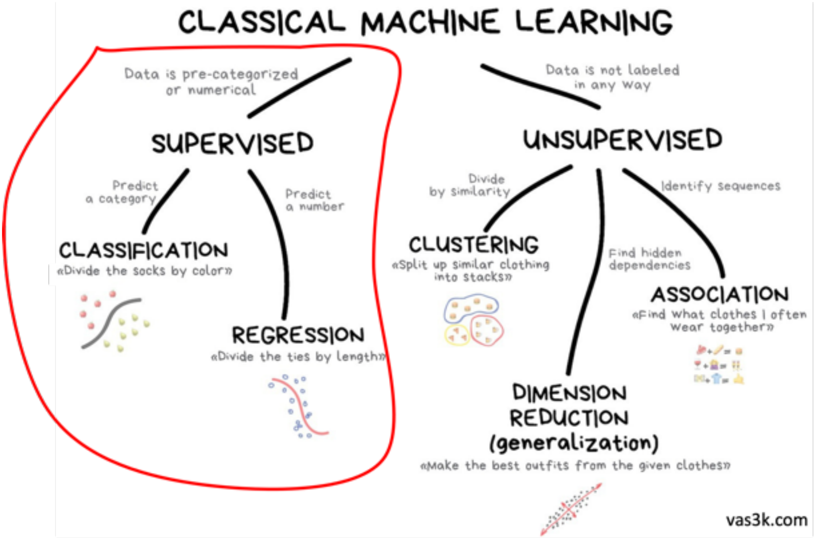
Learning with Linear Models: Foundations of Machine Learning

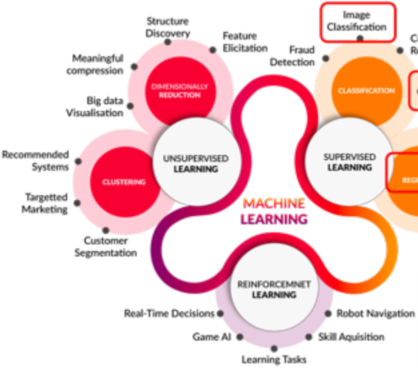
Mário A. T. Figueiredo

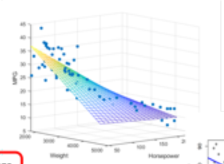
15th Lisbon Machine Learning Summer School, LxMLS 2025

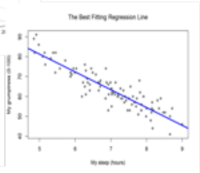

CLASSICAL MACHINE LEARNING
Data is pre-categorized or numerical
Data is not labeled in any way
SUPERVISED
UNSUPERVISED
Predict a category
Predict a number
Divide by similarity
Identify sequences
CLASSIFICATION
«Divide the socks by color»
REGRESSION
«Divide the ties by length»
CLUSTERING
«Split up similar clothing into stacks»
Find hidden dependencies
ASSOCIATION
«Find what clothes I often wear together»
DIMENSION REDUCTION (generalization)
«Make the best outfits from the given clothes»
vas3k.com

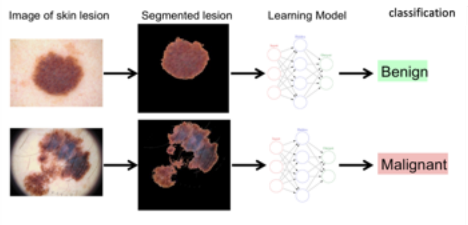
Supervised Learning

Types of Machine Learning









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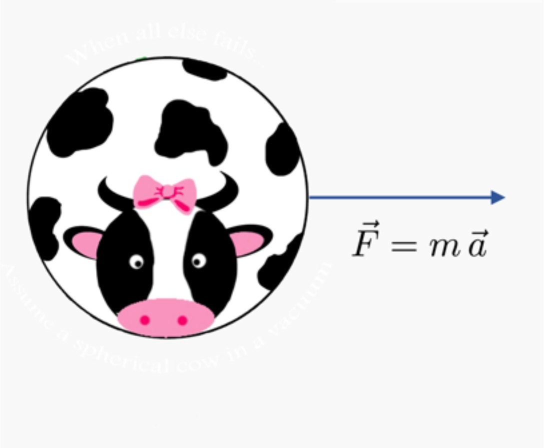
  - ✓ They are a component of DNNs.
  - ✓ Natural starting point for studying ML.

Spherical Cow



Good Advice

Eduardo Ordax · 2nd

Generative AI Lead @ AWS (90k+) | Startup Advisor | Public ...

3d · Edited ·

+ Follow

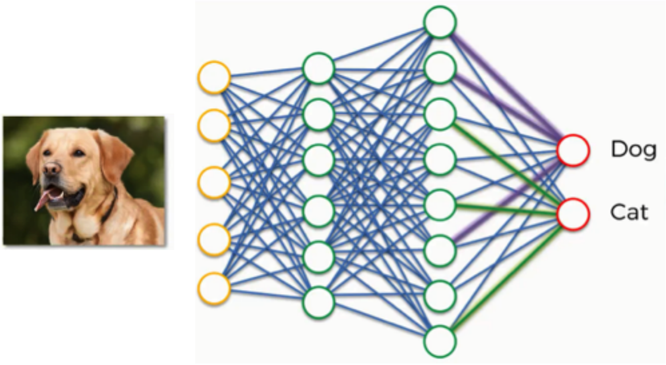
Math Is All You Need! (Or at Least, the Best Place to Start for AI)

I recently came across this advice:

"Don't get an AI degree—the curriculum will be outdated before you graduate. Instead, build a strong foundation in math, statistics, or physics, and stay up to date with AI through code-focused books, blogs, and research papers."

In short, if you're solid in math and willing to refine your coding skills, you'll be a valuable asset to any top AI lab.

Linear Classifiers and Neural Networks



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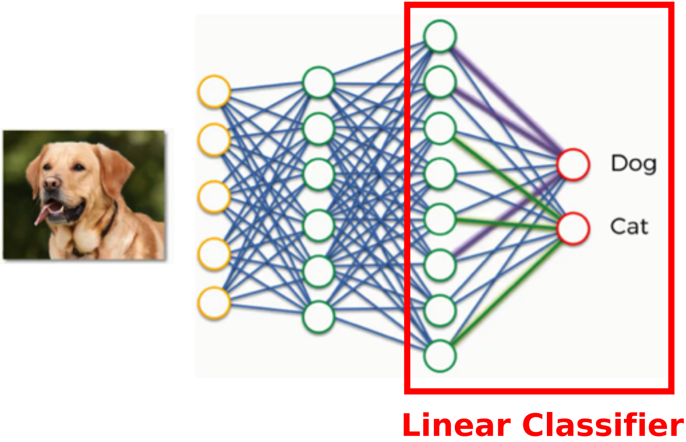

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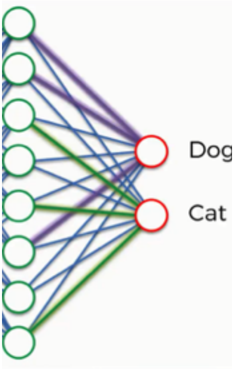

Linear Classifier

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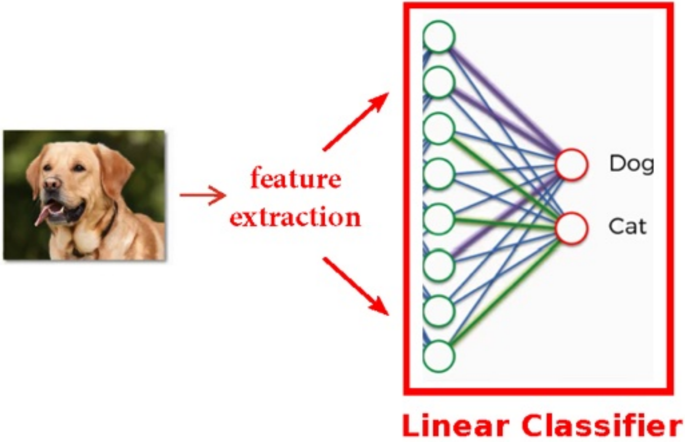

Outline

1. Introduction

2. Regression

3. Classification

4. Optimization for Supervised Learning

Inputs and Outputs

- Input $\boldsymbol{x} \in \mathcal{X}$
  - ✓ e.g., a news article, an email message, a face image, a collection of laboratory test results, features of a credit card transaction, features of a car, features of a house, ...

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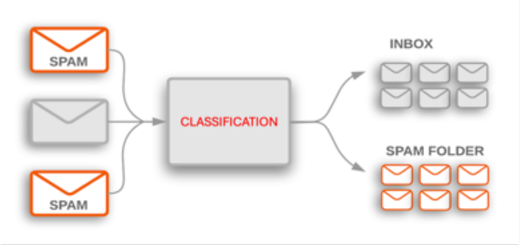
  ✓ e.g., a **news article** together with a **topic**

  ✓ e.g., a **sentence** together with its **translation**

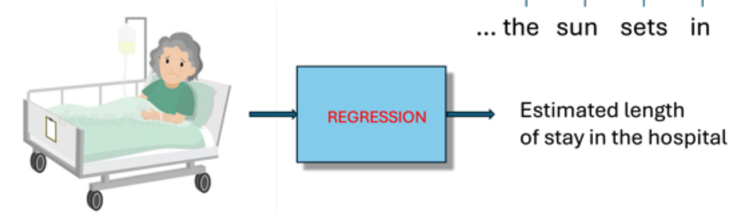
  ✓ e.g., a **sequence of words (tokens)** together with the **next word**

  ✓ e.g., an **image** partitioned into **segmentation regions**

Decisions


SPAM
SPAM
CLASSIFICATION
INBOX
SPAM FOLDER


PREDICTION
... the sun sets in the west


REGRESSION
Estimated length
of stay in the hospital

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- Optimal decision functions minimize the expected loss or risk:

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  where $\mathcal{H}$ is some set of allowed functions.

