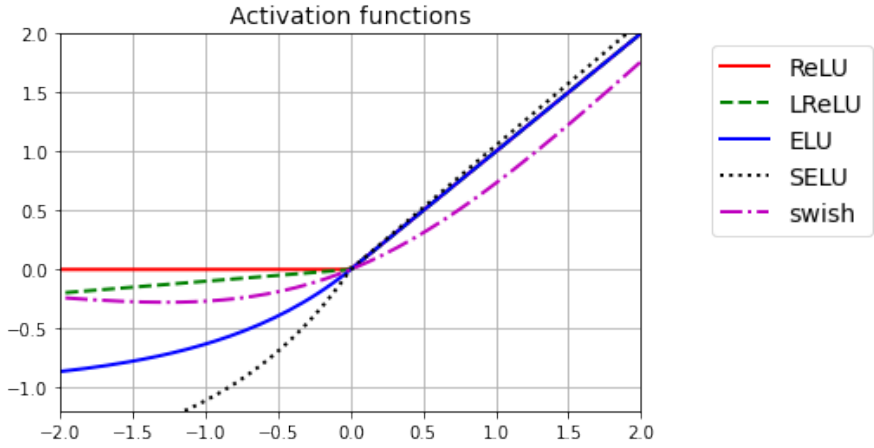
- General purpose architecture
  - Classification, regression
  - Unsupervised learning…

Activation functions

- Nonlinear component







https://colab.research.google.com/github/probml/pyprobml/blob/master/notebooks/book1/02/activation_fun_plot.ipynb

Types of error (binary classification)

- **True Positive (TP):** Positive data (correctly) classified as positive data.
- **True Negative (TN):** Negative data (correctly) classified as negative data.
- **False Positive / Type I Error (FP):** Negative data (not correctly) classified as positive data.
- **False Negative / Type II Error (FN):** Positive data (not correctly) classified as negative data.

	Ground Truth		
Prediction		Positive	Negative
	Positive	TP	FP
	Negative	FN	TN

Metrics: Precision and Recall

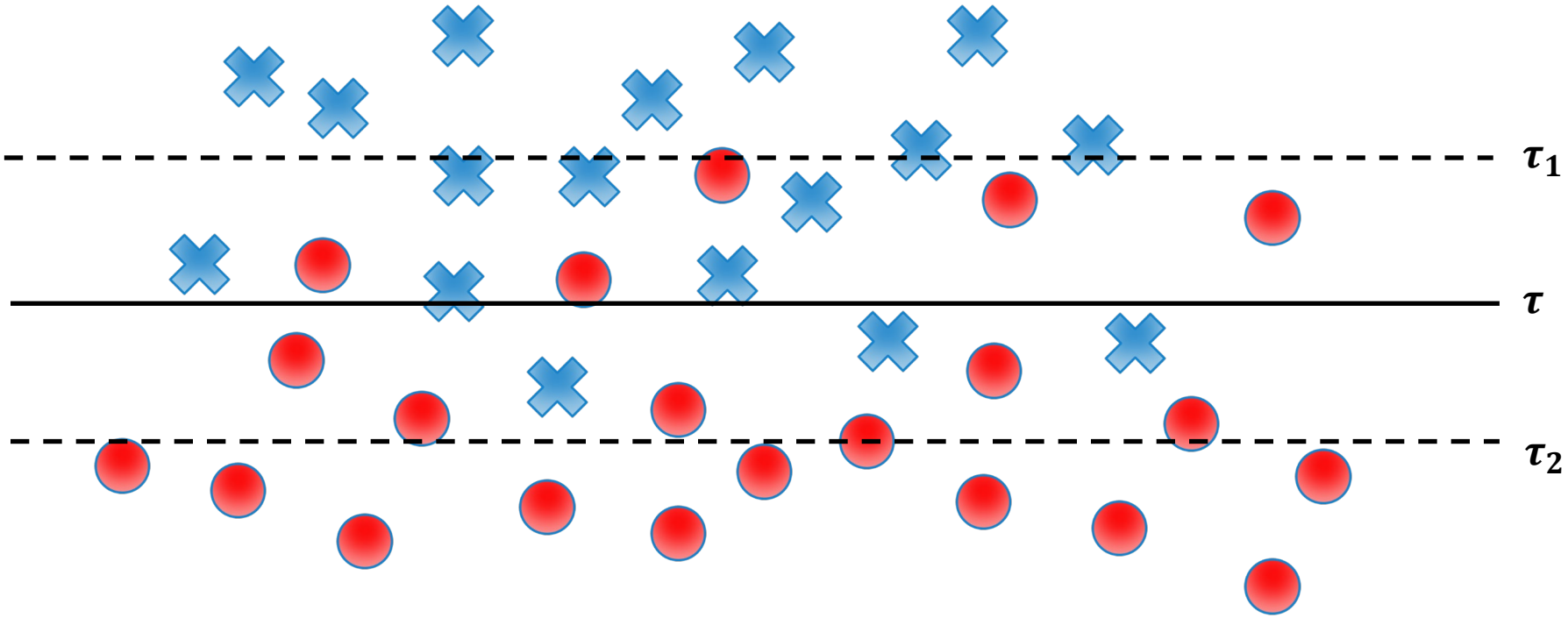
- **Accuracy, success rate, hit rate** $\rightarrow \frac{TP+TN}{TP+FP+TN+FN}$
  - Limitation: Not every error is equally important…
  - Best and worst success rate?
- **Precision** $\rightarrow \frac{TP}{TP+FP} \in [0,1]$
  - Ratio of the true positives over all the positive classifications.
  - Fraction of retrieved elements that are relevant.
- **Recall** $\rightarrow \frac{TP}{TP+FN} \in [0,1]$
  - Ratio of the true positives over all the positive samples.
  - Fraction of relevant elements that are retrieved.
- Both depend on the classification threshold.
- They are dependent, if one increases the other decreases. Sometimes given in pairs (e.g., precision at recall X).

