Learning with Linear Models

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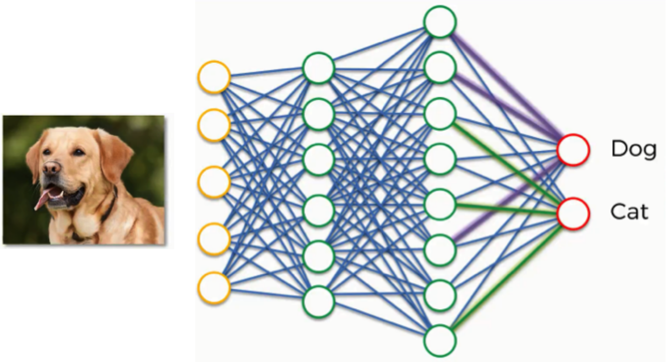
  - ✓ Linear models are **a component of deep networks**.

Linear Classifiers and Neural Networks



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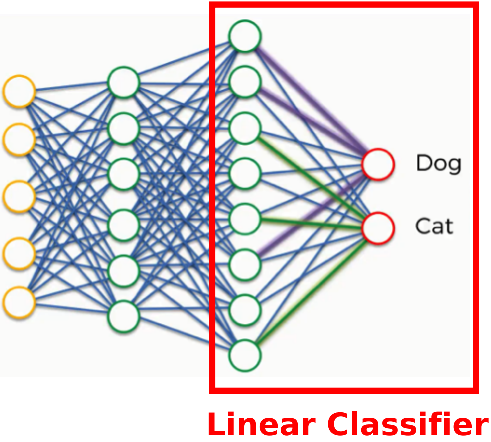

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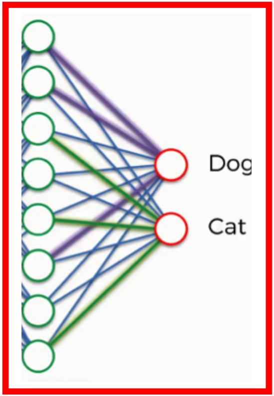

Linear Classifier

Today's Roadmap

- Linear regression
- Binary and multi-class classification
- Linear classifiers: perceptron, logistic regression, SVMs
- Softmax and sparsemax
- Regularization
- Optimization: stochastic gradient descent
- Similarity-based classifiers and kernels.

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  - ✓ e.g., a **news article** together with a **topic**
  - ✓ e.g., a **sentence** together with its **translation**
  - ✓ e.g., an **image** partitioned into **segmentation regions**

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- Standard approach: **empirical risk minimization** (ERM):

$$h = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{N} L\big(h(x_i), y_i\big)$$

where L is a loss function and $\mathcal{H}$ a model class.

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- **Structured classification:** $\mathcal{Y}$ exponentially large and structured
  - ✓ e.g., machine translation, caption generation, image segmentation, ...

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  - ✓ logistic regression reduces classification to regression
  - ✓ one-vs-all reduces multi-class to binary
  - ✓ greedy search reduces structured classification to multi-class
- ... but other times it's better to tackle the problem in its native form.
- More later!

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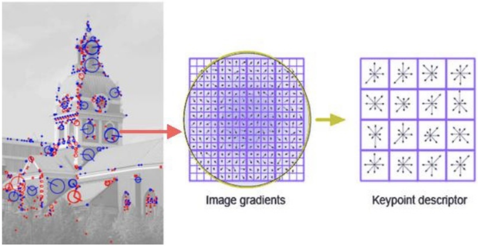

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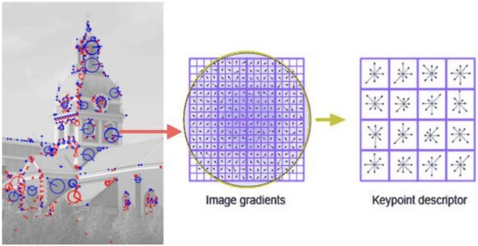

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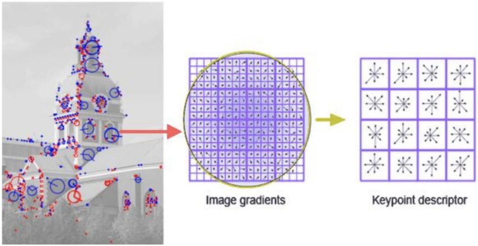

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  - ✓ Decades of research in machine learning, natural language processing, computer vision, image analysis, speech processing, ...

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- $\phi(x)$ is a (maybe high-dimensional) feature vector
- Feature vectors may mix categorical and continuous features
- Categorical features can be reduced to one-hot binary features:

$$\boldsymbol{e}_y := (0, \ldots, 0, \underbrace{1}_{\text{position } y}, 0, \ldots, 0) \in \{0, 1\}^K \text{ represents class } y$$

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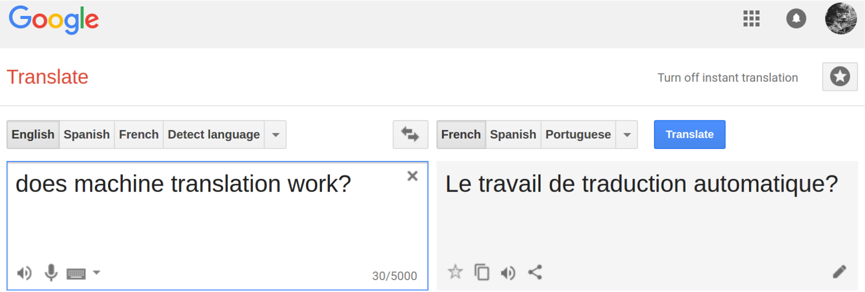
- Each classifier's predictions are used to handcraft features for other classifiers
- Examples of features:
  - ✓ Word occurrences (binary feature)
  - ✓ Word counts (numerical feature)
  - ✓ POS tags; e.g., adjective counts for sentiment analysis
  - ✓ Spell checker; e.g., misspellings counts for spam detection

Example: Translation Quality Estimation



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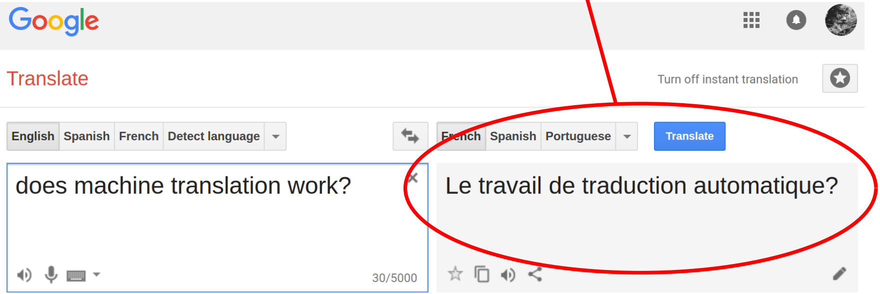

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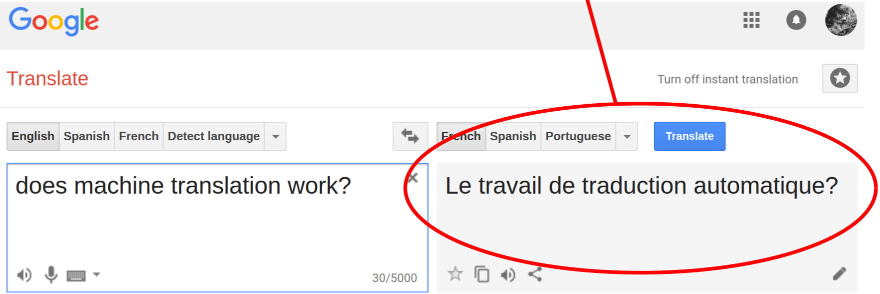

Goal: estimate the quality of a translation on the fly (without a reference)!

Example: Translation Quality Estimation

Hand-crafted features:

- no of tokens in the source/target segment
- language model probability of source/target segment and their ratio
- average number of translations per source word
- ratio of brackets and punctuation symbols in source & target segments
- ratio of numbers, content/non-content words in source & target segments
- ratio of nouns/verbs/etc in the source & target segments
- % of dependency relations b/w constituents in source & target segments
- diff in depth of the syntactic trees of source & target segments
- diff in no of PP/NP/VP/ADJP/ADVP/CONJP in source & target
- diff in no of person/location/organization entities in source & target
- features and global score of the SMT system
- number of distinct hypotheses in the n-best list
- 1–3-gram LM probabilities using translations in the n-best to train the LM
- average size of the target phrases
- proportion of pruned search graph nodes;
- proportion of recombined graph nodes.

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Tomorrow's lecture, by Bhiksha Raj

Outline

1. **Regression**

2. Classification
   - Perceptron
   - Logistic Regression
   - Support Vector Machines
   - Sparsemax

3. Regularization

4. Non-Linear Models

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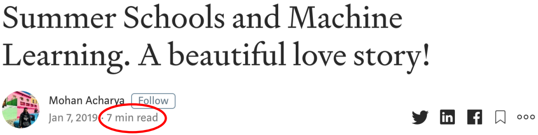

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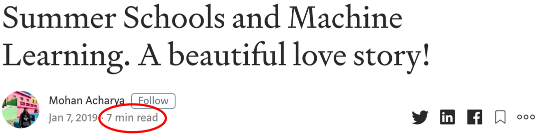

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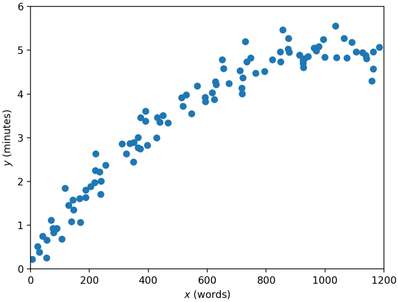
- How to define a model that yields a prediction $\widehat{y}$ from x?

Linear Regression

- First take: assume $\widehat{y} = wx + b$
- Model parameters: w and b
- Given training data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$, how to estimate w and b?