- Unfortunately, $f_{\boldsymbol{X},\boldsymbol{Y}}(\boldsymbol{x},\boldsymbol{y})$ is seldom known: use supervised learning

Supervised Learning

- Rather than knowing $f_{\boldsymbol{X},\boldsymbol{Y}}(\boldsymbol{x},\boldsymbol{y})$, ...
- ... we have a collection of input/output pairs (training data)

$$\mathcal{D} = (\boldsymbol{x}_1,\boldsymbol{y}_1), ..., (\boldsymbol{x}_n,\boldsymbol{y}_n) \in \mathcal{X} \times \mathcal{Y} \qquad\qquad (\boldsymbol{x}_i \in \mathcal{X},\; \boldsymbol{y}_i \in \mathcal{Y})$$

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  ✓ Discriminative: replace the expected risk with the empirical risk,

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- Classical example: next word prediction.

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

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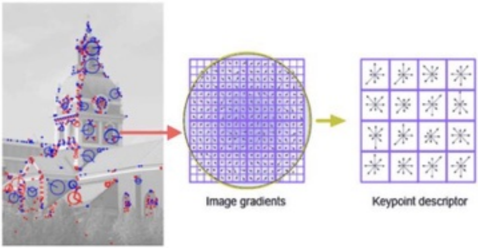

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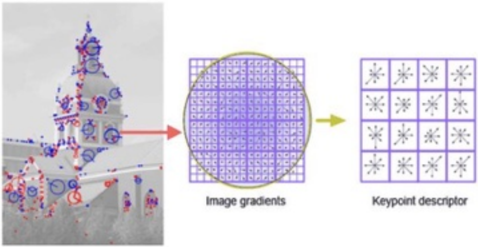

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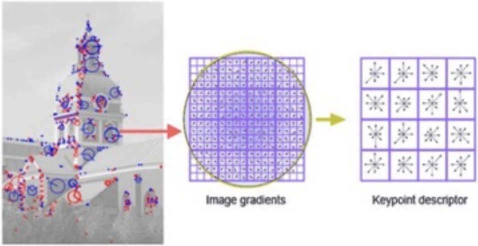

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- Categorical features (e.g., words in a sentence) may be represented by vectors (embeddings).

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Monday's lecture

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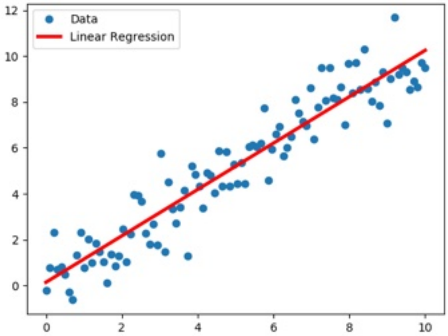
4 Optimization for Supervised Learning

Linear Regression: A Picture



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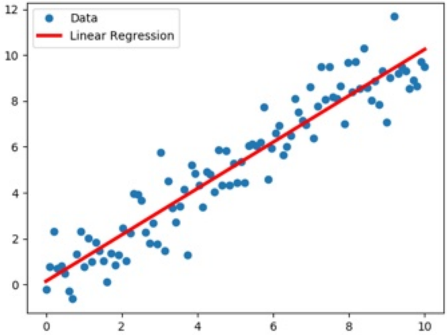


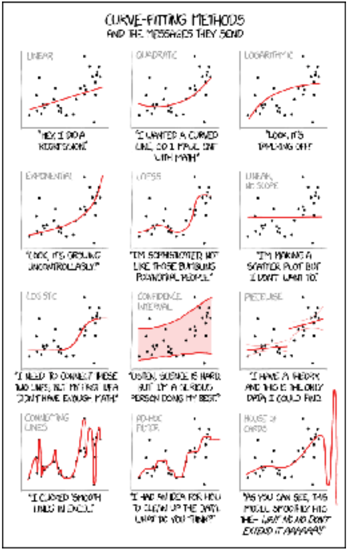
"When you're fundraising, it's AI.

When you're hiring, it's ML.

When you're implementing, it's just linear regression" (B. Schwartz)

Linear (Nonlinear) Regression

- "Linear" regression may be nonlinear (more later)



xkcd.com

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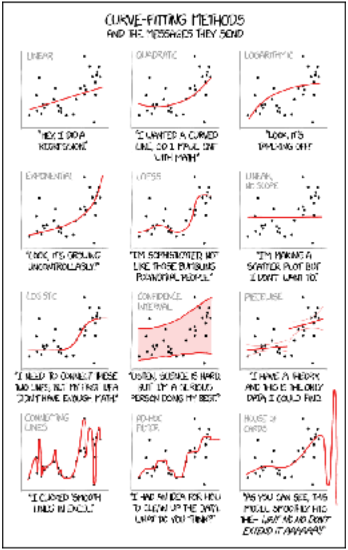
- "Linear" regression may be nonlinear (more later)
- Beware the inductive bias



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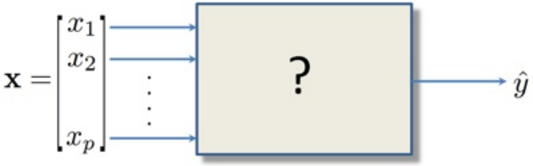
Regression

- In a nutshell: build a "machine" that predicts/estimates/guesses a quantity y from of other "quantities" / "features" $x_1, \ldots, x_p$



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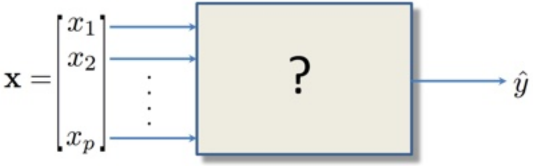

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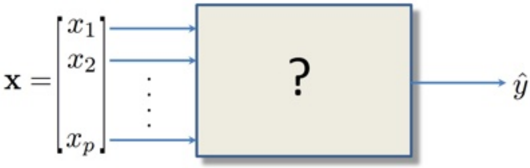

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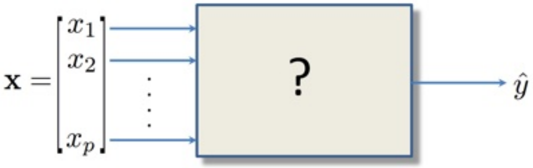

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- Notation: **bold** = vector or matrix (e.g. $\boldsymbol{x}$, $\boldsymbol{X}$).

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- Empirical risk minimization (ERM) = least squares (LS) regression

$$(\hat{\boldsymbol{w}}, \hat{w}_0)_{\mathsf{ERM}} = (\hat{\boldsymbol{w}}, \hat{w}_0)_{\mathsf{LS}} = \arg\min_{\boldsymbol{w}, w_0} R_{\mathsf{emp}}[\boldsymbol{w}, w_0]$$

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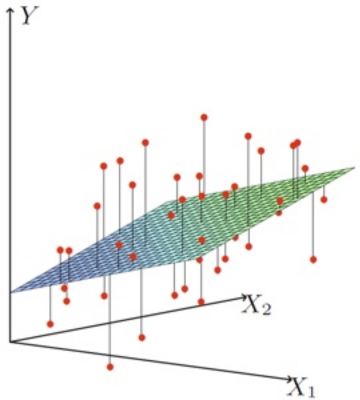
- Maximum likelihood (ML) estimate: $(\hat{\boldsymbol{w}}, \hat{w}_0)_{\text{ML}} = (\hat{\boldsymbol{w}}, \hat{w}_0)_{\text{ERM}}$

Linear Regression: Another Picture



Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of X that minimizes the sum of squared residuals from Y.

From: Hastie, Tibshirani, Friedman, "The Elements of Statistical Learning", Springer, 2009.

Linear Regression: Getting Rid of w_0

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- From now on, we will mostly ignore w_0.

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... if $\boldsymbol{X}^T\boldsymbol{X}$ is invertible, *i.e.*, $\texttt{rank}(\boldsymbol{X}) = p$, requiring $n \geq p$.

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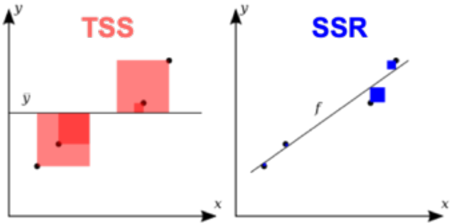

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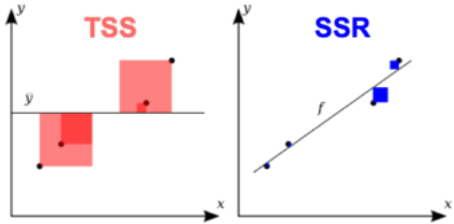

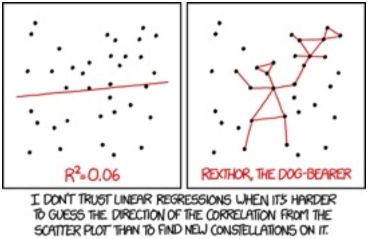

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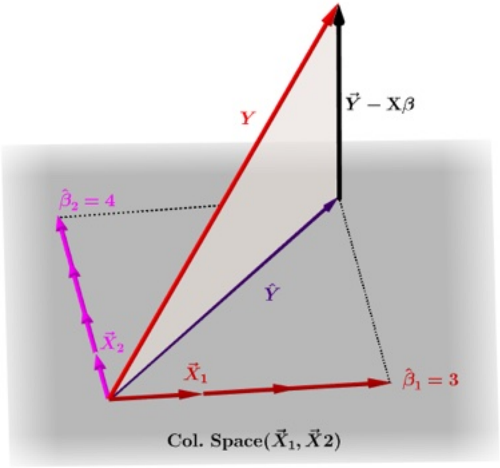
i.e., the orthogonal projection onto $\operatorname{range}(\boldsymbol{X})$.

