Probability Basics and Linear Classification

Machine Learning – Basic Methods

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Learning Outcomes

- Understand probabilistic models and maximum likelihood
- Understand the classification problem
- What is a linear classifier?
- What is the loss function of linear classification?
- What is gradient descent ?

Today‘s Agenda!

Basics: Probability Theory

- Probabilistic Models
- Expectations and Monte Carlo Methods
- Maximum Likelihood

Basics: Gradient Descent

Classification:

- Generative vs. discriminative classification
- Linear Classification
- Logistic Regression

Many slides are based on slides from Shenlon Wang, Yingyu Jiang, Michail Michailidis and Patrick Maiden

Basics: Probability Theory

- *“Probability theory is nothing but common sense reduced to calculation”,* Pierre Laplace, 1812
- We will keep our discussion relatively informal and pick the things we need from probability theory

Notation

- A **random variable** X represents uncertain states or outcomes of the world
- We will write $p(x)$ to mean the probability that X takes the value x
- The sample space is the space of all possible outcomes
  - Might be discrete, continuous or mixed

- $p(x)$ is the **probability mass** (density) function
  - Assigns a number to each point of the sample space
  - Non-negative, sums (integrates) to 1
  - Intuitively: How often does x occur? How much do we believe in x?

Distributions

- **Joint distribution**

  $$p(x, y)$$

  – Probability that X=x and Y=y

- **Conditional distribution**

  $$p(x|y)$$

  – Probability that X=x given Y=y

Conditional Distributions

$P(W|T)$

$P(W|T = hot)$

W	P
sun	0.8
rain	0.2

$P(W|T = cold)$

W	P
sun	0.4
rain	0.6

Joint Distribution

$P(T, W)$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

Rules of Probability

- **Sum rule (marginalization / integrating out):**

$$p(x) = \sum_y p(x, y)$$

$$p(x_1) = \sum_{x_2} \sum_{x_3} \cdots \sum_{x_D} p(x_1, \ldots, x_D)$$

  – **Note:** For continuous distributions, the sums will be replaced by integrals

$P(T, W)$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

$$P(t) = \sum_w P(t, w)$$

$P(T)$

T	P
hot	0.5
cold	0.5

$$P(w) = \sum_t P(t, w)$$

$P(W)$

W	P
sun	0.6
rain	0.4

Rules of Probability

- **Chain / product rule**

$$p(x, y) = p(x|y)p(y)$$

$$p(x_1, \cdots, x_D) = p(x_1)p(x_2|x_1) \ldots p(x_D|x_1, \ldots, x_{D-1})$$

$P(W)$

W	P
sun	0.8
rain	0.2

$P(D|W)$

D	W	P
wet	sun	0.1
dry	sun	0.9
wet	rain	0.7
dry	rain	0.3

$P(D, W)$

D	W	P
wet	sun	0.08
dry	sun	0.72
wet	rain	0.14
dry	rain	0.06

Bayes Rule

Bayes rule is one of the most important equations in probability theory and in machine learning

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)} = \frac{p(y|x)p(x)}{\sum_{x'} p(y|x')p(x')}$$

- Way of “reversing” the conditional probabilities
- Often one conditional is tricky but the other one is simple
- One of the most important equations for ML!

Expectations

The expectation of a function f(x) with respect to a distribution p(x) is given by

$$\mathbb{E}_p[f(x)] = \int p(x)f(x)dx$$

A conditional expectation is given by

$$\mathbb{E}_p[f(x)|Y=y] = \int p(x|y)f(x)dx$$

Chain rule for expectations:

$$\mathbb{E}_p[f(x)] = \int p(y)\overbrace{\mathbb{E}[f(x)|Y=y]}^{g(y)}dy$$

$p(x|y)$ $p(y)$

Monte-carlo estimation

Expectations can always be approximated by samples:

$$\mathbb{E}_p[f(x)] = \int p(x) f(x) dx \approx \frac{1}{N} \sum_{x_i \sim p(x)} f(x_i)$$