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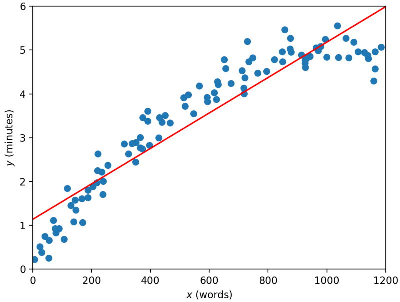

- Least squares (LS) criterion: fit w and b on the training set by solving

$$(\hat{w}_{\text{LS}}, \hat{b}_{\text{LS}}) = \arg\min_{w,\, b} \sum_{i=1}^N \big(y_i - (w\, x_i + b)\big)^2$$

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- Minimize squared loss: $\sum_i \left(y_i - \left(\boldsymbol{w}^T \phi(x_i)\right)\right)^2 = \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2$, where

$$\boldsymbol{X} = \begin{bmatrix} \phi(x_1)^\top \\ \vdots \\ \phi(x_N)^\top \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$$

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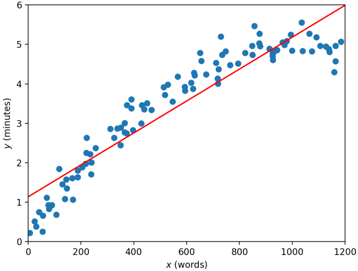
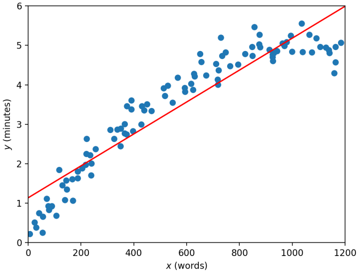
- Still called linear regression: linear w.r.t. the model parameters $\boldsymbol{w}$.



y (minutes)
x (words)
0
1
2
3
4
5
6
0
200
400
600
800
1000
1200

Linear Regression: $D = 1$ vs $D = 2$



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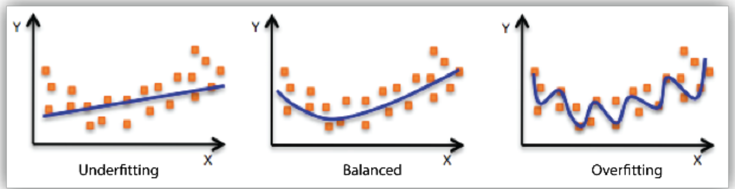

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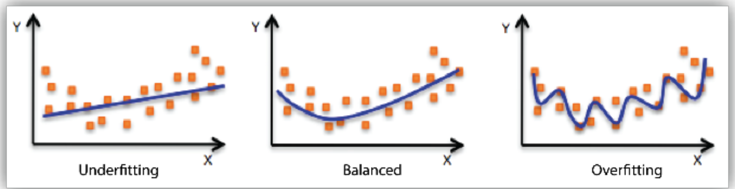
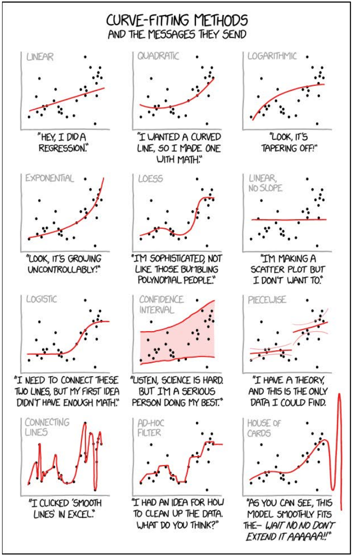


- Avoiding overfitting:
  - ✓ regularization (later)
  - ✓ some way to choose D (model complexity)

Inductive Biases



from xkcd.com

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- That is, $P(y_i|x_i;\boldsymbol{w}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - {\boldsymbol{w}^*}^T \phi(x_i))^2}{2\sigma^2}\right)$

Least Squares: Probabilistic Interpretation

- The least squares criterion has a probabilistic interpretation.
- Assume the following probabilistic observation model:

$$y_i = \boldsymbol{w}^{*T} \phi(x_i) + n_i$$

where

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- Then, $\hat{\boldsymbol{w}}_{\text{LS}}$ is the maximum likelihood (ML) estimate under this model.

One-Slide Proof

- Proof:

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\begin{aligned}
\hat{\boldsymbol{w}}_{\text{ML}} &= \arg\max_{\boldsymbol{w}} P(y_1, \ldots, y_N | x_1, \ldots., x_N; \boldsymbol{w}) \\
&= \arg\max_{\boldsymbol{w}} \prod_{i=1}^{N} P(y_i \mid x_i; \boldsymbol{w}) \\
&= \arg\max_{\boldsymbol{w}} \sum_{i=1}^{N} \log P(y_i \mid x_i; \boldsymbol{w}) \\
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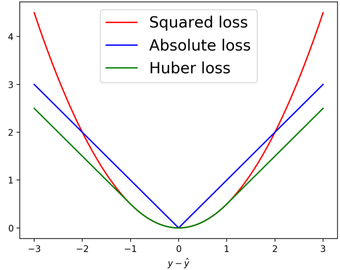
- Conclusion: LS linear regression $\Leftrightarrow$ ML under Gaussian noise.

Other Regression Losses

- Squared loss: $L(y, \widehat{y}) = \frac{1}{2}(y - \widehat{y})^2$.
- Absolute error loss: $L(y, \widehat{y}) = |y - \widehat{y}|$
- Huber loss: $L(y, \widehat{y}) = \begin{cases} \frac{1}{2}(y - \widehat{y})^2 & \text{if } |y - \widehat{y}| \leq 1 \\ |y - \widehat{y}| - \frac{1}{2} & \text{if } |y - \widehat{y}| \geq 1. \end{cases}$



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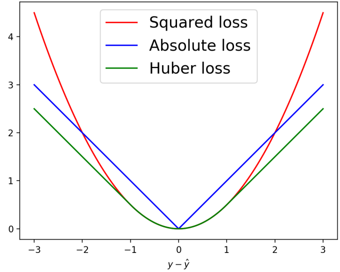

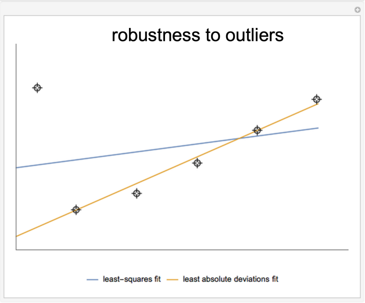

Ridge Regression and Regularization

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- ℓ_2 regularization is also called weight decay, or penalized LS.

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- Conclusion: ℓ_2 regularizarion $\Leftrightarrow$ MAP regression with Gaussian prior.

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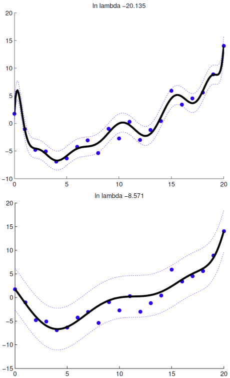

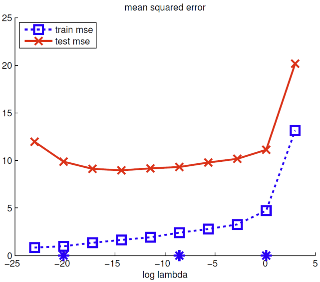

Outline

Binary Classification

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- How to define a model to predict y from x?

Linear Classifier

- Defined by

$$\widehat{y} = \mathrm{sign}(\boldsymbol{w}^T \phi(x) + b) = \begin{cases} +1 & \text{if } \boldsymbol{w}^T \phi(x) + b \geq 0 \\ -1 & \text{if } \boldsymbol{w}^T \phi(x) + b < 0. \end{cases}$$

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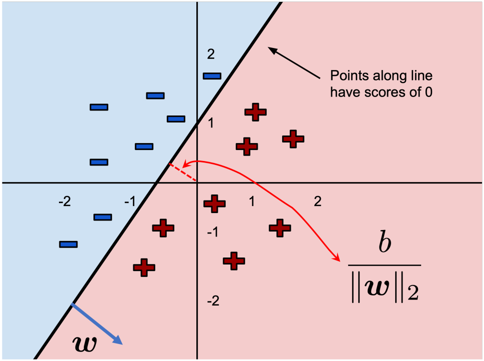
- Decision boundary: $\boldsymbol{w}^T \phi(x) + b = 0$ (hyperplane defined by $\boldsymbol{w}$ and b)
- Also called a hyperplane classifier

Linear Classifier

- $(\boldsymbol{w}, b)$ define an hyperplane that splits the space into two halfs



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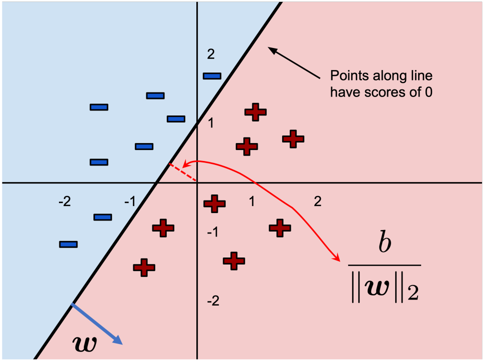
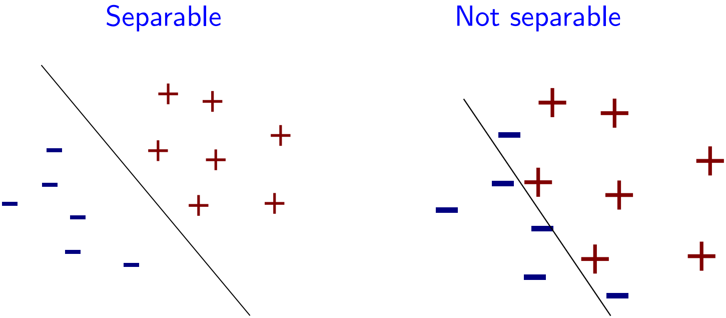


- How to learn it from training data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$?