Geometry of Linear Regression: Euclidean Projection

This picture is in $\mathbb{R}^n$



Going Non-Linear

- To express non-linearities, just replace $\boldsymbol{x}$ with $\boldsymbol{\phi}(\boldsymbol{x})$,

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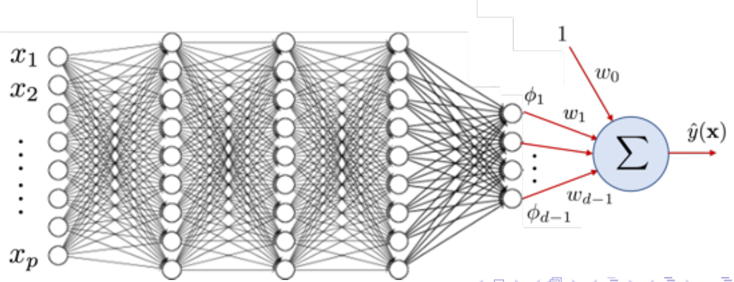
- E.g., final layer of a deep network:



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...exponential in k

Other Types of Non-Linear Regression

- Radial basis functions (RBF): $\phi_j(\boldsymbol{x}) = \psi\Big(\frac{1}{\alpha_j}\|\boldsymbol{x} - \boldsymbol{c}_j\|_2\Big)$

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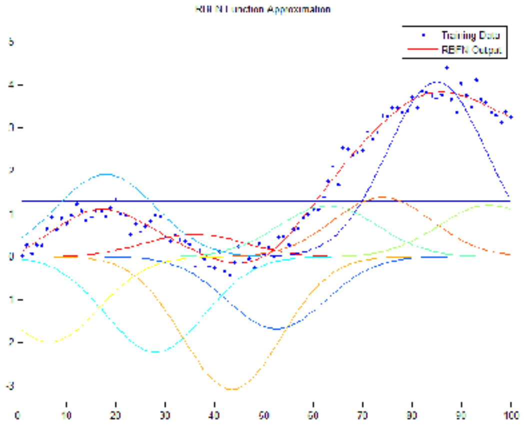
- Kernels: more later.

Example of Gaussian RBF Regression



Ridge Regression

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- Known by other names, in other contexts: *weight decay, penalized least squares, Tikhonov regularization,* ℓ_2 regularization,...

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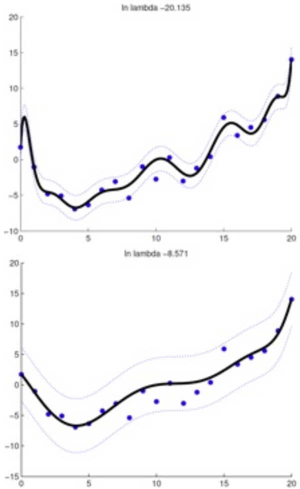
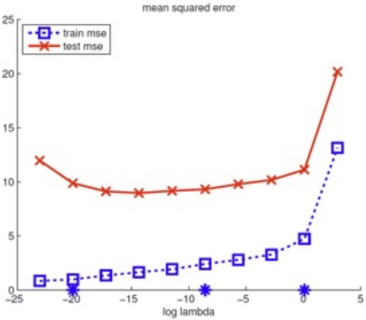
Example: fitting an order-14 polynomial to 21 points in $\mathbb{R}$





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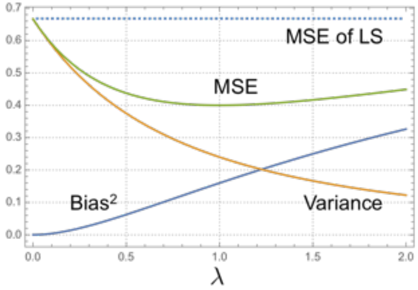

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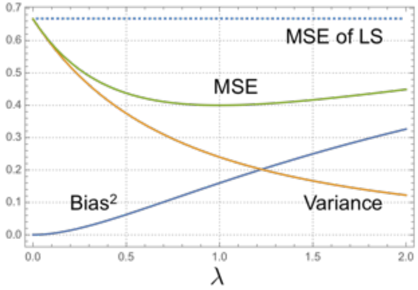
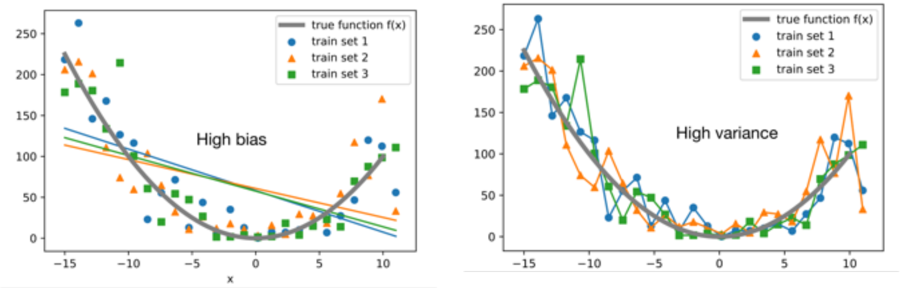


- Bias-variance trade-off. How to choose λ?

Bias-Variance Decomposition: Model Complexity

- Bias-variance trade-off also w.r.t. complexity



linear regression (order-1 polynomial)

Piecewise linear interpolation

Pictures by Sebastian Raschka, 2023.

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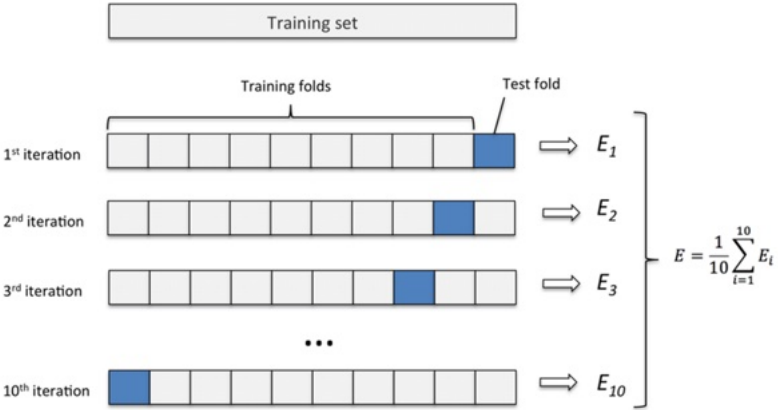
- Extreme case: $K = n$, leave-one-out CV (LOOCV).

Illustration od 10-fold CV



Dual Variables: Ridge Regression

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$$(\boldsymbol{X}^T\boldsymbol{X} + \lambda \boldsymbol{I})\boldsymbol{w} = \boldsymbol{X}^T\boldsymbol{y} \quad \Leftrightarrow \quad \hat{\boldsymbol{w}}_{\text{ridge}}(\boldsymbol{y}) = \frac{1}{\lambda}\boldsymbol{X}^T\big(\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{w}}_{\text{ridge}}(\boldsymbol{y})\big)$$

that is,

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... linear combination of the inner products of $\boldsymbol{x}$ with the $\boldsymbol{x}_i$

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- Motivation example: order 2 polynomial regression in $\mathbb{R}^2$:

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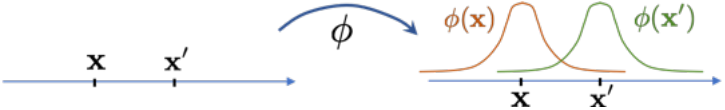

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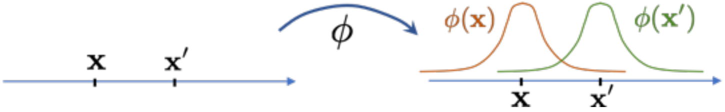

- Why?

$$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}') \rangle = \int \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{u}\|_2^2}{2\sigma^2}\right) \exp\left(-\frac{\|\boldsymbol{x}' - \boldsymbol{u}\|_2^2}{2\sigma^2}\right) d\boldsymbol{u} = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2\sigma^2}\right)$$

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Kernels: Examples

- There are kernels for many other types of objects: sets, strings, images, graphs, probability density or mass functions, ...

- Sets: let $\mathcal{X} = 2^{\mathcal{S}}$ (all subsets of set $\mathcal{S}$, for simplicity, assumed finite).

$$K_\cap(A, A') = |A \cap A'|, \text{ for } A, A' \in \mathcal{X} \quad \text{(intersection kernel)}$$

mapping $\phi : \mathcal{X} \to \mathcal{F}$ (space of real-valued functions in $\mathcal{S}$)

$$\phi(A) = \mathbf{1}_A, \text{ that is } \mathbf{1}_A(x) = \begin{cases} 1 & \Leftarrow \quad x \in A \\ 0 & \Leftarrow \quad x \notin A \end{cases}$$

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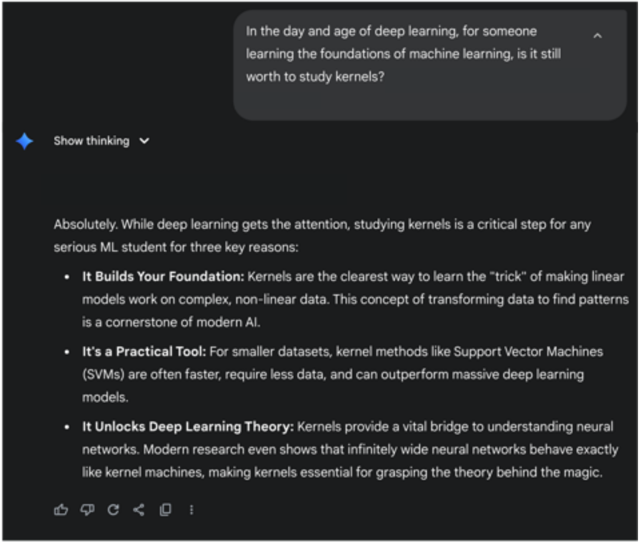
- There are many other kernels for sets.