- Necessary if no analytical solution exists to compute the integral (typical case)

Moments

Moments are expectations:

- 1^{st} moment (mean): $\boldsymbol{\mu} = \mathbb{E}_p[\boldsymbol{x}]$

- 2^{nd} moment: $\boldsymbol{M}_2 = \mathbb{E}_p[\boldsymbol{x}\boldsymbol{x}^T]$

Central moments are always computed relatively to the mean:

- 2^{nd} central moment (covariance):

$$\boldsymbol{\Sigma} = \mathbb{E}_p[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T]$$

- Captures variability (diagonal entries) and correlation (off-diagonal)

Distributions

Bernoulli Distribution:

- Binary random variable $X \in \{0, 1\}$
- One parameter $p(X = 1) = \mu$
- Probability distribution $p(x) = \mu^{x}(1-\mu)^{(1-x)}$

  Depending on x, selects either mu or 1-mu as probability

- Think of it as tossing a coin

Distributions

Multinomial / Categorical Distribution:

- K different events: $C \in \{1, \ldots, K\}$
- Directly specifies probabilities: $p(C = k) = \mu_k, \quad \mu_k \geq 0, \quad \sum_{k=1}^{K} \mu_k = 1$
- Or written with 1-hot-encoding (without an "if" clause)

$$p(c) = \prod_{k=1}^{K} \mu_k^{h_{c,k}}$$

$h_c = [1, 0, 0, \ldots 0]$, $h_c = [0, 0, 1, 0, \ldots]$

Depending on the class label of x, selects the correct μ_k

  – where h_x is the K-dimensional 1-hot encoding vector, which is one for the dimension c = k and 0 elsewhere. $h_{x,k}$ is the k-th element of this vector.

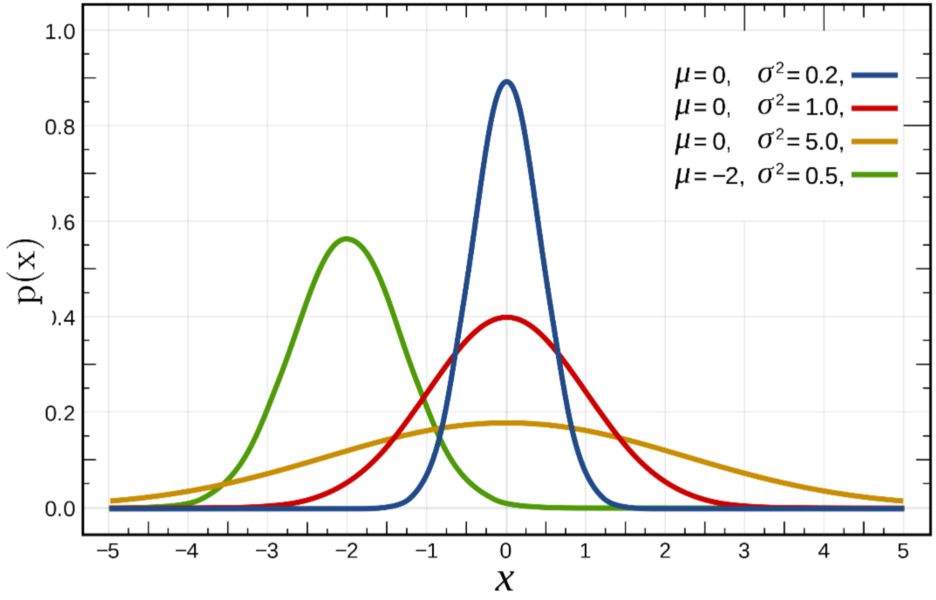
- Think of it as tossing a die

Distributions

Gaussian Distribution

- Continuous RV: $X \in \mathbb{R}$
- Distribution is completely specified by mean μ and variance σ^2