- A dataset $\mathcal{D}$ is linearly separable if there exists $(\boldsymbol{w}, b)$ such that classification is perfect



Linear Separability

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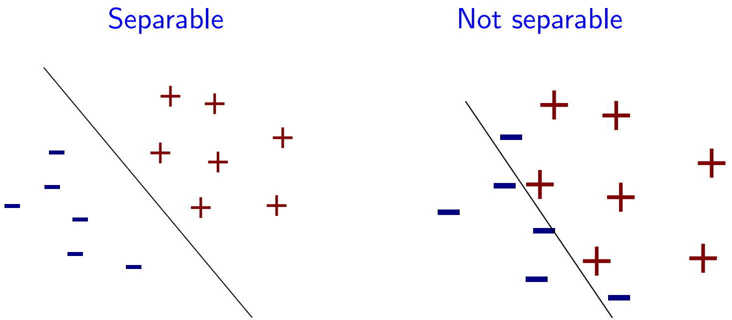

- We next present an (old!) algorithm that finds such an hyperplane, if it exists.

Linear Classifier: No Bias Term

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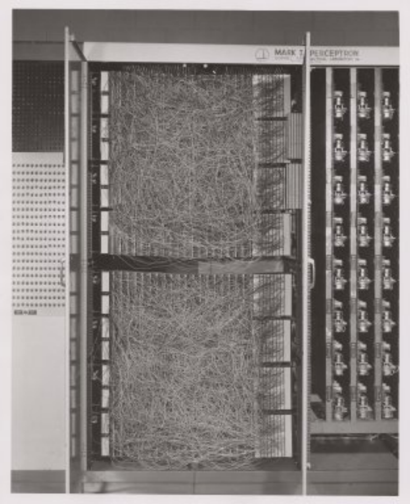
- In this case, the decision boundary is a hyperplane that passes through the origin
- There is no loss of generality:
  - ✓ Add a constant feature to $\phi(x)$: $\phi_0(x) = 1$
  - ✓ The corresponding weight w_0 is a bias term b

Outline

1. Regression
2. **Classification**
   - Perceptron
   - Logistic Regression
   - Support Vector Machines
   - Sparsemax
3. Regularization
4. Non-Linear Models

Perceptron (Rosenblatt, 1958)



(Extracted from Wikipedia)

- Invented in 1957 at the Cornell Aeronautical Laboratory by Frank Rosenblatt
- Implemented in custom-built hardware as the "Mark 1 perceptron," designed for image recognition
- 400 photocells, randomly connected to the "neurons." Weights were encoded in potentiometers
- Weight updates during learning were performed by electric motors.

Perceptron in the News...

1958 New York Times...

NEW NAVY DEVICE LEARNS BY DOING

Psychologist Shows Embryo of Computer Designed to Read and Grow Wiser

WASHINGTON, July 7 (UPI) —The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.

The embryo—the Weather Bureau's $2,000,000 "704" computer—learned to differentiate between right and left after fifty attempts in the Navy's demonstration for newsmen.

The service said it would use this principle to build the first of its Perceptron thinking machines that will be able to read and write. It is expected to be finished in about a year at a cost of $100,000.

Dr. Frank Rosenblatt, designer of the Perceptron, conducted the demonstration. He said the machine would be the first device to think as the human brain. As do human beings, Perceptron will make mistakes at first, but will grow wiser as it gains experience, he said.

Dr. Rosenblatt, a research psychologist at the Cornell Aeronautical Laboratory, Buffalo, said Perceptrons might be fired to the planets as mechanical space explorers.

Without Human Controls

The Navy said the perceptron would be the first non-living mechanism "capable of receiving, recognizing and identifying its surroundings without any human training or control."

The "brain" is designed to remember images and information it has perceived itself. Ordinary computers remember only what is fed into them on punch cards or magnetic tape.

Later Perceptrons will be able to recognize people and call out their names and instantly translate speech in one language to speech or writing in another language, it was predicted.

Mr. Rosenblatt said in principle it would be possible to build brains that could reproduce themselves on an assembly line and which would be conscious of their existence.

In today's demonstration, the "704" was fed two cards, one with squares marked on the left side and the other with squares on the right side.

Learns by Doing

In the first fifty trials, the machine made no distinction between them. It then started registering a "Q" for the left squares and "O" for the right squares.

Dr. Rosenblatt said he could explain why the machine learned only in highly technical terms. But he said the computer had undergone a "self-induced change in the wiring diagram."

The first Perceptron will have about 1,000 electronic "association cells" receiving electrical impulses from an eye-like scanning device with 400 photo-cells. The human brain has 10,000,000,000 responsive cells, including 100,000,000 connections with the eyes.

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Perceptron Algorithm

- Online algorithm: process one data point at each round

  1. Take one x_i; apply the current model to make a prediction for it
  2. If prediction is correct, do nothing
  3. Else, correct $\boldsymbol{w}$ by adding/subtracting feature vector $\phi(x_i)$

- For simplicity, omit the bias b: assume a constant feature $\phi_0(x) = 1$ as explained earlier.

Perceptron Algorithm

input: labeled data $\mathcal{D}$
initialize $\boldsymbol{w}^{(0)} = 0$
initialize $k = 0$ (number of mistakes)
repeat
  get new training example (x_i, y_i)
  predict $\widehat{y}_i = \text{sign}(\boldsymbol{w}^{(k)\,T}\phi(x_i))$
  if $\widehat{y}_i \neq y_i$ **then**
    update $\boldsymbol{w}^{(k+1)} = \boldsymbol{w}^{(k)} + y_i\phi(x_i)$
    increment k
  end if
until maximum number of epochs
output: model weights $\boldsymbol{w}^{(k)}$

Perceptron's Mistake Bound

- Some definitions:

  ✓ the training data is linearly separable with margin $\gamma > 0$ iff there is a weight vector $\boldsymbol{u}$ with $\|\boldsymbol{u}\| = 1$ such that

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- Then, the following bound of the number of mistakes holds:

Theorem (Novikoff, 1962)

The perceptron algorithm is guaranteed to find a separating hyperplane after at most $\frac{R^2}{\gamma^2}$ *mistakes.*

One-Slide Proof

- Recall that $\boldsymbol{w}^{(k+1)} = \boldsymbol{w}^{(k)} + y_i \phi(x_i)$ and that $\|\boldsymbol{u}\| = 1$
- **Lower bound on** $\|\boldsymbol{w}^{(k+1)}\|$:

$$\begin{aligned} \boldsymbol{u}^T \boldsymbol{w}^{(k+1)} &= \boldsymbol{u}^T \boldsymbol{w}^{(k)} + y_i \boldsymbol{u}^T \phi(x_i) \\ &\geq \boldsymbol{u}^T \boldsymbol{w}^{(k)} + \gamma \\ &\geq k\gamma. \end{aligned}$$

Thus: $\|\boldsymbol{w}^{(k+1)}\| = \|\boldsymbol{u}\| \, \|\boldsymbol{w}^{(k+1)}\| \geq \boldsymbol{u}^T \boldsymbol{w}^{(k+1)} \geq k\gamma$ (Cauchy-Schwarz)

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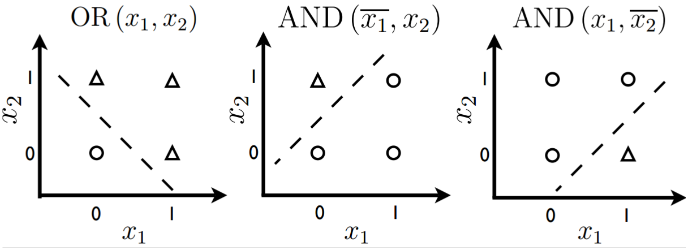
- **Upper bound on $\|\boldsymbol{w}^{(k+1)}\|$:**

$$\begin{aligned}
\|\boldsymbol{w}^{(k+1)}\|^2 &= \|\boldsymbol{w}^{(k)}\|^2 + \|\phi(x_i)\|^2 + 2\,\overbrace{y_i {\boldsymbol{w}^{(k)}}^T \phi(x_i)}^{<0} \\
&\leq \|\boldsymbol{w}^{(k)}\|^2 + R^2 \\
&\leq kR^2.
\end{aligned}$$

- Equating both sides: $(k\gamma)^2 \leq kR^2 \;\Rightarrow\; k \leq R^2/\gamma^2$ (QED).

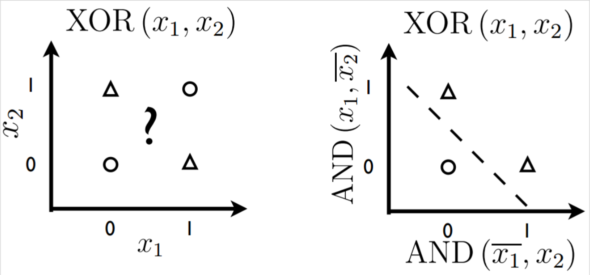
What a Simple Perceptron Can and Can't Do

- Remember: the decision boundary is linear (linear classifier)
- It **can** solve linearly separable problems (OR, AND)



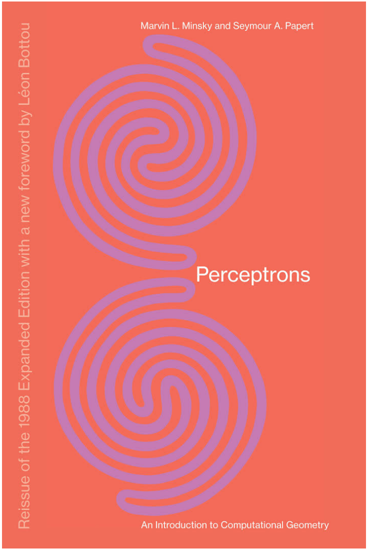
What a Simple Perceptron Can and Can't Do

- ... but it **can't** solve non-linearly separable problems such as simple XOR (unless input is transformed into a better representation):



- This result is often attributed to Minsky and Papert (1969) but was known well before.

Limitations of the Perceptron



- Minsky and Papert (1996) showed limitations of multi-layer perceptrons and fostered an "AI winter" period.

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- Consider multi-class problems, with $|\mathcal{Y}| = K \geq 2$ labels (classes).

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- Here, we consider classifiers that tackle the multiple classes directly.