Kernels in 2025? Let's Ask Gemini 2.5 Pro



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- LS and MN: instances of the Moore-Penrose pseudo-inverse.
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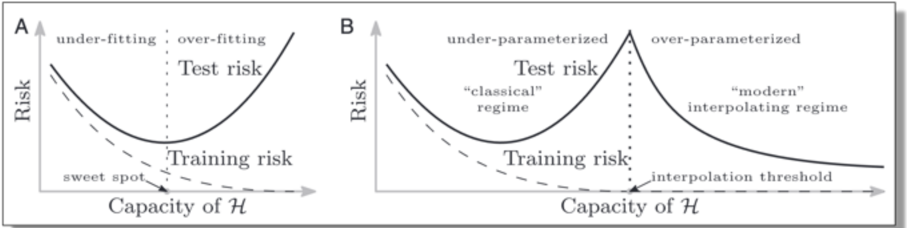
Double Descent

Reconciling modern machine-learning practice and the classical bias–variance trade-off

Mikhail Belkin[a,b,1], Daniel Hsu[c], Siyuan Ma[a], and Soumik Mandal[a]

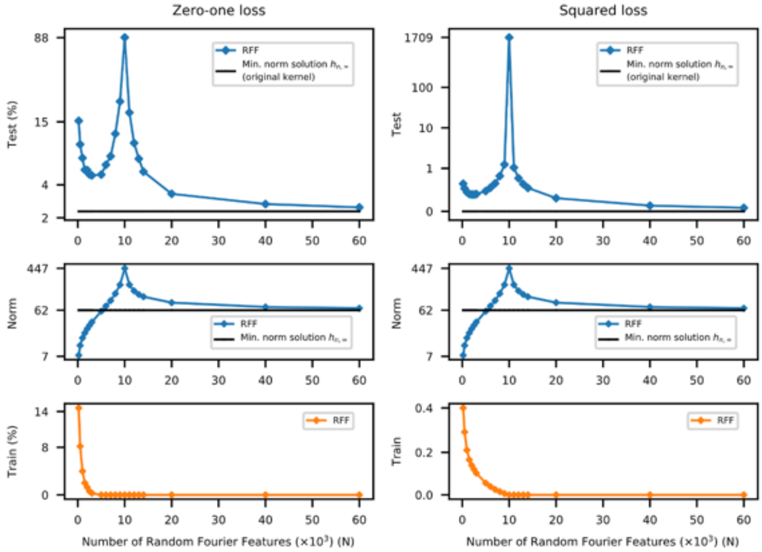
[a]Department of Computer Science and Engineering, The Ohio State University, Columbus, OH 43210; [b]Department of Statistics, The Ohio State University, Columbus, OH 43210; and [c]Computer Science Department and Data Science Institute, Columbia University, New York, NY 10027

Edited by Peter J. Bickel, University of California, Berkeley, CA, and approved July 2, 2019 (received for review February 21, 2019)



Double Descent (2)

- Random Fourier features: $\phi_i(\boldsymbol{x}) = \exp(\sqrt{-1}\langle \boldsymbol{v}_i, \boldsymbol{x}\rangle), \;\; \boldsymbol{v}_i \sim \mathcal{N}(0, \boldsymbol{I})$



Overparametrization and Double Descent

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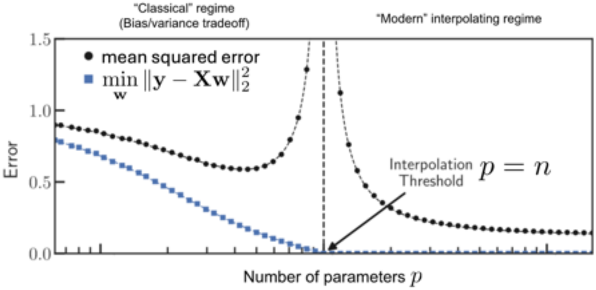

(Image adapted from Rocks and Mehta, 2022.)

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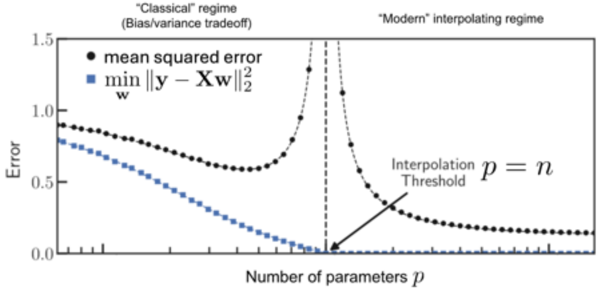
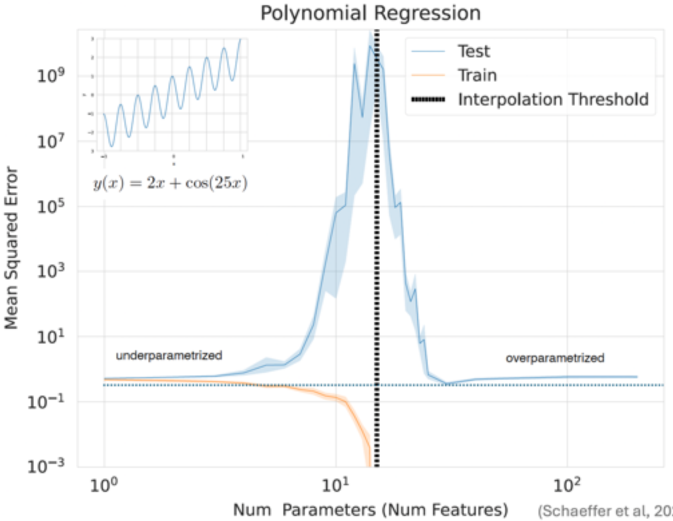


(Image adapted from Rocks and Mehta, 2022.)

- Current research topic.

Overparametrization and Double Descent (cont.)

- Polynomial regression: the ϕ_i are Legendre polynomials.



(Schaeffer et al, 2023)

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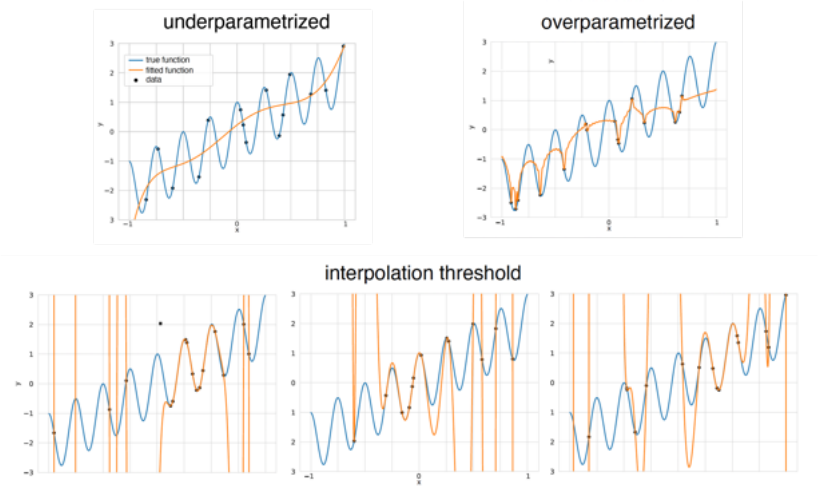

Bayesian View of Ridge Regression

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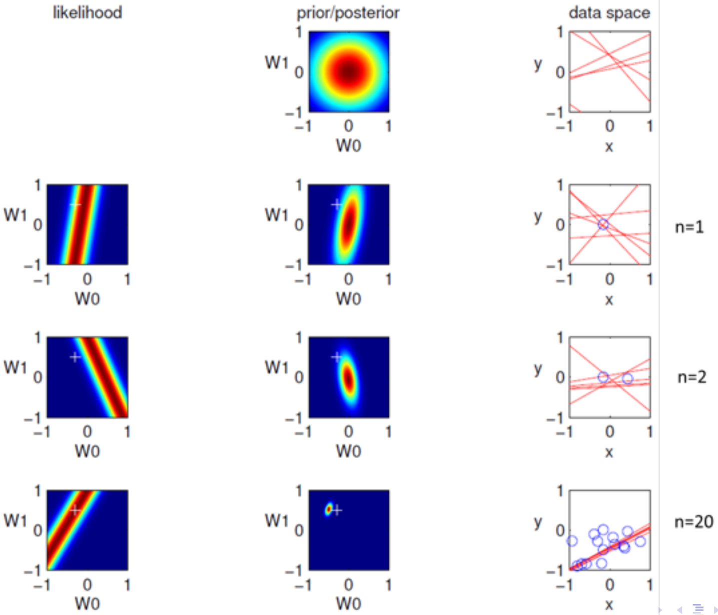
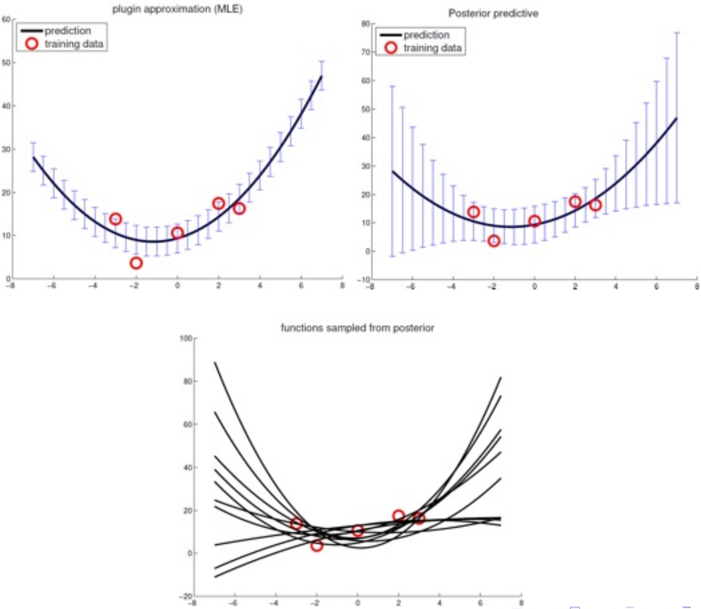
- Example in next slide: $p = 1$, $\boldsymbol{w} = [w_0,\, w_1]^T$, $\boldsymbol{w}_{\text{true}} = [-0.3,\, 0.5]$