Precision and Recall (some intuition)

- The girlfriend/boyfriend example:
  - Your girlfriend/boyfriend makes birthday presents for you every year.
  - One year she/he asks: Do you remember all my presents from the last 10 years?
  - **Precision** is how many are correct from the ones you said you remember.
  - **Recall** is how many correct you can remember from all correct ones.
  - How can we have 100% precision or recall? What happens to the other?
  - What is the relation to the classification threshold?
- The airport security example:
  - FP and FN: Have both errors the same consequences?
  - How can we have 100% precision or recall?
- Do you need precision, recall or both?
  - The solution is, most often, a compromise…

Precision-Recall and thresholds

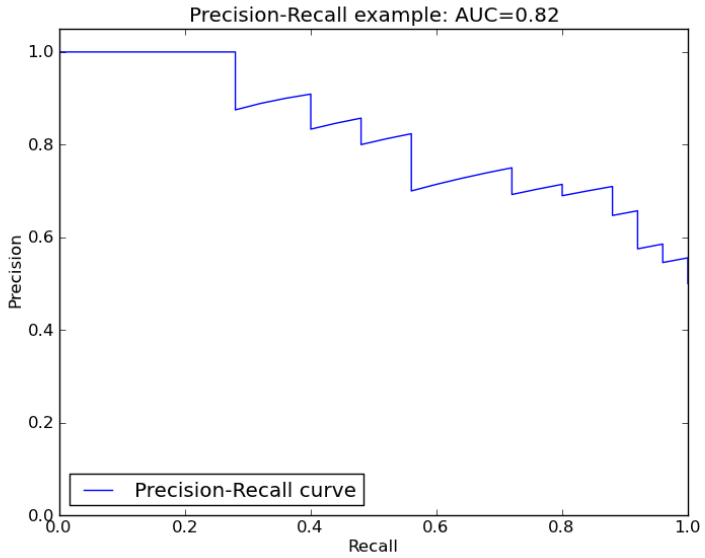
- Two-class problem



- What happens to the TP, TN, FP, FN, precision and recall if we move the boundary from τ to τ_1 or τ_2?

Precision-Recall curve

- 2D plot, recall in x-axis and precision in y-axis.
- It shows the precision-recall pairs when we change the classifier threshold τ
- $\tau \uparrow \Rightarrow FP \downarrow \Rightarrow FN \uparrow \Rightarrow P \rightarrow 1 \;\Rightarrow R \rightarrow 0$
- $\tau \downarrow \Rightarrow FP \uparrow \Rightarrow FN \downarrow \Rightarrow P \rightarrow 0 \;\Rightarrow R \rightarrow 1$
- Changing a classifier threshold τ it operates in different modes. We have to select the more appropriate for our purposes.
- For general purposes, the area under the curve (AUC) is usually taken as a general metric (the higher the better).
- What curve and AUC would have a perfect classifier? What curve and AUC would have the worst possible classifier?



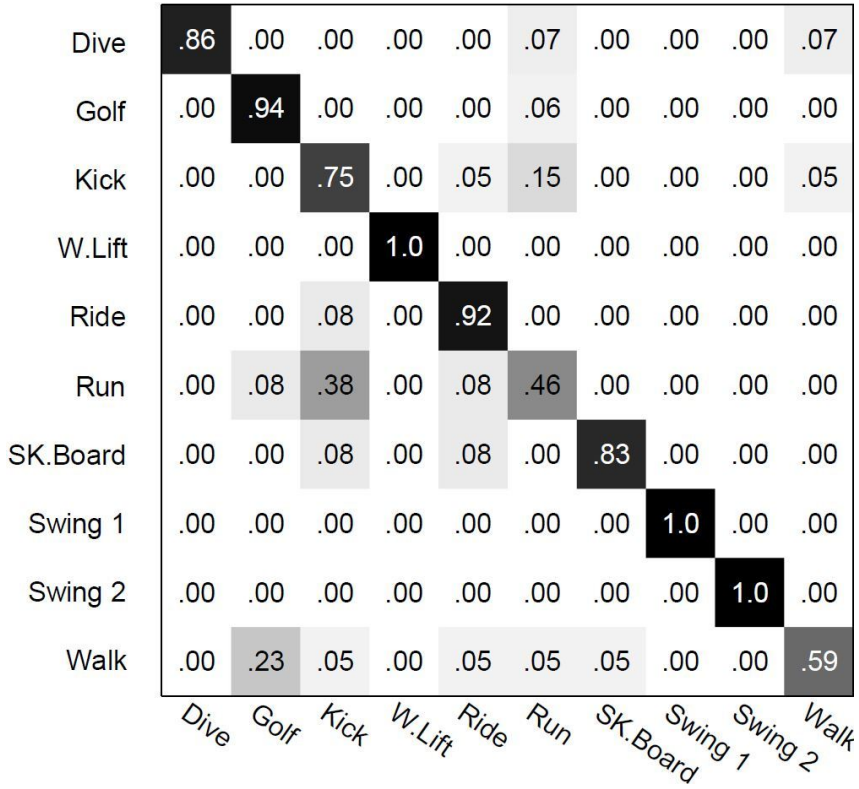
F1 score, confusion matrix

- **F1 score**
  - Harmonic mean of precision and recall (the higher the better)

$$F_1 = \frac{2}{{}^1/_P + {}^1/_R} = 2\frac{precision * recall}{precision + recall} \in [0,1]$$

  - It can be weighed to give β times more importance to precision than recall $F_1 = (1+\beta^2)\frac{precision * recall}{\beta^2 * precision + recall}$

- **Confusion matrix**
  - Rows: true categories.
  - Columns: predicted categories.
  - Cells: number/frequency of ocurrence.
  - More information than other metrics (for example, typical classification mistakes)
  - Difficult to display if many categories.
  - Difficult to summarize…