Multi-Class Linear Classifiers

- Parametrized by a weight matrix $\boldsymbol{W} \in \mathbb{R}^{K \times D}$ (one weight per feature/label pair) and a bias vector $\boldsymbol{b} \in \mathbb{R}^{K}$:

$$\boldsymbol{W} = \begin{bmatrix} \boldsymbol{w}_1^T \\ \vdots \\ \boldsymbol{w}_K^T \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_K \end{bmatrix}.$$

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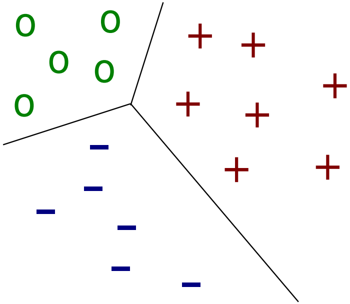
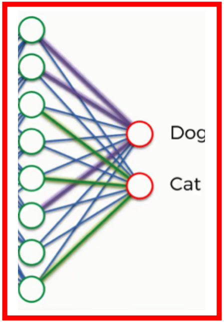
Multi-Class Linear Classifier

- $(\boldsymbol{W}, \boldsymbol{b})$ split the feature space into regions delimited by hyperplanes.
- Each region in the intersection of $K-1$ half-spaces.



Commonly Used Notation in Neural Networks

Handcrafted Features



Linear Classifier

$$\widehat{y} = \operatorname{argmax}\left(\boldsymbol{W}\phi(x) + \boldsymbol{b}\right), \quad \boldsymbol{W} = \begin{bmatrix} \vdots \\ \boldsymbol{w}_y^\top \\ \vdots \end{bmatrix}, \; \boldsymbol{b} = \begin{bmatrix} \vdots \\ b_y \\ \vdots \end{bmatrix}.$$

Multi-Class Recovers Binary

- With two classes (e.g. $\mathcal{Y} = \{+1, -1\}$), we recover the binary classifier:

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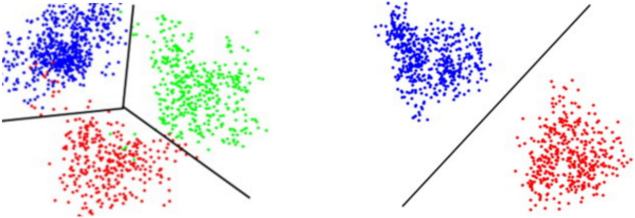
- Only half of the parameters are needed.

Linear Classifiers (Binary vs Multi-Class)

- Prediction rule (omitting the bias term, without loss of generality):

$$\widehat{y} = h(x) = \arg\max_{y \in \mathcal{Y}} \overbrace{\boldsymbol{w}_y{}^T \phi(x)}^{\text{linear in } \boldsymbol{w}_y}$$

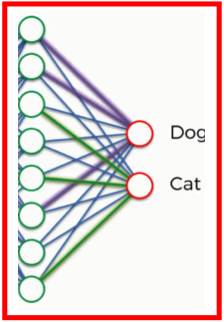
- The decision boundary is defined by the intersection of half spaces
- In the binary case ($|\mathcal{Y}| = 2$) this corresponds to a hyperplane classifier



Perceptron Algorithm: Multi-Class

input: labeled data $\mathcal{D}$
initialize $\boldsymbol{W}^{(0)} = 0$
initialize $k = 0$ (number of mistakes)
repeat
  get new training example (x_i, y_i)
  predict $\widehat{y}_i = \arg\max_{y \in \mathcal{Y}} \boldsymbol{w}_y^{(k)^T} \phi(x_i)$
  if $\widehat{y}_i \neq y_i$ **then**
    update $\boldsymbol{w}_{y_i}^{(k+1)} = \boldsymbol{w}_{y_i}^{(k)} + \phi(x_i)$ $\{$*increase weight of gold class*$\}$
    update $\boldsymbol{w}_{\widehat{y}_i}^{(k+1)} = \boldsymbol{w}_{\widehat{y}_i}^{(k)} - \phi(x_i)$ $\{$*decrease weight of incorrect classes*$\}$
    increment k
  end if
until maximum number of epochs
output: model weights $\boldsymbol{W}^{(k)}$

Reminder



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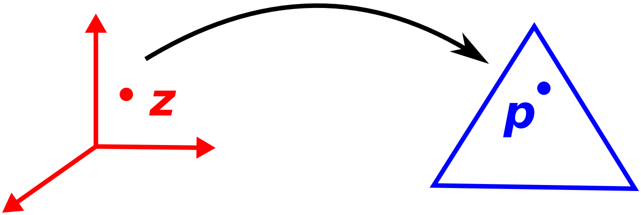

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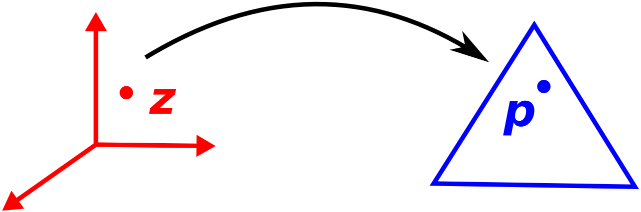

- Two possible mappings: softmax, a.k.a. logistic regression (next) and sparsemax (later).

Outline

Logistic Regression

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- Allows for cost-sensitive decisions, beyond simple MAP.

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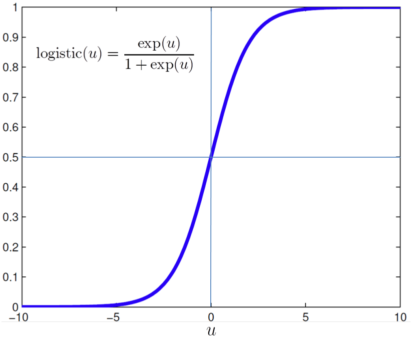
- Sigmoid, or logistic, transformation (more later!)

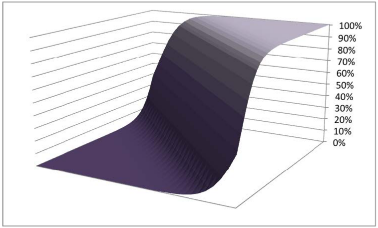
Sigmoid/Logistic Transformation

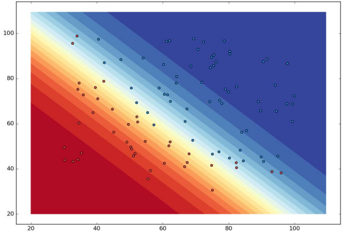
$$\boxed{\sigma(z) = \frac{1}{1 + e^{-z}}}$$



- Widely used in neural networks (more tomorrow!)
- "Squashes" a real number into [0, 1]
- The output can be interpreted as a probability
- Positive, bounded, strictly increasing, differentiable

- In two dimensions, i.e., $\boldsymbol{w}$, $\phi(x) \in \mathbb{R}^2$





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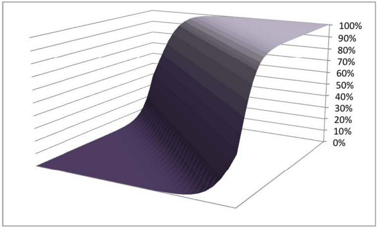

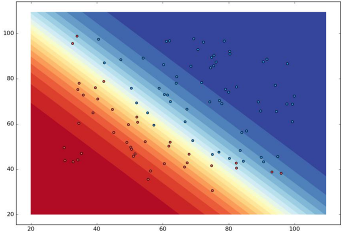

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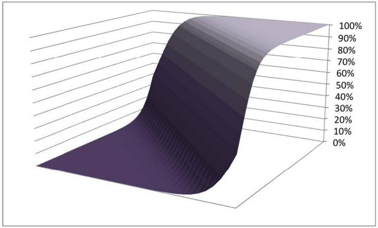

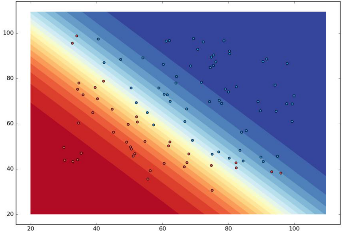

- MAP boundary, $P(y = +1 \mid x) = 1/2 \;\Leftrightarrow\; \boldsymbol{w}^T \phi(x) = 0$, is linear w.r.t. $\phi(x)$.
- Some other threshold, $P(y = +1 \mid x) = \tau \;\Leftrightarrow\; \boldsymbol{w}^T \phi(x) = \log(\frac{\tau}{1-\tau})$; linear w.r.t. $\phi(x)$.

Multinomial Logistic Regression

- Recall $\boldsymbol{W} = [\boldsymbol{w}_1, ..., \boldsymbol{w}_K] \in \mathbb{R}^{K \times D}$ and $P_{\boldsymbol{W}}(y|x) = \frac{\exp(\boldsymbol{w}_y{}^T \phi(x))}{\sum_{y'} \exp(\boldsymbol{w}_{y'}{}^T \phi(x))}$

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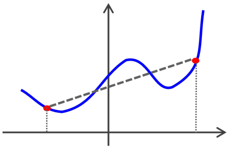
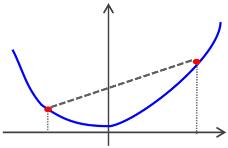
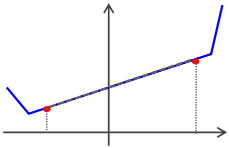
- $\widehat{\boldsymbol{W}}$ is set to assign as much probability as possible to the correct labels!