Bayesian View of Ridge Regression: Example 1



Bayesian View of Ridge Regression: Example 2



Epistemic and Aleatoric Uncertainty

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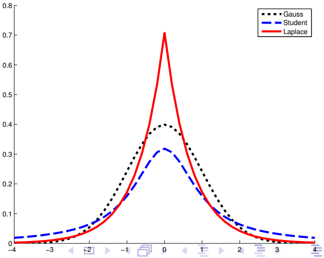
- Can be seen as MAP estimate of $\boldsymbol{w}$, under Laplacian prior

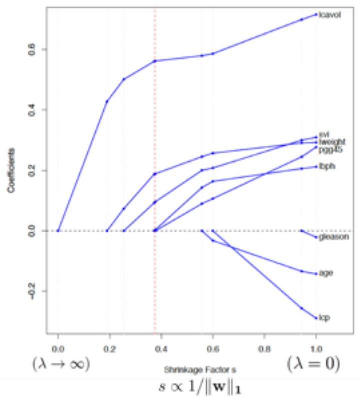
$$f_{\boldsymbol{W}}(\boldsymbol{w}) = \prod_{i=1}^{p} \frac{\lambda}{2} \exp\Big(-\lambda |w_i|\Big)$$
$$= \left(\frac{\lambda}{2}\right)^p \exp\Big(-\lambda \|\boldsymbol{w}\|_1\Big)$$



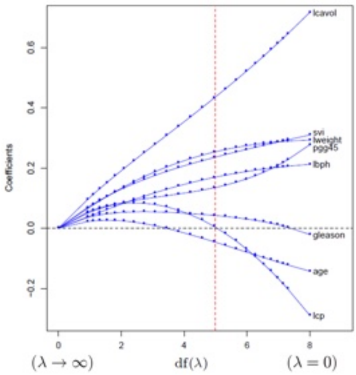
LASSO versus Ridge

- Example (prostate cancer data)

LASSO



Ridge



Solving LASSO Regression

- Ridge regression: simply a linear system:

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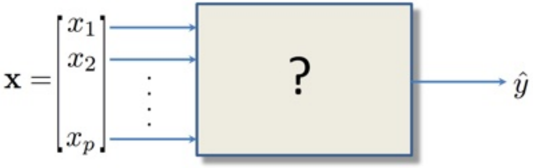
- Using gradient descent (*e.g.*, in deep learning), simply pretend that ℓ_1 is differentiable (derivative in $\{-1, 0, 1\}$), carefully adapt the step size.

Outline

1. Introduction
2. Regression
3. **Classification**
4. Optimization for Supervised Learning

Classification (a.k.a. Pattern Recognition)

- In a nutshell: produce a "machine" that predicts/estimates/guesses a class $y \in \{1, ..., K\}$, from variables/features x_1,...,x_p



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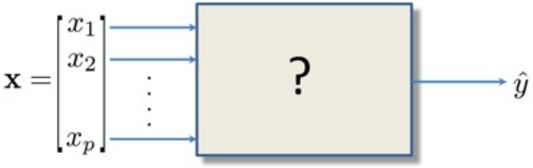

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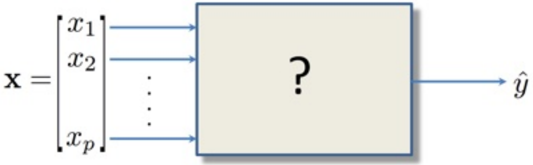

- Maybe the core machine learning problem, with countless applications.
- Learning/training: given a collection of examples (training data)

$$\mathcal{D} = \big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big)$$

..find the "best" possible machine.

Generalized Linear Models

- Conditional probability of class y for sample $\boldsymbol{x}$:

$$f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}) = \frac{\exp\left((\boldsymbol{\eta}^{(y)})^T \boldsymbol{\phi}(\boldsymbol{x})\right)}{\sum_{u=1}^{K} \exp\left((\boldsymbol{\eta}^{(u)})^T \boldsymbol{\phi}(\boldsymbol{x})\right)}$$

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- Parameters $\boldsymbol{\eta} = \left(\boldsymbol{\eta}^{(1)}, ..., \boldsymbol{\eta}^{(K)}\right)$, log-likelihood function:

$$\log f_{Y_1,...,Y_n}(y_1, ..., y_n; \boldsymbol{x}_1, ..., \boldsymbol{x}_n, \boldsymbol{\eta}) = \sum_{i=1}^{n} \log f_{Y|\boldsymbol{X}}(y_i|\boldsymbol{x}_i, \boldsymbol{\eta})$$

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moderly called cross-entropy loss.

The Binary Case: A Detailed Look

- Binary classification, $y \in \{1,\, 0\}$, thus

$$f_{Y|\boldsymbol{X}}(1|\boldsymbol{x}) = \frac{\exp\left((\boldsymbol{\eta}^{(1)})^T \boldsymbol{\phi}(\boldsymbol{x})\right)}{\exp\left((\boldsymbol{\eta}^{(1)})^T \boldsymbol{\phi}(\boldsymbol{x})\right) + \exp\left((\boldsymbol{\eta}^{(0)})^T \boldsymbol{\phi}(\boldsymbol{x})\right)}$$

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where $\boldsymbol{w} = \boldsymbol{\eta}^{(1)} - \boldsymbol{\eta}^{(0)}$.

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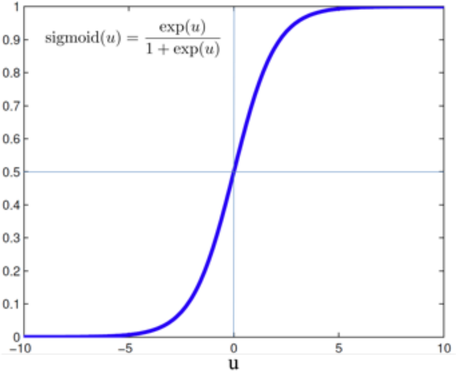

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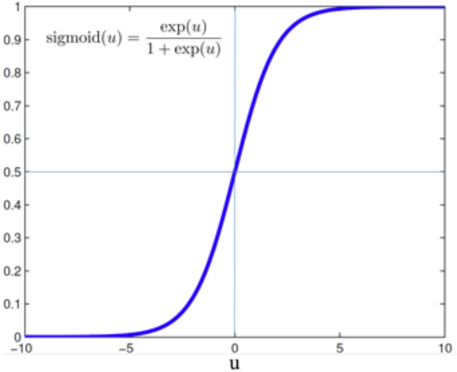
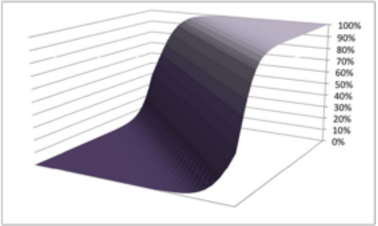
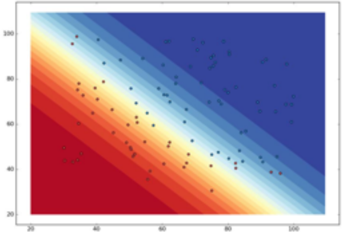


- Obviously $f_{Y|\mathbf{X}}(0|\boldsymbol{x}) = 1 - f_{Y|\mathbf{X}}(1|\boldsymbol{x})$.

Binary Logistic Regression

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





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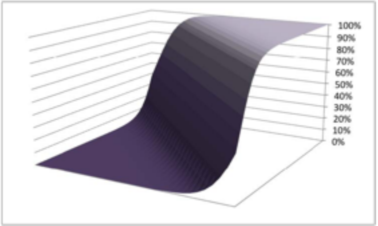

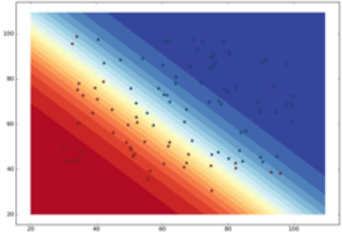

- Classical decision boundary, $f_{Y|\mathbf{X}}(1|\boldsymbol{x}) = 1/2 \;\Leftrightarrow\; \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}) = 0$, is linear with respect to $\boldsymbol{\phi}(\boldsymbol{x})$.

Binary Logistic Regression: Log-Likelihood

- $f_Y(y|\boldsymbol{x}) = \left(\dfrac{\exp\left(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})\right)}{1 + \exp\left(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})\right)} \right)^y \left(\dfrac{1}{1 + \exp\left(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})\right)} \right)^{(1-y)}$

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- Negative log-likelihood (NLL), given $\mathcal{D} = \Big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\Big)$,

$$\mathcal{L}(\boldsymbol{w}) = -\sum_{i=1}^{n}\left(y_i \log \frac{\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_i)\right)}{1+\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_i)\right)} + (1-y_i)\log\frac{1}{1+\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_i)\right)}\right)$$

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- $\mathcal{L}(\boldsymbol{w})$ is smooth and convex (should not be too hard to optimize)

Ridge and LASSO Logistic Regression

- Ridge logistic regression:

$$\hat{\boldsymbol{w}}_{\mathsf{ridge}} = \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

still smooth and convex.

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still smooth and convex.

- Sparse (LASSO) logistic regression:

$$\hat{\boldsymbol{w}}_{\text{sparse}} = \arg\min_{\boldsymbol{w}} \mathcal{L}(\boldsymbol{w}) + \lambda\|\boldsymbol{w}\|_1$$

still convex, but not smooth.

Multi-class Logistic Regression

- Recall the GLM,

$$f_{Y|\boldsymbol{X}}(y|\boldsymbol{x},\boldsymbol{w}) = \frac{\exp\left(\phi(\boldsymbol{x})^T \boldsymbol{w}^{(y)}\right)}{\sum_{u=1}^{K} \exp\left(\phi(\boldsymbol{x})^T \boldsymbol{w}^{(u)}\right)}$$

... with $\boldsymbol{w} = (\boldsymbol{w}^{(1)}, ..., \boldsymbol{w}^{(K)})$.