$$p(x) = \mathcal{N}(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

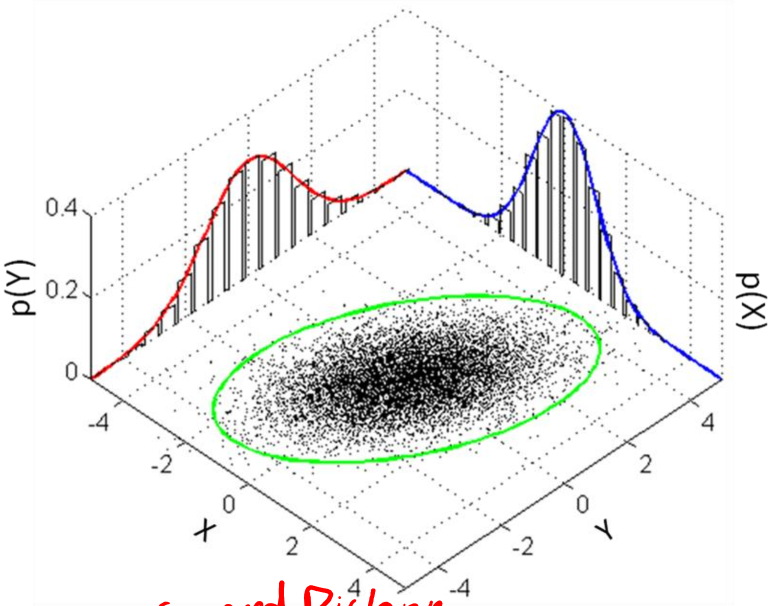


Distributions

Multivariate Gaussian Distribution

- Continuous RV: $X \in \mathbb{R}^d$

- Distribution is completely specified by mean vector $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$



Squared Distance

$$p(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{|2\pi\boldsymbol{\Sigma}|}} \exp\left\{-\frac{(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}{2}\right\}$$

Normalizer

Distributions

Important Properties of Gaussians:

- All marginals of a Gaussian are again Gaussian
- Every conditional is Gaussian
- The product of 2 Gaussians is again Gaussian
- Even the sum of 2 Gaussian RVs is again Gaussian

Maximum Likelihood Estimation (MLE)

- Given: the training data $D = \{(x_i, y_i)\}_{i=1\ldots N}$ **identically independently distributred (iid)** from the data distribution p_{data}
- Let $p_{\boldsymbol{\theta}}(x, y)$ be a family of distributions parametrized by $\boldsymbol{\theta} \in \boldsymbol{\Theta}$
- We want to find $\boldsymbol{\theta}$ such that p fits the data well

Fitness of $\boldsymbol{\theta}$ for one single data point:

$$\mathrm{lik}(\boldsymbol{\theta}; x_i, y_i) = p_{\boldsymbol{\theta}}(x_i, y_i)$$

Fitness of $\boldsymbol{\theta}$ for whole dataset (iid. assumption):

$$\mathrm{lik}(\boldsymbol{\theta}; D) = \prod_i p_{\boldsymbol{\theta}}(x_i, y_i)$$

Maximum Likelihood Estimation (MLE)

Log-likelihood is easier to optimize:

$$\text{loglik}(\boldsymbol{\theta}; D) = \sum_i \log p_{\boldsymbol{\theta}}(x_i, y_i)$$

- Log is monotonous -> same optimum
- Sums are “nicer” to optimize than products
- Log cancels exponential form (most distributions are in the exponential family)

The MLE solution is given by:

$$\boldsymbol{\theta}_{\text{ML}} = \text{argmax}_{\boldsymbol{\theta}} \text{loglik}(\boldsymbol{\theta}; D)$$

Example: Gaussian

Gaussian density function:

$$\mathrm{loglik}(\boldsymbol{\theta}; D) = -N \log \sqrt{2\pi\sigma^2} - \sum_i \frac{(x_i - \mu)^2}{2\sigma^2}$$