Logistic Regression

- This objective function is strictly convex


non-convex


convex
strictly convex


convex, not strictly

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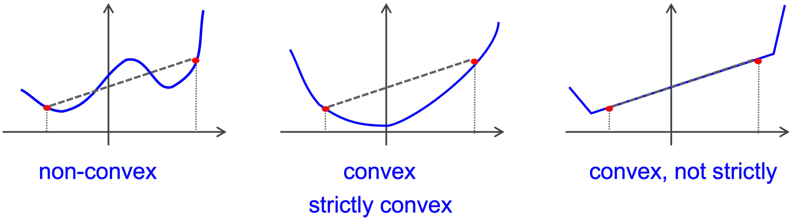

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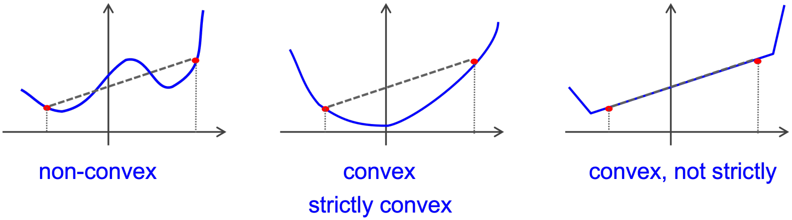

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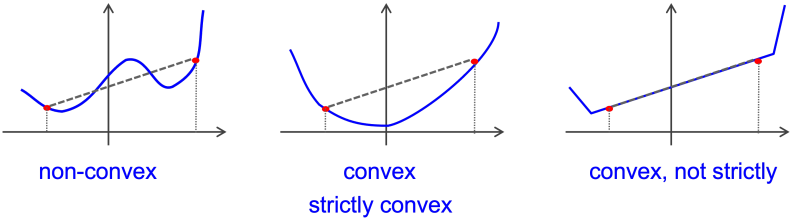

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- Therefore any local minimum is a global minimum
- No closed form solution, but many numerical techniques
  - ✓ Gradient methods (gradient descent, conjugate gradient)
  - ✓ Quasi-Newton methods (L-BFGS, ...)

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- Take small steps in the negative gradient direction until a stopping criterion is met:
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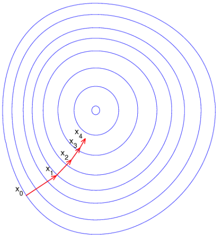
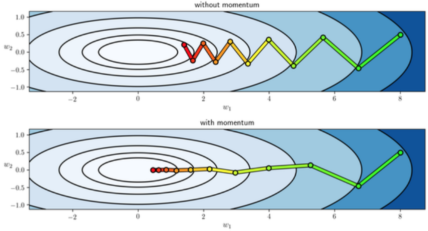
- Choosing the step-size: crucial for convergence and performance.

- Goal: minimize $f : \mathbb{R}^d \to \mathbb{R}$, for differentiable objective function f
- Take small steps in the negative gradient direction until a stopping criterion is met:

$$x^{(t+1)} \leftarrow x^{(t)} - \eta_{(t)} \nabla f(x^{(t)})$$

- Choosing the step-size: crucial for convergence and performance.
- GD may work well, or not so well. There are many ways to improve it.





Gradient Descent

- Objective function in logistic regression:

$$\sum_{t=1}^{N} L(\boldsymbol{W};(x_t,y_t)) = \sum_{t=1}^{N}\left(\log\sum_{y'}\exp({\boldsymbol{w}_{y'}}^T\phi(x)) - {\boldsymbol{w}_y}^T\phi(x)\right)$$

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- Gradient descent:

  ✓ Set $\boldsymbol{W}^{(0)} = 0$

  ✓ Iterate until convergence (for suitable stepsize η_k):

$$\begin{aligned} \boldsymbol{W}^{(k+1)} &= \boldsymbol{W}^{(k)} - \eta_k \nabla_{\boldsymbol{W}} \left(\textstyle\sum_{t=1}^{N} L(\boldsymbol{W}^{(k)}; (x_t, y_t)) \right) \\ &= \boldsymbol{W}^{(k)} - \eta_k \textstyle\sum_{t=1}^{N} \nabla_{\boldsymbol{W}} L(\boldsymbol{W}^{(k)}; (x_t, y_t)) \end{aligned}$$

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- $\nabla_{\boldsymbol{W}} L(\boldsymbol{W}^{(k)})$ is gradient of w.r.t. $\boldsymbol{W}$, computed at $\boldsymbol{W}^{(k)}$
- L convex $\Rightarrow$ gradient descent converges to global optimum

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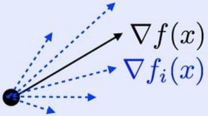
- Variants exist in-between batch and stochastic: mini-batches
- All guaranteed to find the optimal $\boldsymbol{W}$ (for suitable step sizes)

SGD: Visual Summary

Finite sums

$$f(x) \overset{\text{def.}}{=} \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$
$$\nabla f(x) = \frac{1}{n}\sum_i \nabla f_i(x)$$

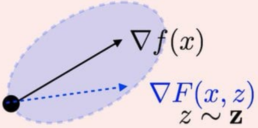


Draw $i \in \{1, \dots, n\}$ uniformly.

$$x_{k+1} = x_k - \tau_k \nabla f_i(x_k)$$

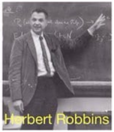
Expectation

$$f(x) \overset{\text{def.}}{=} \mathbb{E}_{\mathbf{z}}(f(x, \mathbf{z}))$$
$$\nabla f(x) = \mathbb{E}_{\mathbf{z}}(\nabla F(x, \mathbf{z}))$$



Draw $z \sim \mathbf{z}$

$$x_{k+1} = x_k - \tau_k \nabla F(x, z)$$



Theorem: If f is strongly convex and $\tau_k \sim 1/k$,

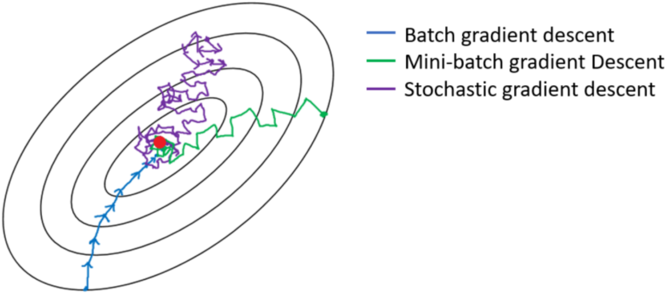
$$\mathbb{E}(\|x_k - x^\star\|^2) = O(1/k)$$

Figure by Gabriel Peyre. Highly recommended: twitter.com/gabrielpeyre

Batch, Stochastic, and Minibatch Gradient Descent

- Minibatch: instead of single sample, sample subset $B \subset \{1, \ldots, N\}$.
- Use average gradient on minibatch:

$$\boldsymbol{W}^{(k+1)} = \boldsymbol{W}^{(k)} - \eta_k \frac{1}{|B|} \sum_{t \in B} \nabla_{\boldsymbol{W}} L(\boldsymbol{W}^{(k)}; (x_t, y_t))$$



Computing the Gradient

- All this requires computing $\nabla_{\boldsymbol{W}} L(\boldsymbol{W}; (x_t, y_t))$, where

$$L(\boldsymbol{W}; (x, y)) = \log \sum_{y'} \exp(\boldsymbol{w}_{y'}{}^T \phi(x)) - \boldsymbol{w}_y{}^T \phi(x)$$

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- Some reminders:

✓ $\nabla_{\boldsymbol{W}} \log F(\boldsymbol{W}) = \frac{1}{F(\boldsymbol{W})} \nabla_{\boldsymbol{W}} F(\boldsymbol{W})$

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- One-hot vector representation of class y:

$$\boldsymbol{e}_y = [0, \ldots, 0, \underbrace{1}_{y}, 0, \ldots, 0]^\top \in \{0,1\}^K, \text{ such that } 1^T \boldsymbol{e}_y = 1$$

Computing the Gradient: Step by Step

$$\nabla_{\boldsymbol{W}} L(\boldsymbol{W}; (x, y)) \quad = \quad \nabla_{\boldsymbol{W}} \left(\log \sum_{y'} \exp({\boldsymbol{w}_{y'}}^T \phi(x)) - {\boldsymbol{w}_y}^T \phi(x) \right)$$

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\nabla_{\boldsymbol{W}} L(\boldsymbol{W};(x,y)) &= \nabla_{\boldsymbol{W}} \left(\log \sum_{y'} \exp(\boldsymbol{w}_{y'}{}^T \phi(x)) - \boldsymbol{w}_y{}^T \phi(x) \right) \\
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- Conditional class probabilities:

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- Gradient can be computed

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thus (S)GD (or any gradient-based algorithm) can be used.

The Story So Far

- Logistic regression is discriminative: maximizes conditional likelihood
  - ✓ also called log-linear model and max-entropy classifier
  - ✓ no closed form solution.
  - ✓ stochastic gradient updates (SGD):

$$\boldsymbol{W}^{(k+1)} = \boldsymbol{W}^{(k)} + \eta_k \left(\boldsymbol{e}_y \phi(x)^\top - \sum_{y'} P_{\boldsymbol{W}^{(k)}}(y'|x)\, \boldsymbol{e}_{y'}\, \phi(x)^\top \right)$$

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- Logistic regression SGD updates and perceptron updates look similar!

Outline

Maximizing Margin

- Let $\gamma > 0$ denote the margin, and set the goal of maximizing it

$$\max_{\boldsymbol{U}} \ \gamma$$

subject to

$$\|\boldsymbol{U}\| = 1$$

$$\boldsymbol{u}_{y_t}^T \phi(x_t) - \boldsymbol{u}_{y'}^T \phi(x_t) \geq \gamma$$

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- Fix $||\boldsymbol{U}|| = 1$ since increasing $\|\boldsymbol{U}\|$ trivially produces larger margin

Maximum Margin $\Leftrightarrow$ Minimum Norm

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$\Leftrightarrow$

Min Norm:

$$\min_{\boldsymbol{W}} \quad \frac{1}{2} ||\boldsymbol{W}||^2$$

such that:

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- Instead of fixing $||\boldsymbol{U}||$ we fix the margin to 1
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- Quadratic programming (QP) problem: well known convex problem, for which there are several techniques.