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- The negative log-likelihood function (cross-entropy loss):

$$\sum_{i=1}^{n}\log f_{Y|\boldsymbol{X}}(y_i|\boldsymbol{x}_i,\boldsymbol{w}) = \sum_{i=1}^{n}\sum_{k=1}^{K}\mathbf{1}_{y_i=k}\log f_{Y|\boldsymbol{X}}(k|\boldsymbol{x}_i,\boldsymbol{\eta}),$$

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- Using one-hot encoding: $\boldsymbol{y}_i \in \{0,1\}^K$, $y_{ik} = 1$ if $\boldsymbol{x}_i$ is in class k

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can be written as

$$\mathcal{L}(\boldsymbol{w}) = \sum_{i=1}^{n} \left[\log \left(\sum_{k=1}^{K} \exp(\boldsymbol{x}_i^T \boldsymbol{w}^{(k)}) \right) - \left(\sum_{k=1}^{K} y_{ik}\, \boldsymbol{x}_i^T \boldsymbol{w}^{(k)} \right) \right]$$

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- Notice: if $\boldsymbol{x}_i$ is in class k, minimizing $\mathcal{L}(\boldsymbol{w})$ pushes $\boldsymbol{x}_i^T \boldsymbol{w}^{(k)}$ up.

Bayesian Logistic Regression

- Using some estimate $\hat{\boldsymbol{w}}$, obtained from data $\mathcal{D}$, and plugging it into $f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}, \hat{\boldsymbol{w}})$ ignores the randomness/uncertainty in $\hat{\boldsymbol{w}}$

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- Unfortunately, none of these have closed-form expressions.

Bayesian Logistic Regression (2)

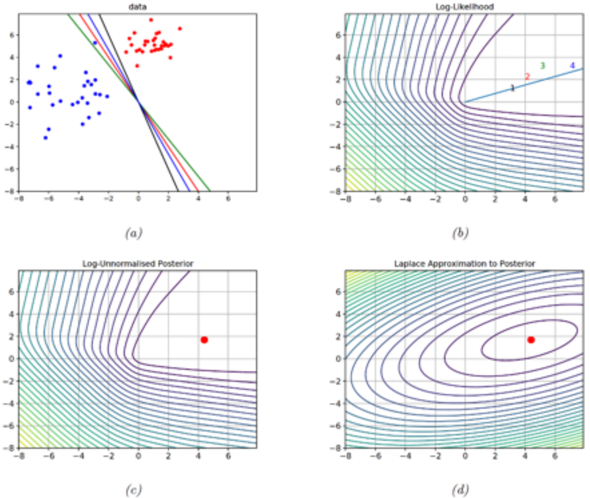


Figure 10.13: (a) Illustration of the data. (b) Log-likelihood for a logistic regression model. The line is drawn from the origin in the direction of the MLE (which is at infinity). The numbers correspond to 4 points in parameter space, corresponding to the lines in (a). (c) Unnormalized log posterior (assuming vague spherical prior). (d) Laplace approximation to posterior. Adapted from a figure by Mark Girolami. Generated by code at figures.probml.ai/book1/10.13.

Bayesian Logistic Regression (3)

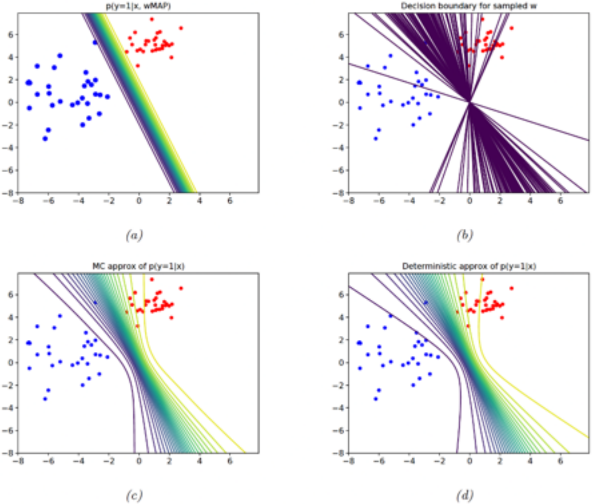
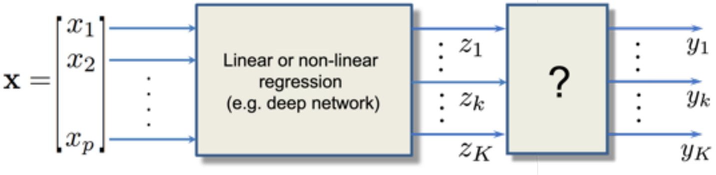


Figure 10.14: Posterior predictive distribution for a logistic regression model in 2d. (a): contours of $p(y = 1|\boldsymbol{x}, \hat{\boldsymbol{w}}_{map})$*. (b): samples from the posterior predictive distribution. (c): Averaging over these samples. (d): moderated output (probit approximation). Adapted from a figure by Mark Girolami. Generated by code at* *figures.probml.ai/book1/10.14.*

Another View of (and Beyond) Softmax



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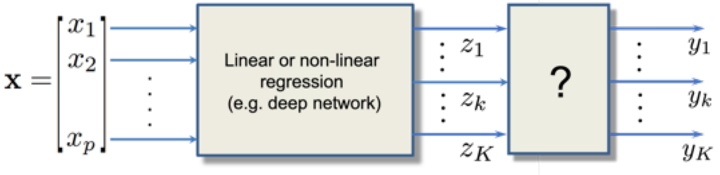

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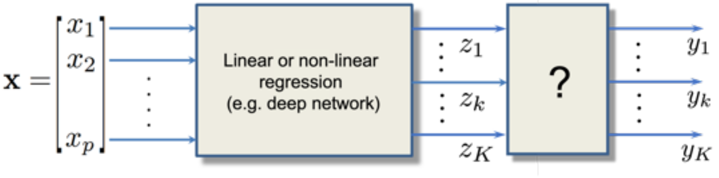
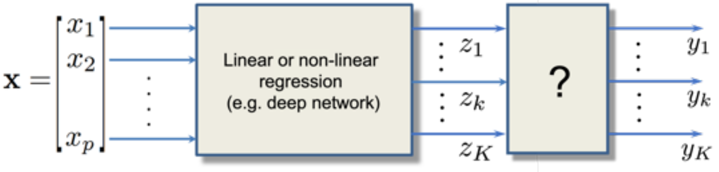


- Scores: $\boldsymbol{z} \in \mathbb{R}^K$, without constraints/restrictions.

- Probabilities: $y_k = \mathbb{P}[\text{class } k|\boldsymbol{x}]$, thus $\boldsymbol{y} \in \Delta_{K-1}$, where

$$\Delta_{K-1} = \left\{\boldsymbol{y} \in \mathbb{R}^K, \text{ s.t. } y_1, ..., y_K \geq 0 \text{ and } \sum_{k=1}^{K} y_i = 1\right\} \qquad \text{(simplex)}$$

Another View of (and Beyond) Softmax



- Scores: $\boldsymbol{z} \in \mathbb{R}^K$, without constraints/restrictions.

- Probabilities: $y_k = \mathbb{P}[\text{class } k|\boldsymbol{x}]$, thus $\boldsymbol{y} \in \Delta_{K-1}$, where

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- How to map from $\boldsymbol{z} \in \mathbb{R}^K$ to $\boldsymbol{y} \in \Delta_{K-1}$, such that

$$z_i = z_j \;\Rightarrow\; y_i = y_j \quad \text{and} \quad z_i > z_j \Rightarrow y_i \geq y_j$$

Argmax and Softmax

- First possibility: probability vector "most aligned" with $\boldsymbol{z}$:

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- Choosing λ to satisfy the constraint $\mathbf{1}^T \boldsymbol{p} = 1$ determines $Z(\beta, \lambda)$

$$y_i = \frac{e^{\beta\, z_i}}{\sum_{j=1}^K e^{\beta\, z_j}} = \big[\mathbf{softmax}(\beta\, \boldsymbol{z})\big]_i$$

Beyond Softmax: Sparsemax

- A third possibility[1]: simply project $\boldsymbol{z}$ onto Δ_{K-1}

$$\boldsymbol{y} = \arg\min_{\boldsymbol{p}\in\Delta_{K-1}} \|\boldsymbol{p} - \boldsymbol{z}\|_2^2 \quad \Longrightarrow \quad \boldsymbol{y} = \textbf{sparsemax}(\boldsymbol{z})$$

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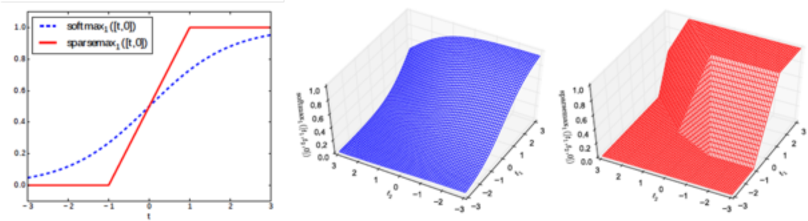
- Sparsemax versus softmax:



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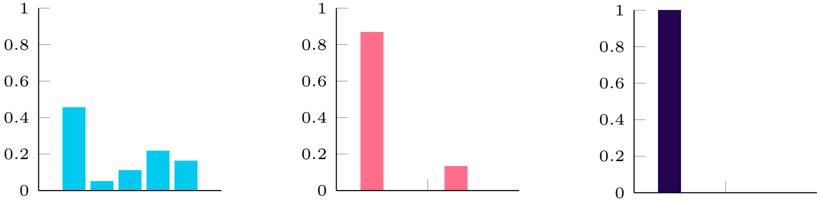
- Sparsemax is in-between softmax and argmax
- For $\boldsymbol{z} = [1.0716, -1.1221, -0.3288, 0.3368, 0.0425]$

$\mathbf{softmax}(\boldsymbol{z})$ $\mathbf{sparsemax}(\boldsymbol{z})$ $\mathrm{argmax}(\boldsymbol{z})$



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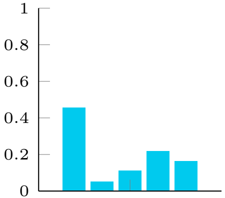

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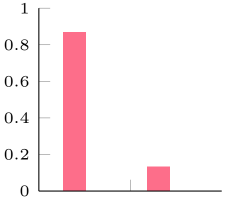

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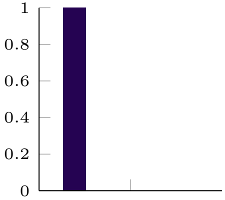

- Sparsemax, unlike softmax, may yield exact zeros.