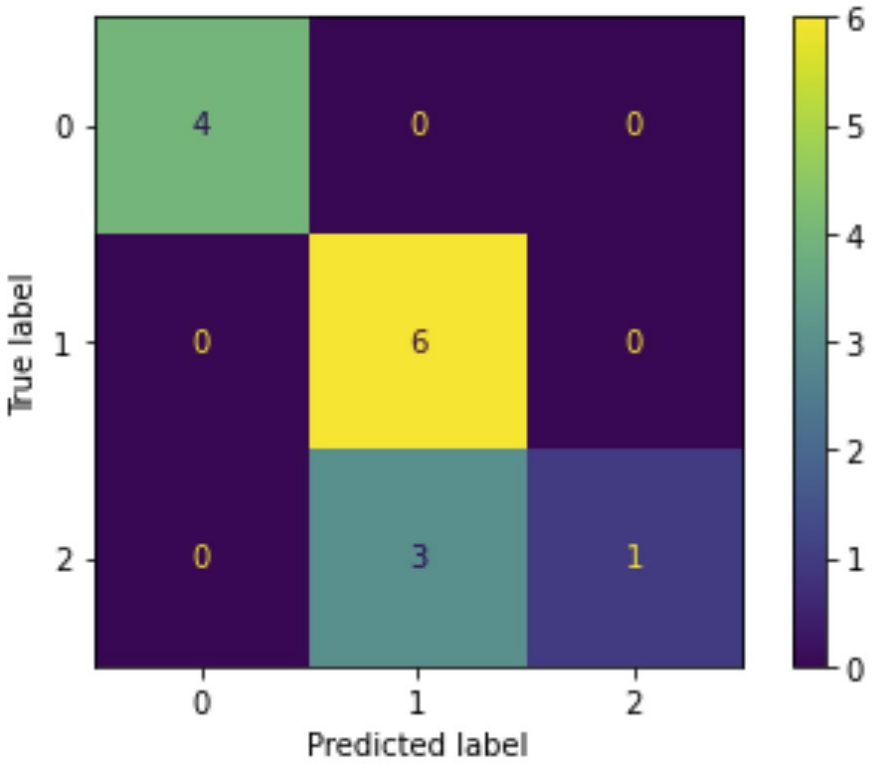


Confusion matrix for action recognition from videos

Taken from Qiu, Jiang, and Chellappa, "Sparse Dictionary-based Representation and Recognition of Human Action Attributes", ICCV 2011

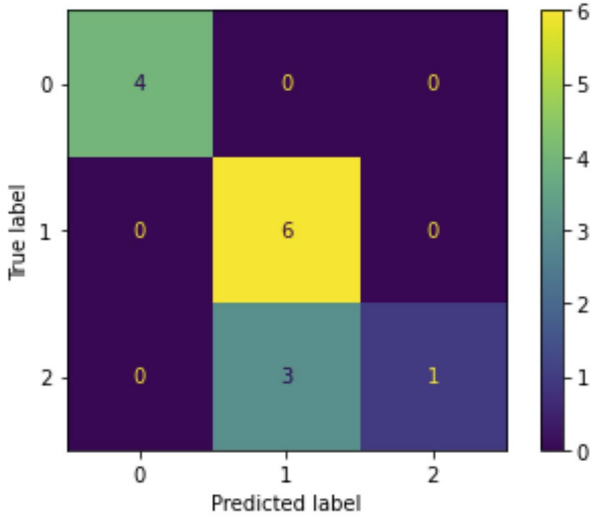
TP, TN, FP and FN from the confusion matrix

- Remember:
  - Rows: true categories.
  - Columns: predicted categories.
- **True positives per class:**
  - Diagonal elements [4, 6, 1]
- **False positives per class:**
  - Sum of the off-diagonal elements of each column [0, 3, 0]
- **False negatives per class:**
  - Sum of the off-diagonal elements of each row [0, 0, 3]
- **True negatives per class:**
  - Sum of all matrix elements except the row and column of the class [10, 5, 10]



Multiclass Precision/Recall

- **True positives per class:** [4, 6, 1], **True negatives per class:** [10, 5, 10]
- **False positives per class:** [0, 3, 0], **False negatives per class:** [0, 0, 3]



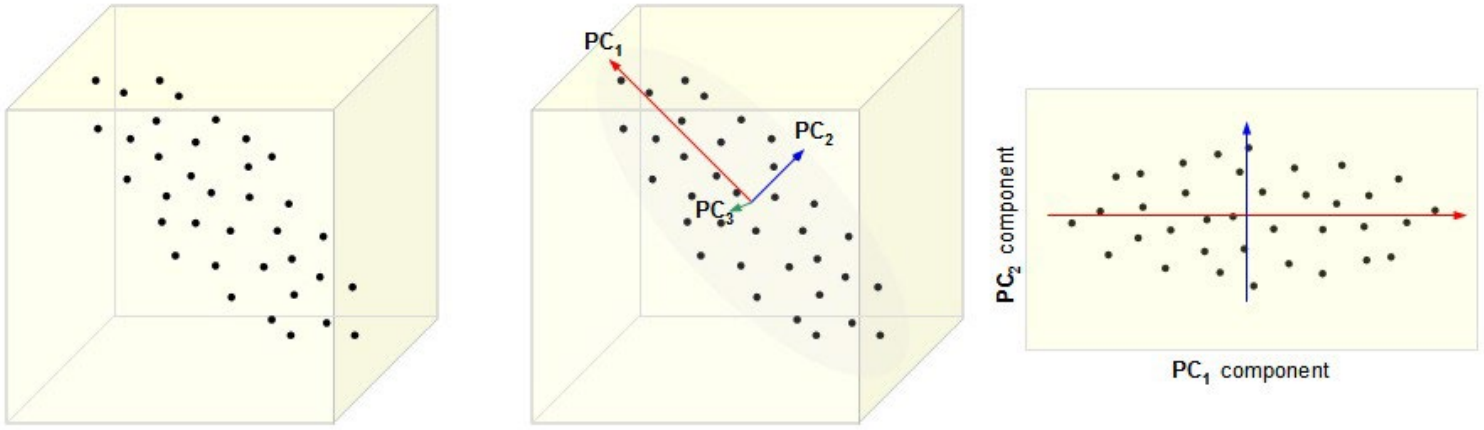
	Accuracy	Precision	Recall
Class 1	$\frac{4+10}{4+6+1+3} = \mathbf{1.0}$	$\frac{4}{4+0} = \mathbf{1.0}$	$\frac{4}{4+0} = \mathbf{1.0}$
Class 2	$\frac{6+5}{4+6+1+3} = \mathbf{0.79}$	$\frac{6}{6+3} = \mathbf{0.66}$	$\frac{6}{6+0} = \mathbf{1.0}$
Class 3	$\frac{1+10}{4+6+1+3} = \mathbf{0.79}$	$\frac{1}{1+0} = \mathbf{1.0}$	$\frac{1}{1+3} = \mathbf{0.25}$