Support Vector Machines

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- Slacks allow (penalized) violation of the margin constraints

$$\widehat{\boldsymbol{W}} = \arg\min_{\boldsymbol{W},\xi} \; \frac{1}{2}||\boldsymbol{W}||^2 + C\sum_{t=1}^{N}\xi_t$$

subject to

$$\boldsymbol{w}_{y_t}^T\phi(x_t) - \boldsymbol{w}_{y'}^T\phi(x_t) \geq 1 - \xi_t \text{ and } \xi_t \geq 0$$

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- If data is separable, optimal solution has $\xi_i = 0$, $\forall i$

Support Vector Machines: Hinge Loss View

$$\boldsymbol{W} = \arg\min_{\boldsymbol{W},\xi} \; \frac{1}{2}||\boldsymbol{W}||^2 + C\sum_{t=1}^{N}\xi_t$$

subject to

$$\boldsymbol{w}_{y_t}^T\phi(x_t) - \boldsymbol{w}_{y'}^T\phi(x_t) \geq 1 - \xi_t \quad \forall y' \neq y_t$$

Support Vector Machines: Hinge Loss View

$$\boldsymbol{W} = \arg\min_{\boldsymbol{W},\xi} \ \frac{1}{2}||\boldsymbol{W}||^2 + C\sum_{t=1}^{N}\xi_t$$

subject to

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$$L(\boldsymbol{W}; (x_t, y_t)) = \max \left(0, 1 + \max_{y' \neq y_t} \ \boldsymbol{w}_{y'}^T \phi(x_t) - \boldsymbol{w}_{y_t}^T \phi(x_t)\right)$$

Support Vector Machines: Hinge Loss View

- SVM QP formulation:

$$\widehat{\boldsymbol{W}} = \arg\min_{\boldsymbol{W},\xi} \ \frac{\lambda}{2}||\boldsymbol{W}||^2 + \sum_{t=1}^{N} \xi_t$$

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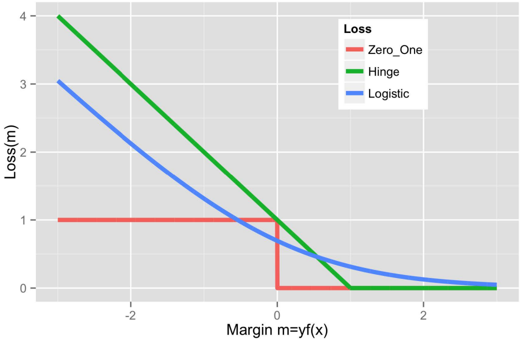
- Hinge loss equivalent:

$$\boldsymbol{W} = \arg\min_{\boldsymbol{W}} \left(\sum_{t=1}^{N} \underbrace{\max\left(0, 1 - \overbrace{\left(\boldsymbol{w}_{y_t}^T \phi(x_t) - \max_{y' \neq y_t} \boldsymbol{w}_{y'}^T \phi(x_t)\right)}^{\text{margin of sample } t}\right)}_{L(\boldsymbol{W};(x_t,y_t))} \right) + \frac{\lambda}{2}||\boldsymbol{W}||^2$$

Hinge Loss



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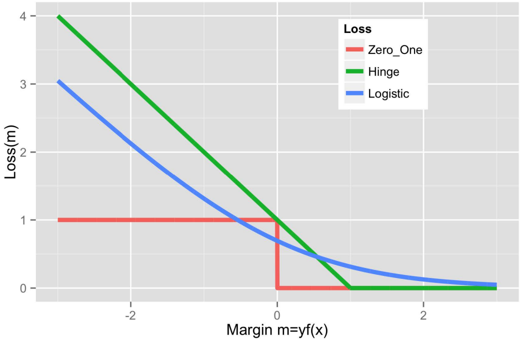

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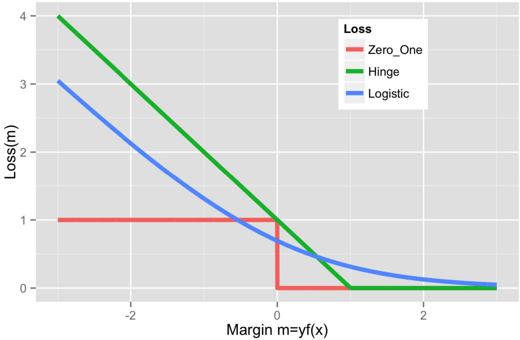
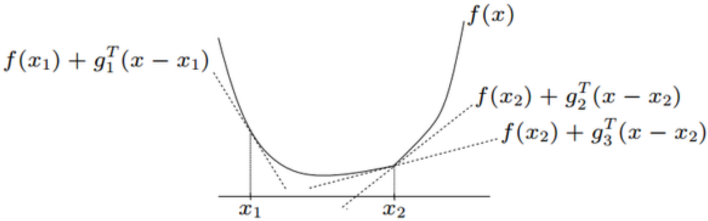


- Hinge: $h(u) = \max\{0, 1 - u\}$: piecewise linear, not everywhere differentiable.
- Cannot use gradient descent
- But can use subgradient descent (almost the same)!

Subgradients



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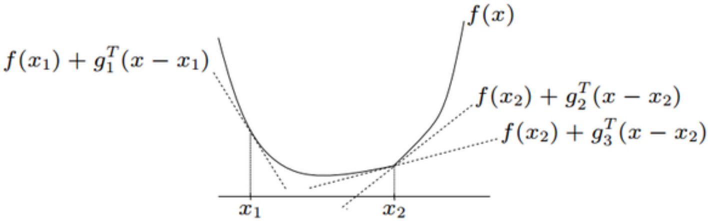

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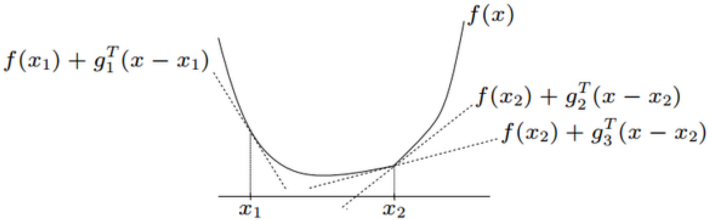

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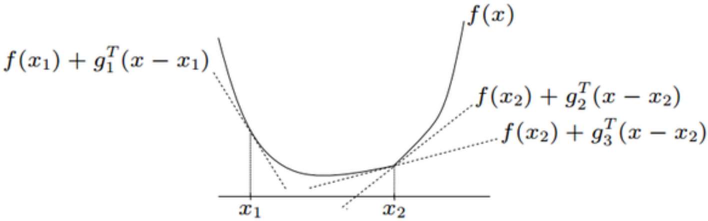

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- At points where f is non-differentiable, there are infinitely many subgradients (an interval for $D = 1$).
- For $D = 1$ (figure above), a subgradient at x_2 is the slope of any tangent that stays below the function.

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- For some $f(x) = h(g(x))$, if g is differentiable, a valid choice is thus

$$\tilde{\nabla} f(x) = \begin{cases} 0, & \text{if } g(x) \geq 1 \\ -\nabla g(x), & \text{if } g(x) < 1 \end{cases}$$

Perceptron and Hinge-Loss

- SVM subgradient update (ignoring $\|\boldsymbol{W}\|^2$ term):

$$\boldsymbol{W}^{(k+1)} = \boldsymbol{W}^{(}k) - \eta \begin{cases} 0, & \text{if } \boldsymbol{w}_{y_t}^T \phi(x_t) - \max_{y \neq y_t} \boldsymbol{w}_y^T \phi(x_t) \geq 1 \\ (\boldsymbol{e}_y - \boldsymbol{e}_{y_t}) \phi(x_t)^T, & \text{otherwise, w/ } y = \arg\max_{y \neq y_t} \boldsymbol{w}_y^T \phi(x_t) \end{cases}$$

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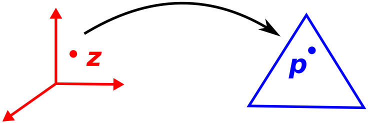
- Perceptron = SGD with zero-margin hinge-loss:

$$\max\left(0, \max_{y \neq y_t} \boldsymbol{w}_y^T \phi(x_t) - \boldsymbol{w}_{y_t}^T \phi(x_t)\right) = \mathrm{ReLU}(\max_{y \neq y_t} \boldsymbol{w}_y^T \phi(x_t) - \boldsymbol{w}_{y_t}^T \phi(x_t))$$

Outline

Obtaining Probabilities

- Mapping from score vector $\boldsymbol{z} \in \mathbb{R}^{|\mathcal{Y}|}$ to probability distribution over $\mathcal{Y}$



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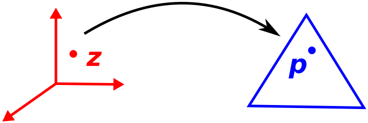

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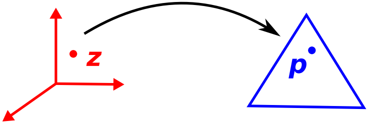

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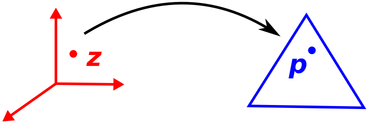

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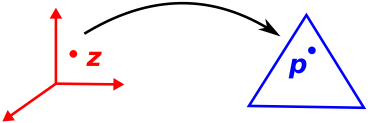

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- We already saw one such mapping: softmax. Next: sparsemax.

Recap: Softmax Transformation

- Classical choice is softmax : $\mathbb{R}^{|\mathcal{Y}|} \to \Delta_{|\mathcal{Y}|-1}$:

$$\boxed{\mathrm{softmax}(\boldsymbol{z}) = \left[\frac{\exp(z_1)}{\sum_j \exp(z_j)}, \ldots, \frac{\exp(z_{|\mathcal{Y}|})}{\sum_j \exp(z_j)}\right]}$$

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- Common workaround: threshold and renormalize.

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- Essentially: sorting, shifting, and thresholding.