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

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  ... underlies support vector machines (SVM)

Classification: The Loss Function Perspective (2)

- Both the hinge and the logistic loss can be seen as convex replacements for the error loss (or misclassification loss)

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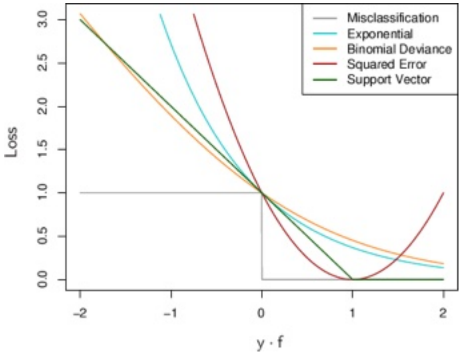

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- Logistic regression and SVMs solve regularized ERM problems, with convex surrogates of the error loss

Outline

1 Introduction

2 Regression

3 Classification

4 Optimization for Supervised Learning

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- Absolute error loss: $L_{\text{abs}}(f, y) \propto |f - y|$ (not covered today)

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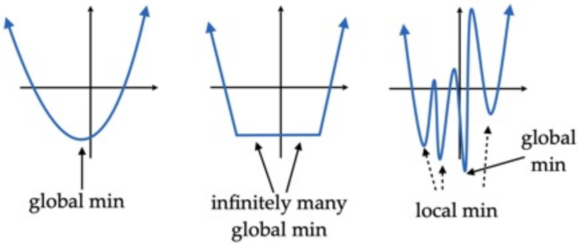
  - ✓ local, if $F(\boldsymbol{\theta}^*) \leq F(\boldsymbol{\theta})$, for any $\boldsymbol{\theta} \in \mathbb{R}^d$ s.t. $\|\boldsymbol{\theta} - \boldsymbol{\theta}\| \leq \varepsilon$, for some ε.



Minimizers

- Goal: find $\boldsymbol{\theta}^*$, a minimizer of $F(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta} \in \mathbb{R}^d$
- Types of minimizers:
  - ✓ global, if $F(\boldsymbol{\theta}^*) \leq F(\boldsymbol{\theta})$, for any $\boldsymbol{\theta} \in \mathbb{R}^d$
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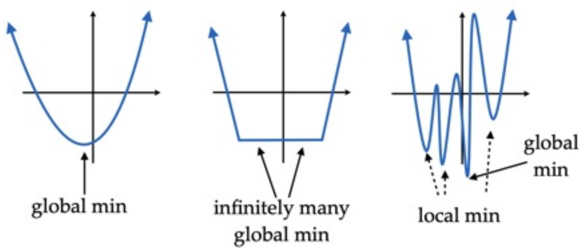

- Minimizers: global $\Rightarrow$ local; local $\not\Rightarrow$ global.

Convexity

- F is a convex function if, for all $\boldsymbol{\theta}_1,\, \boldsymbol{\theta}_2 \in \mathbb{R}^d$,

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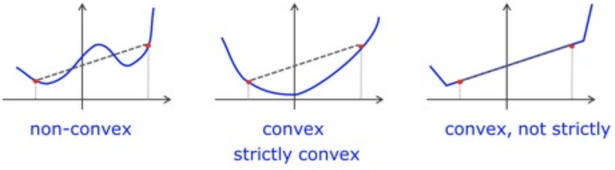

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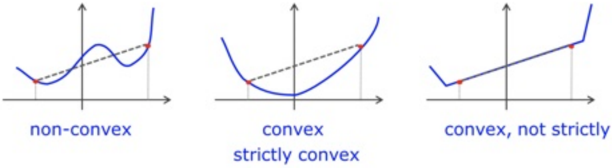

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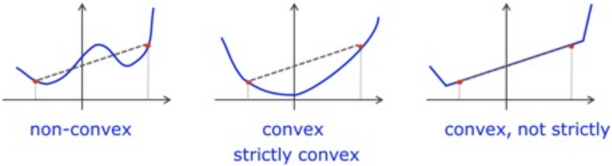

- Convexity $\Rightarrow$ all local minima are global minima.

- Convexity $\Rightarrow$ continuity.

Hessian

- For F twice differentiable, the Hessian is

$$H(\boldsymbol{\theta}) = \nabla^2 F(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial^2 F}{\partial \theta_1^2} & \frac{\partial^2 F}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 F}{\partial \theta_1 \partial \theta_d} \\ \frac{\partial^2 F}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 F}{\partial \theta_2^2} & \cdots & \frac{\partial^2 F}{\partial \theta_2 \partial \theta_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 F}{\partial \theta_d \partial \theta_1} & \frac{\partial^2 F}{\partial \theta_d \partial \theta_2} & \cdots & \frac{\partial^2 F}{\partial \theta_d^2} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

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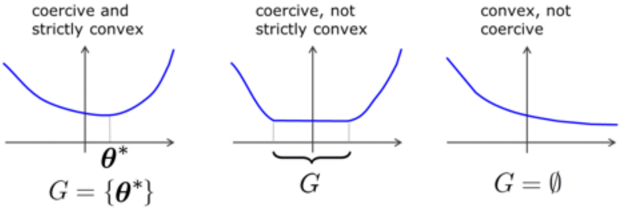

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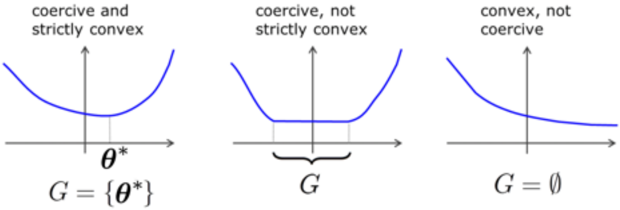

- Non-coercivity examples: logistic regression on separable data; linear regression for $n < p$.

Descent Directions

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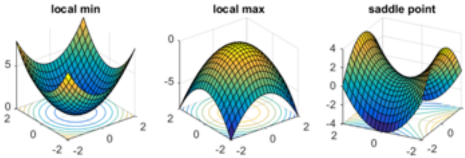

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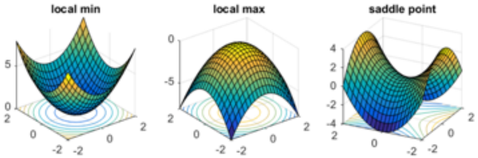

- If F is convex, $\boldsymbol{\theta}^*$ is a global minimizer $\Leftrightarrow \nabla F(\boldsymbol{\theta}^*) = 0$

Gradient Descent

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- Some stopping criterion is used; *e.g.*, $\|\nabla F(\boldsymbol{\theta}_t)\| \leq \delta$

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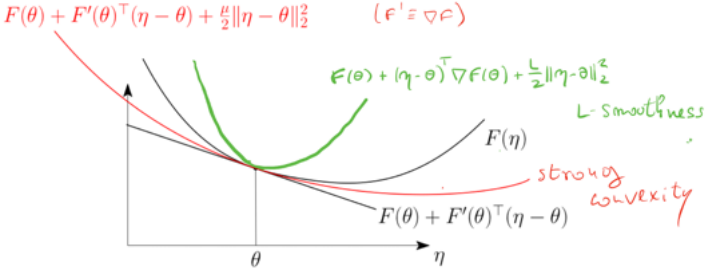
- Condition number $\kappa = \dfrac{L}{\mu}$.

L-smoothness and $\mu-$Strongly Convex

- L-smooth and $\mu-$strongly convex function: upper and lower bounded by quadratics.



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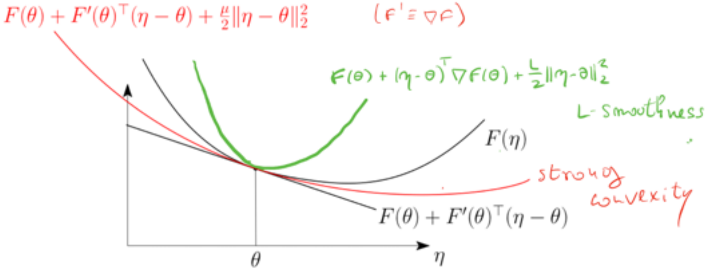

- Regularization: if $F(\boldsymbol{\theta})$ is convex, $F(\boldsymbol{\theta}) + \frac{\mu}{2}\|\boldsymbol{\theta}\|_2^2$ is μ-strongly convex.

Gradient Descent for Convex Functions

- Gradient descent with step-size $\alpha = 1/L$,

$$F(\boldsymbol{\theta}_t) - F(\boldsymbol{\theta}^*) \leq \left(\frac{\kappa - 1}{\kappa}\right)^t \big(F(\boldsymbol{\theta}_0) - F(\boldsymbol{\theta}^*)\big)$$

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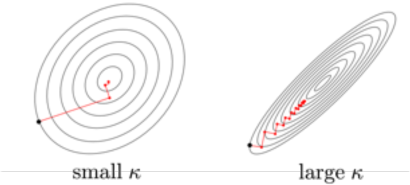
- Proofs: see recommended reading (F. Bach).

Gradient Descent: Strongly Convex Case

- The condition number κ expresses the problem difficulty.