- **Overall accuracy** $= \frac{correct}{total} = \frac{4+6+1}{4+6+1+3} = 0.78$
- **Average accuracy** $= \frac{1.0+0.79+0.79}{3} = 0.86$
- **Average Precision** $= \frac{1.0+0.66+1.0}{3} = 0.89$
- **Average Recall** $= \frac{1.0+1.0+0.25}{3} = 0.75$

If data is imbalanced, average metrics may be weighted…

Dimensionality reduction (unsupervised learning)

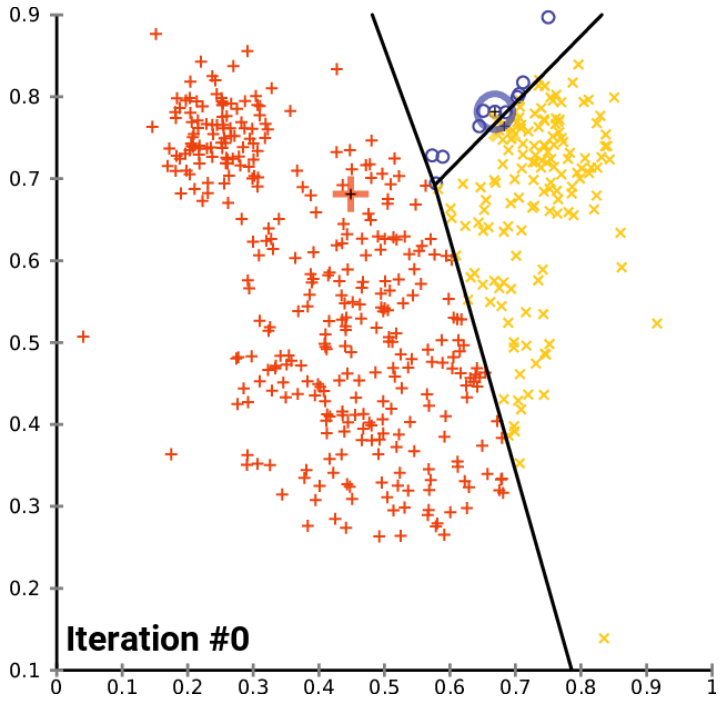
- PCA → Principal Component Analysis.
  - **Motivation:** in high dimensional data, some dimensions are redundant, or are highly correlated…
  - **Intuition:** Project the data into a low-dimensional space preserving the dimensions of maximum variance
  - SVD decomposition ($X = U\Sigma V^T$) of the training matrix $X = [x^{(1)} \quad \dots \quad x^{(N)}]$, the columns of V are the unit vectors of the principal components.
  - The low-d data is computed as $X_{d'} = XW_{d'}$; $W_{d'} \coloneqq V[1:d']$



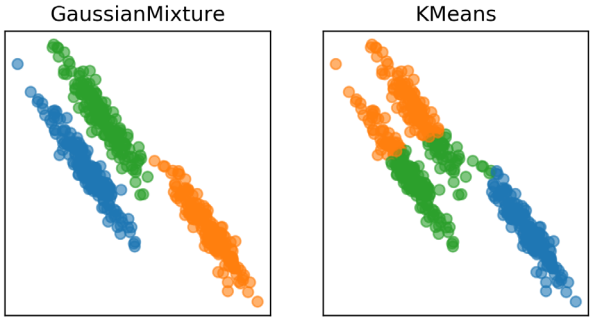
For more details, check Deisenroth chapter 10

Clustering (unsupervised learning)

- K-means:
  - Start with K random points (cluster means).
  - Repeat until convergence:
    - Assign each data point to the closest mean.
    - Recalculate means based on the new assignments



- Isotropic: clusters are spheres
  - Alternative: Gaussian mixture model (GMM) with expectation-maximization (EM)



- Requires knowing K
  - Alternative: X-means

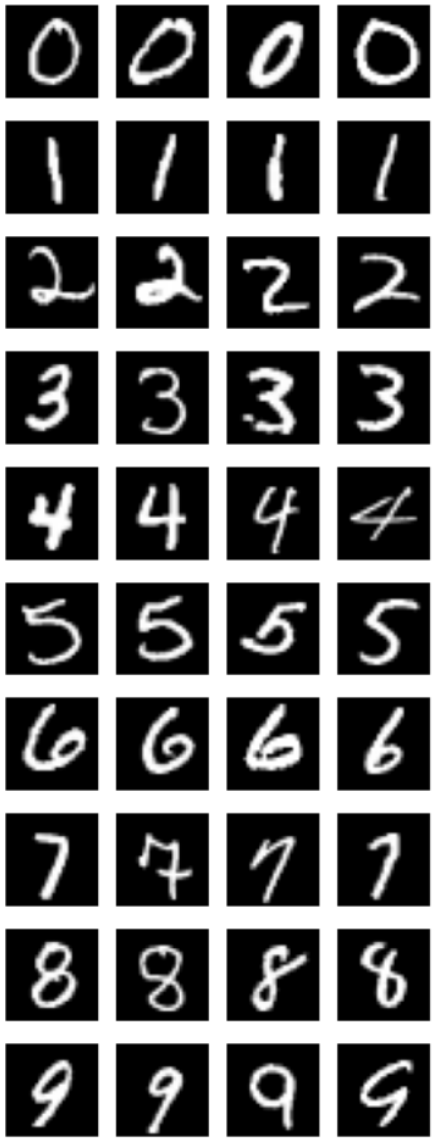
1-NN with and without PCA in MNIST

- Time per 10,000 queries in the test set
- Full-size input, $x \in \mathbb{R}^{784}$:

```
k=1, accuracy=97.22%, time=849.6 s
```

- Removing lowest-variance dimensions with PCA, up to 98% time reduction and same accuracy!