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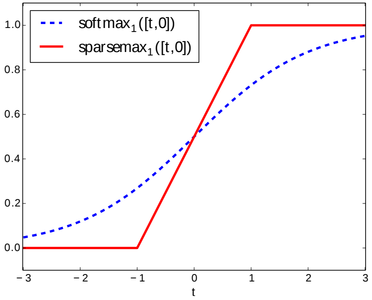

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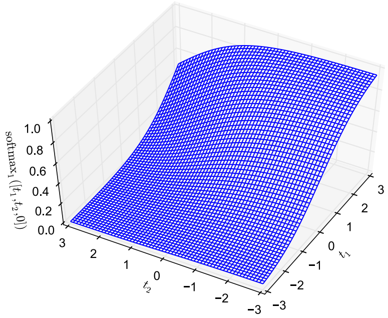
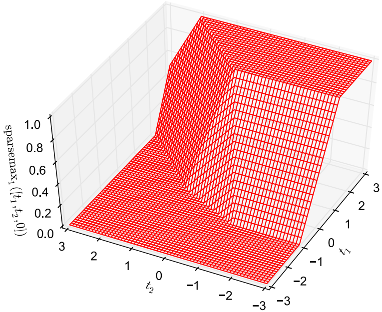
- sparsemax is piecewise linear, but asymptotically similar to softmax





Softmax, sparsemax, and argmax

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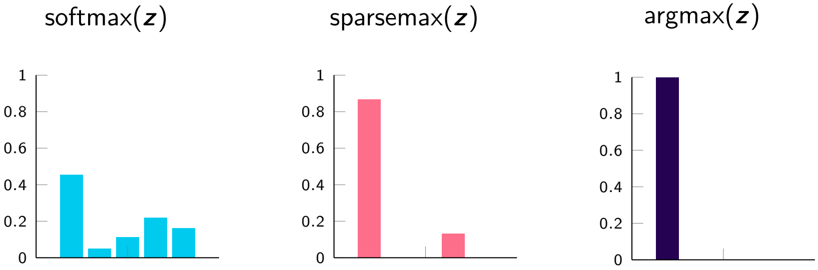

(Same $\boldsymbol{z} = [1.0716, -1.1221, -0.3288, 0.3368, 0.0425]$)

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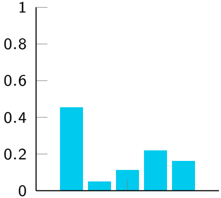

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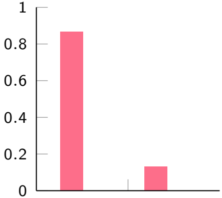

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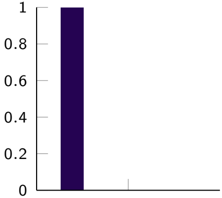

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- It is (it may be) **sparse**, but **differentiable**.

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- The temperature controls how peaked the softmax is and how sparse the sparsemax is.

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- Not directly applicable to sparsemax: cannot compute $log(0)$

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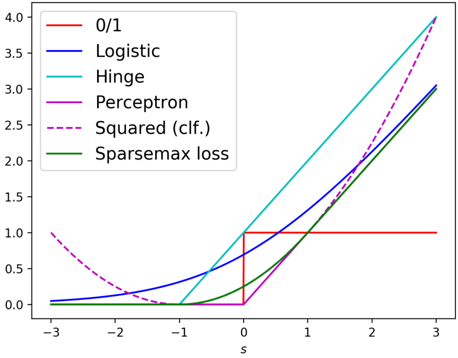
- This is achieved with the sparsemax loss:

$$L(\boldsymbol{W}; (x, y)) = -z_y(x) + \frac{1}{2}\|\text{sparsemax}(\boldsymbol{z}(x))\|^2 - \boldsymbol{z}(x)^\top \text{sparsemax}(\boldsymbol{z}(x)),$$

where $z_y(x)$ is the score of class y.

Classification Losses (Binary Case)

- Let the correct label be $y = 1$ and define $s = z_2 - z_1$.
- Sparsemax loss in 2D becomes a "classification Huber loss":

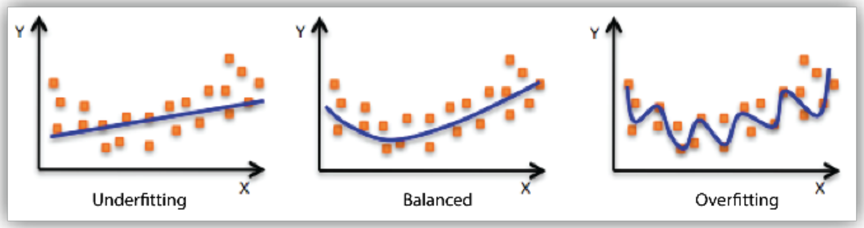


Outline

1. Regression
2. Classification
   - Perceptron
   - Logistic Regression
   - Support Vector Machines
   - Sparsemax
3. **Regularization**
4. Non-Linear Models

Overfitting

- If a model is too complex (too many parameters), there is a the risk of overfitting:



- We saw one example already with polynomial regression.

Regularization

- Regularization aims at preventing overfitting

$$\widehat{\boldsymbol{W}} = \arg\min_{\boldsymbol{W}} \sum_{t=1}^{N} L(\boldsymbol{W}; (x_t, y_t)) + \lambda\, \Omega(\boldsymbol{W}),$$

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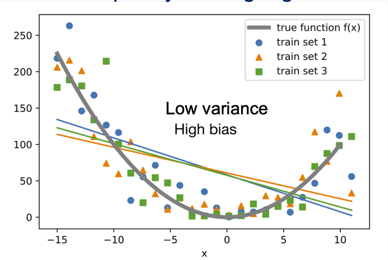
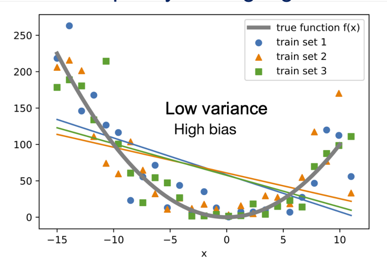
- Not so easy to use ℓ_1 regularization.

low complexity / strong regularization



Bias, Variance, and their Tradeoff

low complexity / strong regularization



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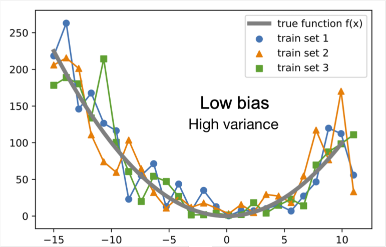

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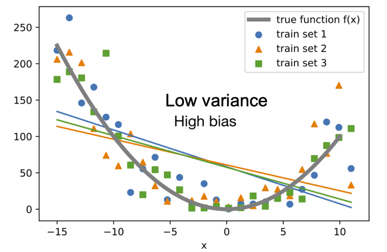

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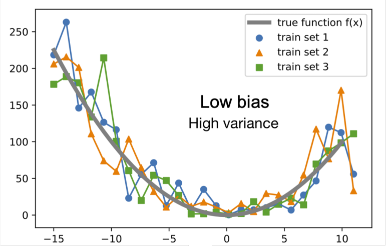
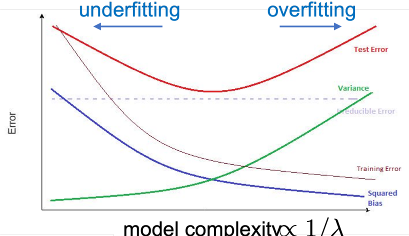
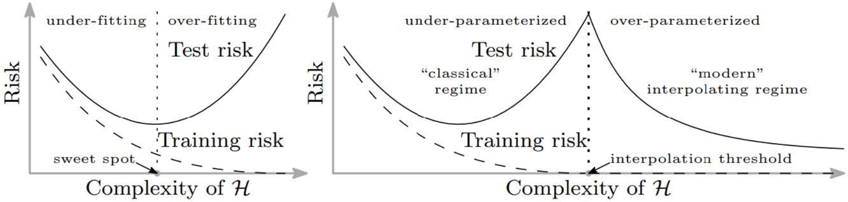




model complexity $\propto 1/\lambda$

- A more modern view, compatible with large deep networks:



(a) U-shaped "bias-variance" risk curve (b) "double descent" risk curve

Double Descent

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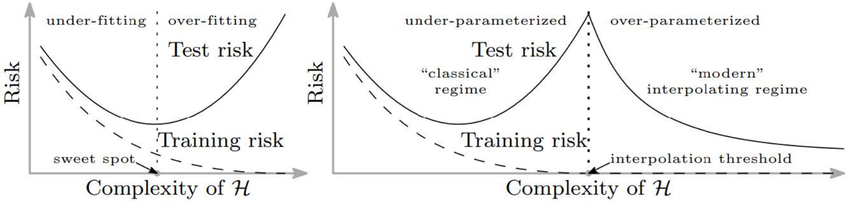

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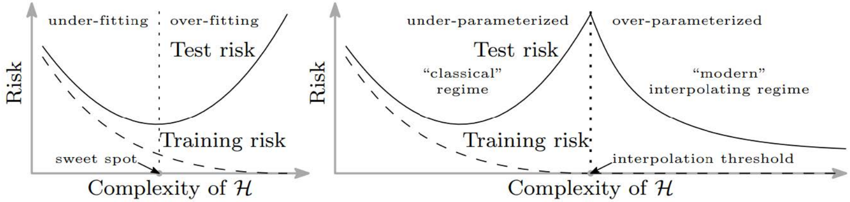

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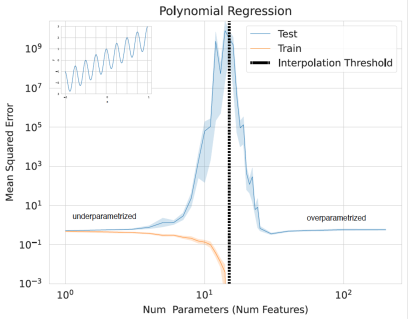
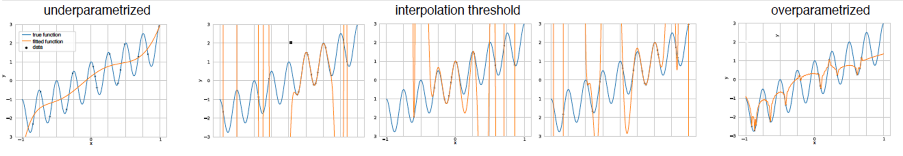
- Active research topic, pioneered by M. Belkin (2018).