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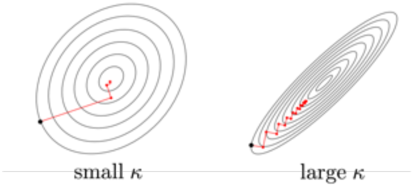
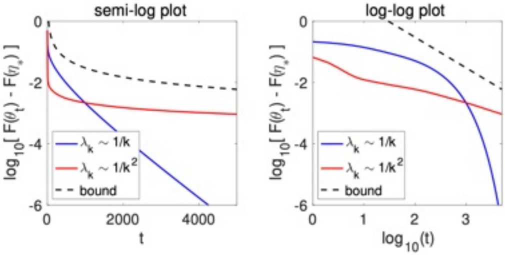
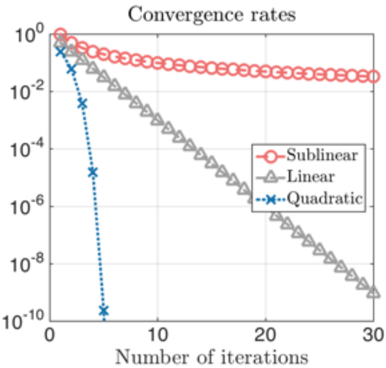


- Convergence for different distributions of eigenvalues.



(pictures from F. Bach).

Linear vs Sublinear Convergence



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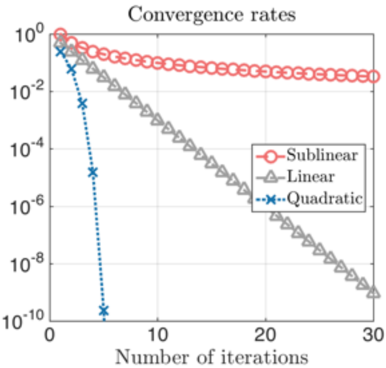

- Quadratic ($\frac{\Delta_t}{\Delta_{t-1}^2} \rightarrow \beta < \infty$) and super-linear ($\frac{\Delta_t}{\Delta_{t-1}} \rightarrow 0$) convergence: not achievable using only gradient information.
- Optimization is a central tool in machine learning; it is a huge field.

Stochastic Gradient "Descent"

- Back to empirical risk minimization: $\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} F(\boldsymbol{\theta})$

$$F(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} L(f(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i) \quad \big(\text{maybe } + R(\boldsymbol{\theta})\big)$$

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- Alternative: stochastic gradient "descent" (SGD):
  - ✓ Start at some initial point $\boldsymbol{\theta}_0 \in \mathbb{R}^d$
  - ✓ For $t = 1, 2, ...,$
    - ▷ sample $i \in \{1, ..., n\}$ at random and choose step-size α_t,
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- Thus, $\nabla L(f(\boldsymbol{X};\boldsymbol{\theta}),Y)$ is an unbiased estimate of $\nabla\mathcal{R}(\boldsymbol{\theta})$

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Convergence of Stochastic Gradient Descent

- SGD uses noisy gradients: $\boldsymbol{G}(\boldsymbol{\theta})$, such that $\mathbb{E}[\boldsymbol{G}(\boldsymbol{\theta})] = \nabla F(\boldsymbol{\theta})$
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- Important: not practical to compute $F(\boldsymbol{\theta}_t)$. Selecting the best iterate is thus impractical and would beat the purpose of SGD.

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- Regularization: $F(\boldsymbol{\theta}) = \dfrac{1}{n}\sum_{i=1}^{n} L(f(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i) + \dfrac{\mu}{2}\|\boldsymbol{\theta}\|_2^2$

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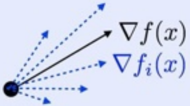
- Strong convexity speeds up convergence from $O(1/\sqrt{t})$ to $O(1/t)$

Visual Summary

Finite sums

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

$$\nabla f(x) = \frac{1}{n}\sum_i \nabla f_i(x)$$



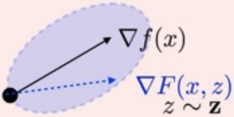
Draw $i \in \{1, \ldots, n\}$ uniformly.

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

Expectation

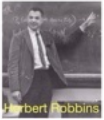
$$f(x) \overset{\text{def.}}{=} \mathbb{E}_{\mathbf{z}}(f(x, \mathbf{z}))$$

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



Draw $z \sim \mathbf{z}$

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



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

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

(Picture by Gabriel Peyré)

Stochastic Gradient Descent: Linear Classification

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showing that $\nabla \ell(y_i \boldsymbol{\theta}^T \boldsymbol{x}_i)$ is co-linear with $\boldsymbol{x}_i$.

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- Each SGD update moves $\boldsymbol{\theta}_t$ in a direction parallel to sample $\boldsymbol{x}_i$.

The Perceptron Algorithm

- Hinge loss: $\ell(u) = \max\{0, 1 - \tau\}$, thus

$$\frac{d\,\ell(u)}{d\,u} = \begin{cases} -1, & \text{if } u \leq \tau \\ 0, & \text{otherwise.} \end{cases}$$

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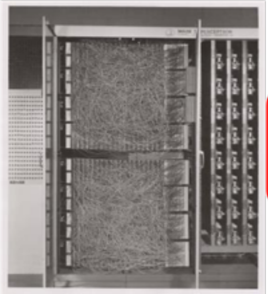
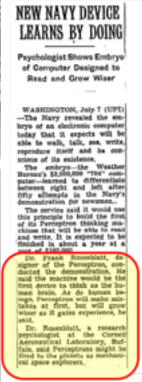
- This is the famous Perceptron algorithm, proposed in 1957 by Frank Rosenblatt (with $\tau = 0$), the percursor of modern neural networks.

A Bit of History: The Perceptron





NEW NAVY DEVICE LEARNS BY DOING

Psychologist Shows Embryo of Computer Designed to Read and Grow Wiser

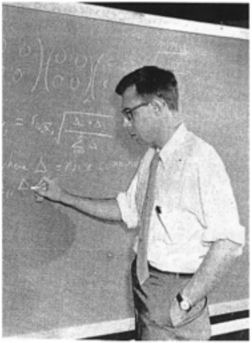
WASHINGTON, July 7 (UPI) —The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.

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.



The New York Times, 1958

Minsky and Pappert, 1969

Perceptron Mistake Bound

- 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

$$y_n \, \boldsymbol{u}^T \boldsymbol{x}_n \geq \gamma, \quad \forall n.$$

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- Then, the following bound of the number of mistakes holds[2]

Theorem

The perceptron algorithm is guaranteed to find a separating hyperplane after at most $\frac{R^2}{\gamma^2}$ mistakes (non-zero updates).

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Novikoff's Theorem: One-Slide Proof

- Recall that non-zero updates (mistakes) are: $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + y_i\, \boldsymbol{x}_i$.

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- Equating both sides, $(M\gamma)^2 \leq \|\boldsymbol{\theta}_t\|^2 \leq M\,R^2 \;\Rightarrow\; M \leq R^2/\gamma^2$ ■

Implicit Regularization

- SGD in linear prediction, with i_t denoting the sample at iteration t,

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- This is sometimes called the overparametrized or interpolating regime and is a central tool in the understanding of modern deep learning.

Explicit Regularization: Weight Decay

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- $\boldsymbol{\theta}_{t-1}$ is shrunk/decayed before being updated: weight decay

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- Minibatching: instead of a single sample, use minibatches (size m)

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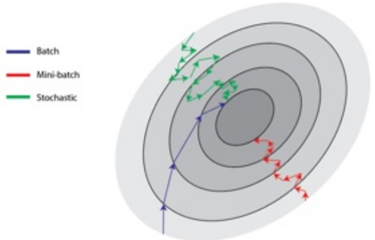

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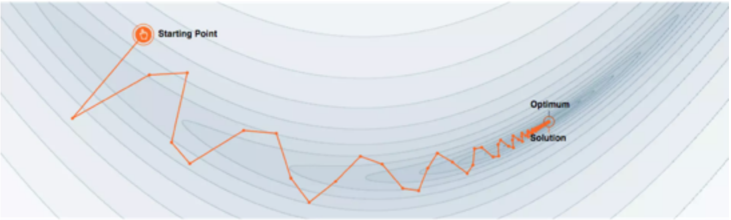
- Advantage: reduces the update in directions with changing gradients; increases the update in directions with stable gradient.



Adaptive Gradient (AdaGrad)

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Adam Algorithm: Adaptive Moment Estimation

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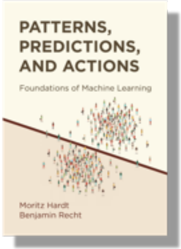
Recommended Books



https://mlstory.org/
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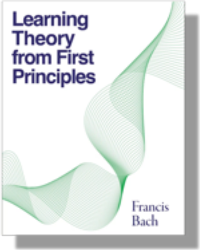

www.di.ens.fr/~fbach/ltfp_book.pdf
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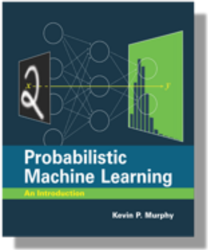

probml.github.io/pml-book
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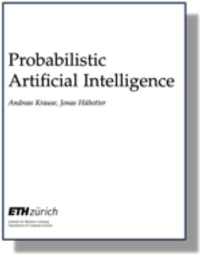

arxiv.org/abs/2502.05244
2025

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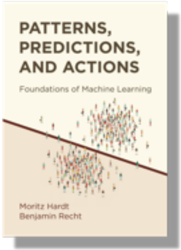

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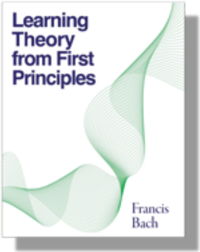

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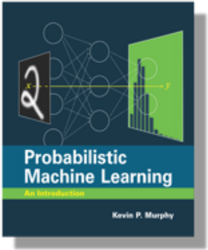

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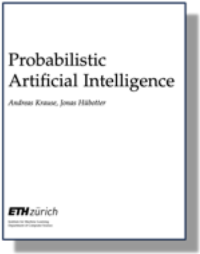

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Thank you!   Questions?