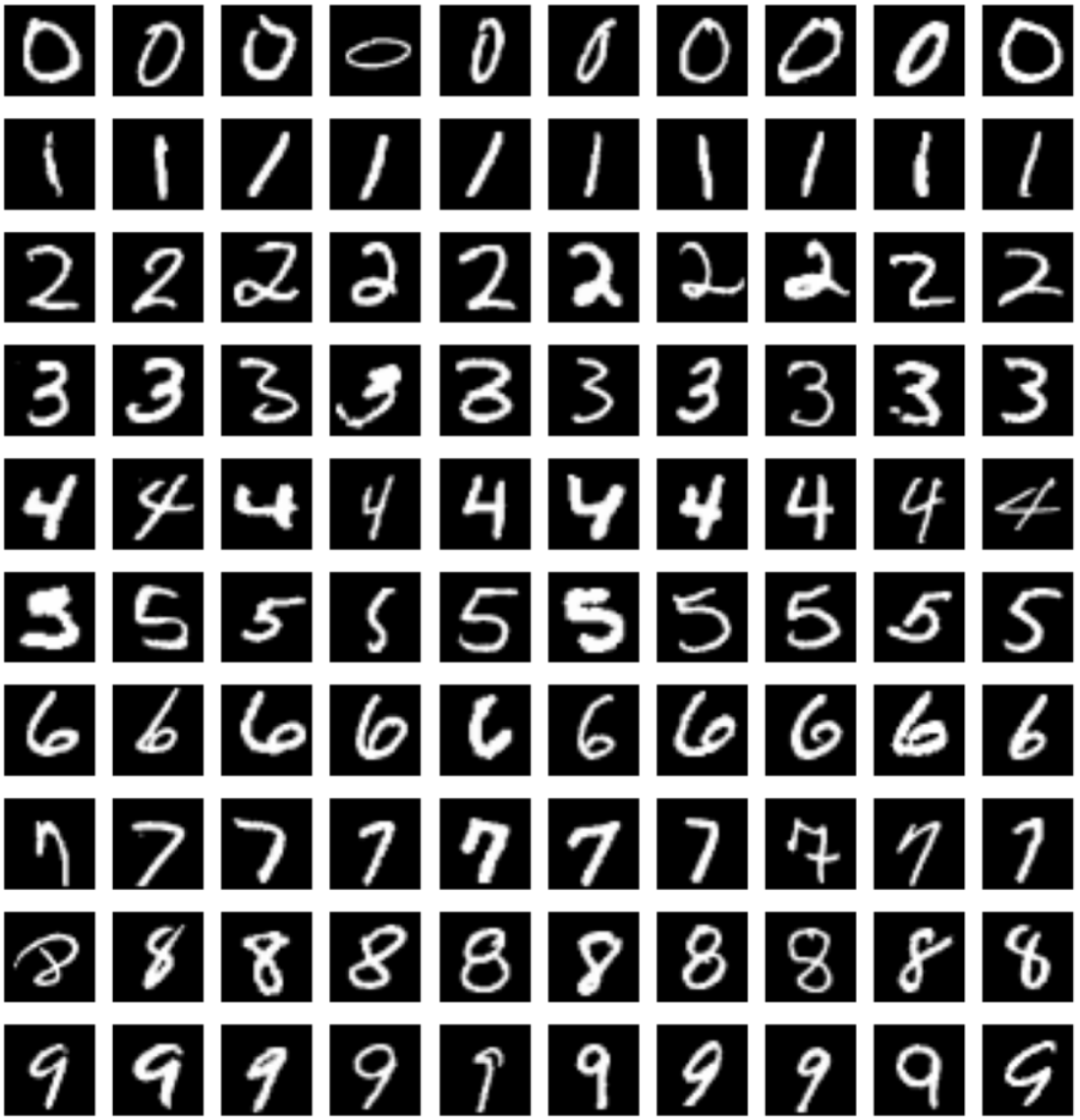
```
dims after PCA=10, accuracy=91.95%, time=1.3 s
dims after PCA=20, accuracy=96.60%, time=6.1 s
dims after PCA=30, accuracy=97.60%, time=14.8 s
dims after PCA=40, accuracy=97.43%, time=24.6 s
dims after PCA=50, accuracy=97.45%, time=36.3 s
dims after PCA=60, accuracy=97.56%, time=48.9 s
dims after PCA=70, accuracy=97.48%, time=62.0 s
dims after PCA=80, accuracy=97.51%, time=69.3 s
dims after PCA=90, accuracy=97.44%, time=81.7 s
dims after PCA=100, accuracy=97.54%, time=93.8 s
dims after PCA=200, accuracy=97.29%, time=159.8 s
dims after PCA=300, accuracy=97.24%, time=243.2 s
dims after PCA=400, accuracy=97.22%, time=318.2 s
dims after PCA=500, accuracy=97.24%, time=400.1 s
dims after PCA=600, accuracy=97.22%, time=473.3 s
```



Colab link:
https://colab.research.google.com/drive/1EdemME5vbZr01Q6CijYh0eo3hnRsjjKE