Double Descent: Intuition



Schaeffer et al, 2023
arXiv:2303.14151v1



Outline

Summary: Linear Classifiers

- We have covered:
  - ✓ Perceptron
  - ✓ Logistic and Sparsemax regression
  - ✓ Support vector machines
- All lead to convex optimization problems $\Rightarrow$ no issues with local minima/initialization
- All assume the feature map ϕ is well engineered such that the data is (nearly) linearly separable

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- Use one of many other methods: trees, random forests, nearest neighbors, ...
- Use deep neural networks (tomorrow's lecture!)
  - ✓ embrace non-convexity and local minima
  - ✓ instead of engineering features/kernels, engineer the model architecture,
  - ✓ ...and use many tricks of the trade.

Nearest Neighbor Classifiers

- Instead of "training", **keep** all the data $\mathcal{D} = \{(x_i, y_i)_{i=1}^N\}$
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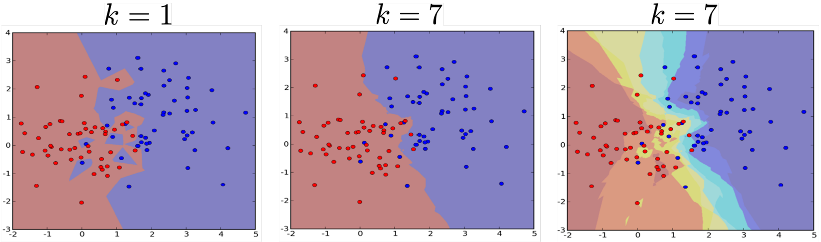

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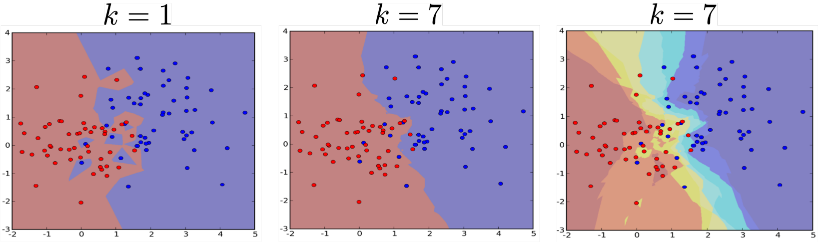

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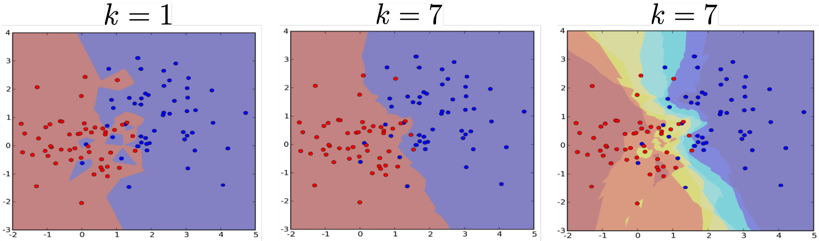

class probability estimates

- Pros: no training, easy implementation, few assumptions, intuitive, intrinsically explainable
- Cons: store all the data, need to define distance, not top (but decent) performance, slow with large high-dim datasets (but there are tricks!)

Nearest Neighbor Classifiers: Obsolete?

"Low-Resource" Text Classification: A Parameter-Free Classification Method with Compressors

Zhiying Jiang[1,2], Matthew Y.R. Yang[1], Mikhail Tsirlin[1], Raphael Tang[1], Yiqin Dai[2] and Jimmy Lin[1]

ACL 2023, July 9-14

alternative to DNNs that's easy, lightweight, and universal in text classification: a combination of a simple compressor like *gzip* with a k-nearest-neighbor classifier. Without any training parameters, our method achieves results that are competitive with non-pretrained deep learning methods on six in-distribution datasets. It even outperforms BERT on all five OOD datasets, including four low-resource languages. Our method also excels in the few-shot setting, where labeled data are too scarce to train DNNs effectively. Code is available at

Model/Dataset	KinyarwandaNews		KirundiNews		DengueFilipino		SwahiliNews		SogouNews	
Shot#	Full	5-shot	Full	5-shot	Full	5-shot	Full	5-shot	Full	5-shot
Bi-LSTM+Attn	0.843	0.253±0.061	0.872	0.254±0.053	0.948	0.369±0.053	0.863	0.357±0.049	0.952	0.534±0.042
HAN	0.820	0.137±0.033	0.881	0.190±0.099	0.981	0.362±0.119	0.887	0.264±0.042	0.957	0.425±0.072
fastText	0.869	0.170±0.057	0.883	0.245±0.242	0.870	0.248±0.108	0.874	0.347±0.255	0.930	0.545±0.053
W2V	0.874	0.281±0.236	0.904	0.288±0.189	0.993	0.481±0.158	0.892	0.373±0.341	0.943	0.141±0.005
SentBERT	0.788	0.292±0.062	0.886	0.314±0.060	0.992	0.629±0.143	0.822	0.436±0.081	0.860	0.485±0.043
BERT	0.838	0.240±0.060	0.879	0.386±0.099	0.979	0.409±0.058	0.897	0.396±0.096	0.952	0.221±0.041
mBERT	0.835	0.229±0.066	0.874	0.324±0.071	0.983	0.465±0.048	0.906	0.558±0.169	0.953	0.282±0.060
gzip (ours)	**0.891**	**0.458±0.065**	**0.905**	**0.541±0.056**	**0.998**	**0.652±0.048**	**0.927**	**0.627±0.072**	**0.975**	**0.649±0.061**

Table 5: Test accuracy on OOD datasets with 95% confidence interval over five trials in five-shot setting.

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- Sometimes the diference is unclear

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$$K_{i,j} = \kappa(x_i, x_j)$$

- The kernel is positive semi-definite if, for all $N \in \mathbb{N}$, all sets of N objects $\{x_1, ..., x_N\} \subseteq \mathcal{X}$, and any $\mathbf{v} \in \mathbb{R}^N$

$$\mathbf{v}\boldsymbol{K}\mathbf{v}^T \geq 0$$

Kernels

- Mercer's Theorem: for any kernel $\kappa : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, there exists some feature mapping $\phi : \mathcal{X} \rightarrow \mathcal{H}$, such that

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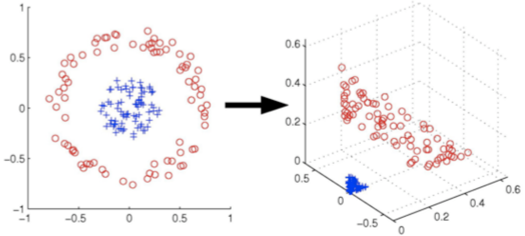
- Extremely popular idea in the 1990-2000s!

Kernel Trick Illustration



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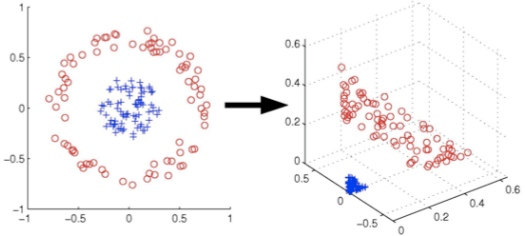

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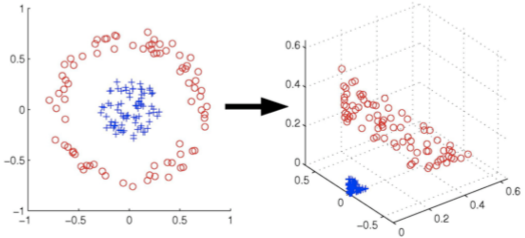
$$
\begin{aligned}
\phi(x) \cdot \phi(z) &= [x_1^2, \sqrt{2} x_1 x_2, x_2^2] \cdot [z_1^2, \sqrt{2} z_1 z_2, z_2^2] \\
&= x_1^2 z_1^2 + 2 x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\
&= ([x_1 \, x_2] \cdot [z_1, z_2])^2 \\
&= \kappa(x, z)
\end{aligned}
$$



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- The inner product in $\mathbb{R}^3$ is a function of the inner product in $\mathbb{R}^2$

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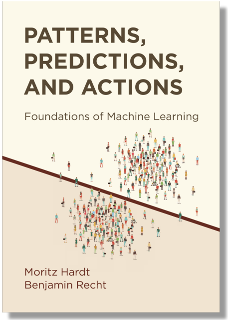
- Many models can be "kernelized" – learning algorithms generally solve the dual optimization problem (also convex)
- Drawback: quadratic dependency on dataset size
- Kernels decouple the learning algorithm (e.g., logistic, SVM) from the nature of the data: strings, images, sets, signals, graphs, probability distributions, ...

Conclusions

- Linear models are a broad class including the well-known perceptron, logistic regression, support vector machines
- They all involve manipulating weights and features
- They either lead to closed-form solutions or convex optimization problems (no local minima)
- Stochastic gradient descent is useful if training datasets are large
- However, linear models rely on specification of feature representations
- **Tomorrow:** methods that learn internal representations

Recommended Books



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Learning Theory from First Principles

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April 19, 2023

Francis Bach

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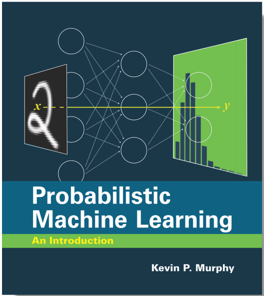
https://www.di.ens.fr/~fbach/ltfp_book.pdf



https://probml.github.io/pml-book/book1.html

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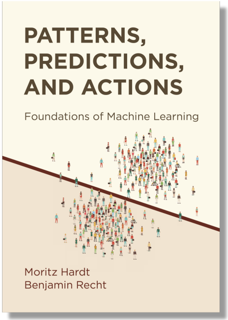

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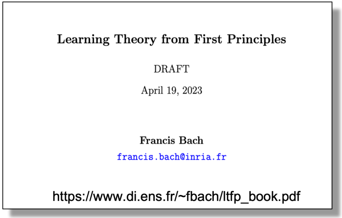
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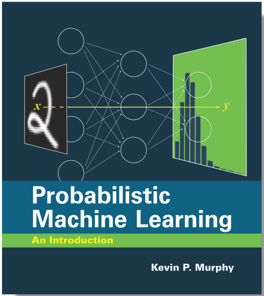

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Thank you! Questions?