Assignment: Logistic regression in MNIST

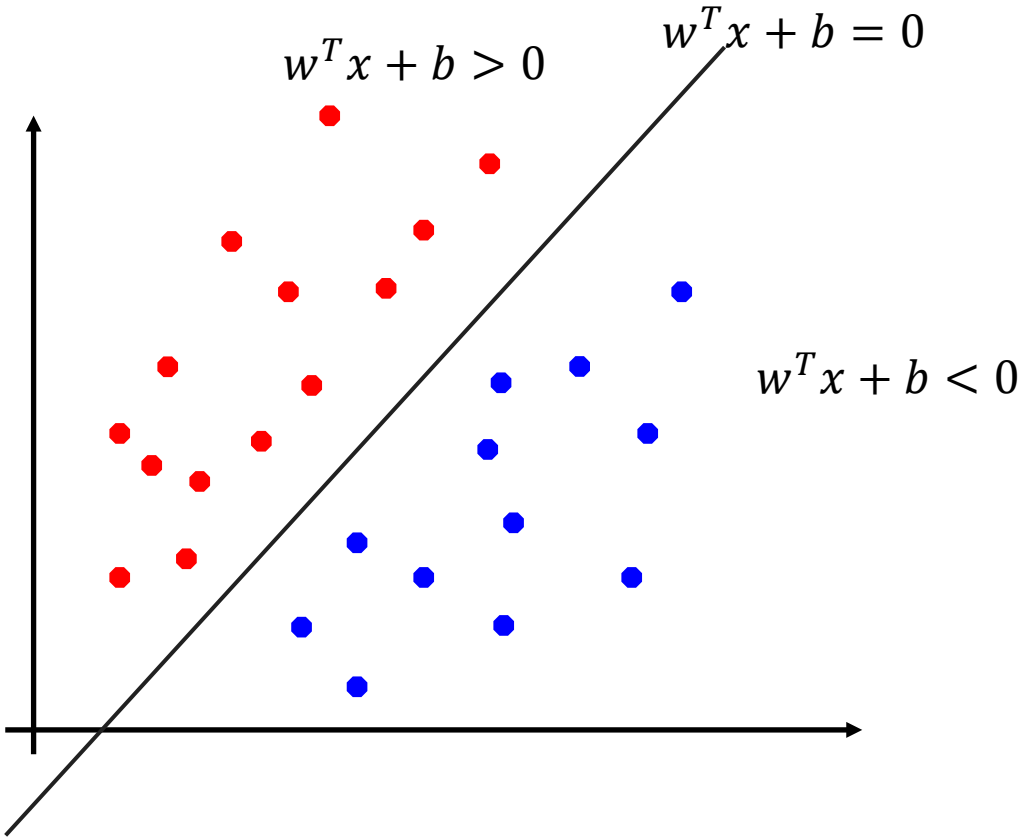
- Spoilers:
  - Excruciatingly slow!
    - Due to high dimensionality and large dataset size
    - Shortlist promising models using a reduced version of the data!
    - Use PCA!
  - 1-NN better than logistic regression…
    - why?



https://colab.research.google.com/drive/1HS9988xVWD6yqw9FRbe4z7qQfAFejL_V

Support Vector Machines (SVM)

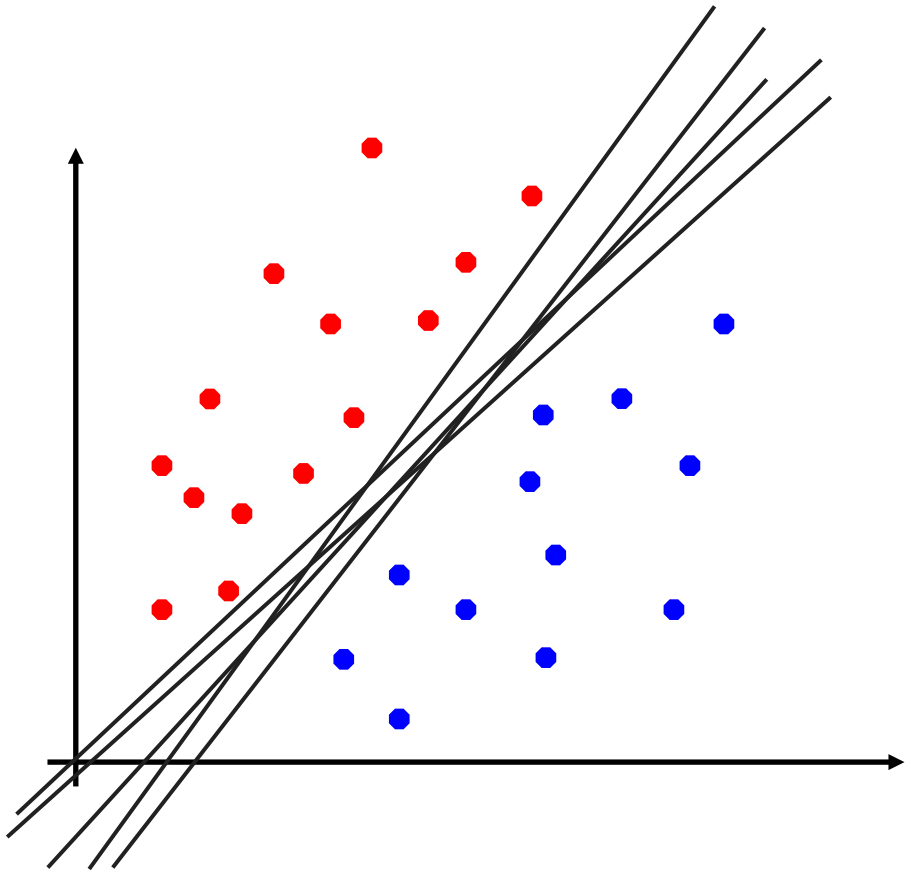
- Recap: Linear classification consists of finding an hyperplane in the feature space that separates the training data



For more details, check Deisenroth chapter 12

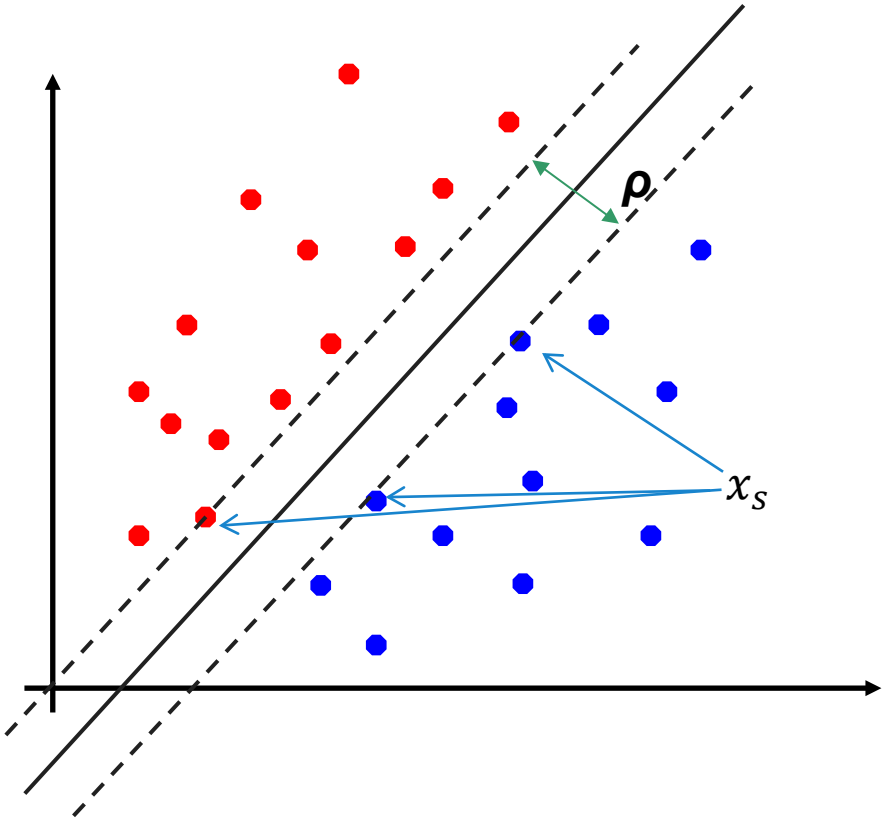
Support Vector Machines (SVM)

- But… which one of these hyperplanes would be the best one?



Support Vector Machines (SVM)

- SVM idea: let's take the one with **maximum margin** ρ
- Maximum margin:
  - The closest samples to the hyperplane are the support vectors x_s
  - The margin is the distance between the support vectors
  - Only support vectors matter! (which seems reasonable…)



"Hard-margin" SVM

- For each training example $(x^{(i)}, y^{(i)}), y^{(i)} \in \{-1, +1\}$

$$\begin{aligned} w^T x^{(i)} + b &\leq {}^{-\rho}/_{2} \quad if\ y^{(i)} = -1 \\ w^T x^{(i)} + b &\geq {}^{\rho}/_{2} \quad if\ y^{(i)} = +1 \end{aligned} \Rightarrow y^{(i)}\left(w^T x^{(i)} + b\right) \geq {}^{\rho}/_{2}$$

- If $x_s^{(i)}$ is a support vector, the above inequality is an equality
- After re-scaling w and b by ${}^{\rho}/_{2}$, the distance between each support vector $x_s^{(i)}$ and the hyperplane is ${}^{1}/_{\|w\|}$
- The margin is then $\rho = {}^{2}/_{\|w\|}$
- And the margin maximization can be formulated as

$$\hat{w}, \hat{b} = \arg max_{w,b}\ {}^{2}/_{\|w\|} \text{ (alternatively } \arg min_{w,b}\ \frac{1}{2}\|w\|^2\text{)}$$

subject to $y^{(i)}\left(w^T x^{(i)} + b\right) \geq 1$ (for re-scaled w and b)

"Soft-margin" SVM

- "Hard-margin SVM" does not allow data to be on the wrong side of the hyperplane
- For noisy data, we might want to allow that
- Idea: introduce a per-sample slack variable $\xi^{(i)} > 0$ modelling deviations from the correct side of the hyperplane
- The optimization is now

$$\hat{w}, \hat{b} = \arg min_{w,b} \frac{1}{2} \|w\|^2 + C \sum_i \xi^{(i)}$$

$$\text{subject to } y^{(i)}\left(w^T x^{(i)} + b\right) \geq 1 - \xi^{(i)} \text{(re-scaled } w \text{ and } b\text{)}$$

- C trades off the margin and the amount of slack we have
  - $C \downarrow\downarrow$ regularizes the solution (favors simple decision functions)
  - Usually tuned by cross-validation

Non-linear SVM

- The SVM parameters are learnt by solving the dual form of the optimization

$$\hat{\alpha} = \arg max_{\alpha}\ {}^{1}/_{2} \sum_{i}\sum_{j} y^{(i)} y^{(j)} \alpha^{(i)} \alpha^{(j)} \left\langle \boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)} \right\rangle - \sum_{i} \alpha^{(i)}$$

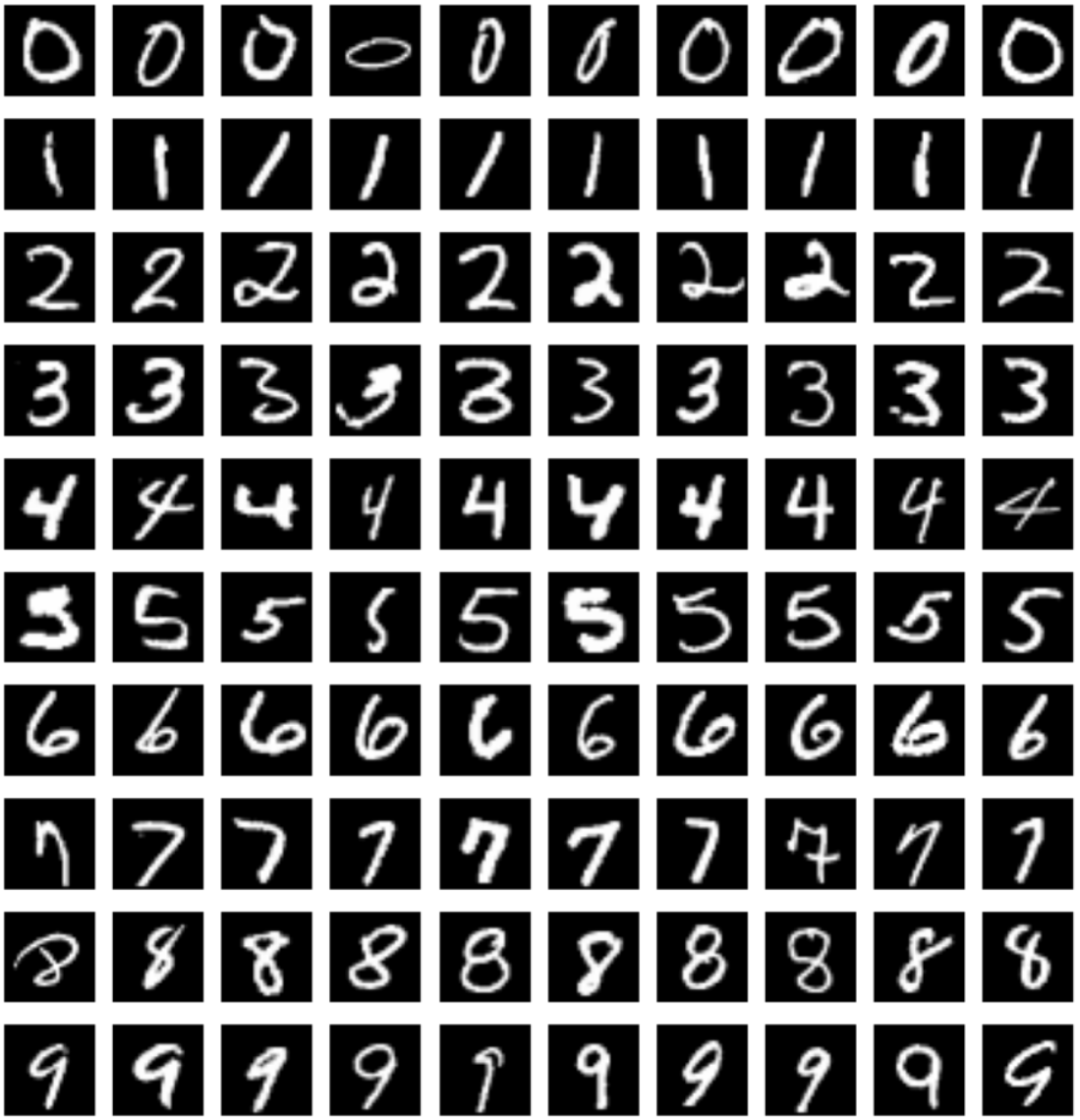
$$\text{subject to } \textstyle\sum_i y^{(i)} \alpha^{(i)} = 0,\ 0 \leq \alpha^{(i)} \leq \mathrm{C}$$

- The objective function is based in the inner product $\left\langle \boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)} \right\rangle$
- For non-linear functions of the data $\phi(x^{(i)})$, the only modification is on the inner product $\left\langle \boldsymbol{\phi}(\boldsymbol{x}^{(i)}), \boldsymbol{\phi}(\boldsymbol{x}^{(j)}) \right\rangle$
- Instead of choosing the non-linear function $\phi(x^{(i)})$, we choose the similarity function $k(x^{(i)}, x^{(j)}) = \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle_{\mathcal{H}}$
- The similarity function $k(x^{(i)}, x^{(j)})$ is a kernel (more about kernels later in the course…)

Non-linear SVM hyperparameters

- Obtained by cross-validation
- C parameter
  - Trades off the margin and the slack allowed to the data
- Kernel and kernel parameters. Usual choices
  - Linear kernel: $k\left(x^{(i)}, x^{(j)}\right) = x^{(i)}x^{(j)}$
  - Polynomial kernel: $k\left(x^{(i)}, x^{(j)}\right) = \left(\gamma x^{(i)}x^{(j)} + r\right)^d$
  - Gaussian kernel: $k\left(x^{(i)}, x^{(j)}\right) = \exp\left(-\frac{\left\|x^{(i)} - x^{(j)}\right\|^2}{\sigma^2}\right)$
  - Radial basis function: $k\left(x^{(i)}, x^{(j)}\right) = \exp\left(-\gamma\left\|x^{(i)} - x^{(j)}\right\|^2\right)$
  - Sigmoid kernel: $k\left(x^{(i)}, x^{(j)}\right) = \tanh\left(\gamma x^{(i)}x^{(j)} + r\right)$

Assignment: SVM in MNIST??



https://colab.research.google.com/drive/1HS9988xVWD6yqw9FRbe4z7qQfAFejL_V

Ensembling

- The machine learning equivalent to the wisdom of the crowd
  - Aggregating predictions from several models improve over the individual ones
- Example (from Géron 2019):
  - Aggregating the votes of 1,000 binary classifiers with individual accuracies of 51% gives us an accuracy of 75%!
- **Practical trick:** when, at the end of a machine learning project, you trained several good models, combine their predictions to obtain an even better one.

Aurélien Géron, Hands-on Machine Learning with Scikit-Learn, Keras and TensorFlow, O'Reilly, 2nd edition, 2019

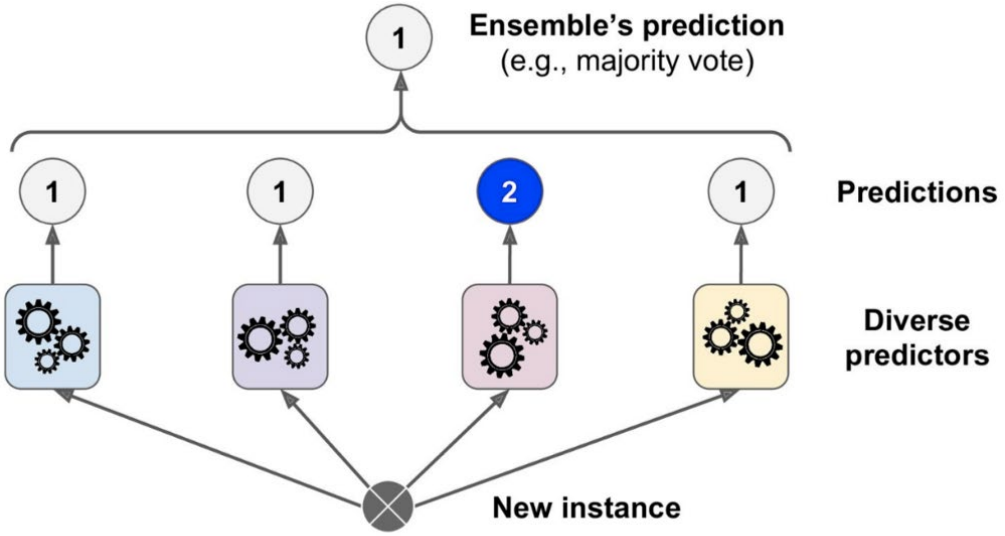


Figure 7-2. Hard voting classifier predictions

Universidad Zaragoza

Machine Learning (69152)

Máster in Robotics, Graphics and Computer Vision