MLE solution for μ **:**

MLE: conditional log-likelihood

- Given the training data $D = \left\{(x_i, y_i)\right\}_{i=1 \ldots N}$ iid. from the data distribution p_{data}
- Let $p_{\boldsymbol{\theta}}(y|x)$ be a family of distributions parametrized by $\boldsymbol{\theta} \in \boldsymbol{\Theta}$
- We only care about distribution of y, not of x
- Typical case in supervised learning

Log-likelihood:

$$\mathrm{loglik}(\boldsymbol{\theta}; D) = \sum_i \log p_{\boldsymbol{\theta}}(y_i|x_i)$$

Example: Linear Gaussian model

We consider the following conditional Gaussian model:

$$p_{\boldsymbol{\theta}}(y|\boldsymbol{x}) = \mathcal{N}(y|\boldsymbol{w}^T\tilde{\boldsymbol{x}}, \sigma^2), \quad \boldsymbol{\theta} = \{\boldsymbol{w}, \sigma^2\}$$

Log-likelihood:

$$\mathrm{loglik}(\boldsymbol{\theta}; D) = -\log\sqrt{2\pi\sigma^2} - \sum_i \frac{(y_i - \boldsymbol{w}^T\tilde{\boldsymbol{x}}_i)^2}{2\sigma^2}$$

- For obtaining **w**, only the squared errors matter, i.e.

$$\mathrm{loglik}(\boldsymbol{\theta}; D) = \mathrm{const}_1 - \mathrm{const}_2 \sum_i (y_i - \boldsymbol{w}^T\tilde{\boldsymbol{x}}_i)^2$$

- Hence, the MLE solution is equivalent to the least squares solution!
- **But:** we can also obtain the variance!

Takeaway messages

What have we learned so far?

- Basic rules of probabilities … nothing new so far
- Expectations can be evaluated by samples
- How to compute the ML estimator
- Maximum likelihood is equivalent to minimizing the squared loss for:
  - Conditional Gaussian models
  - With constant noise

Today‘s Agenda!

Basics: Probability Theory

- Probabilistic Models
- Expectations and Monte Carlo Methods
- Maximum Likelihood

Linear Classification:

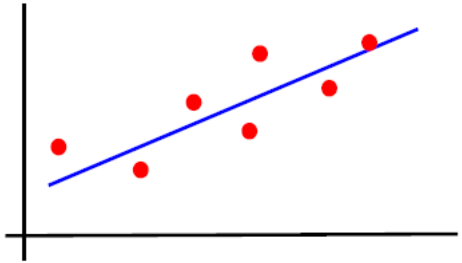
- Linear Classifiers
- Logistic Regression

Basics: Gradient Descent

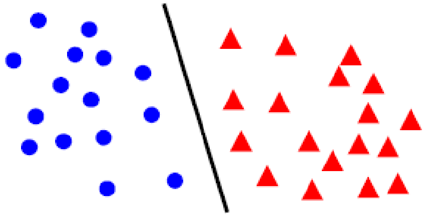
Supervised Learning

Training data includes targets

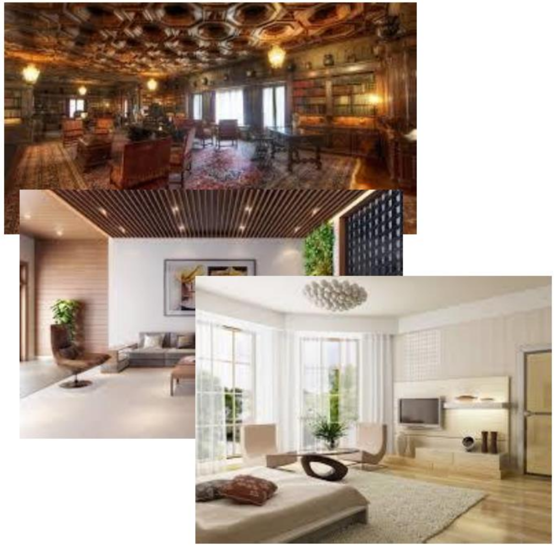
- **Regression:**
  - Learn continuous function
  - Example: line



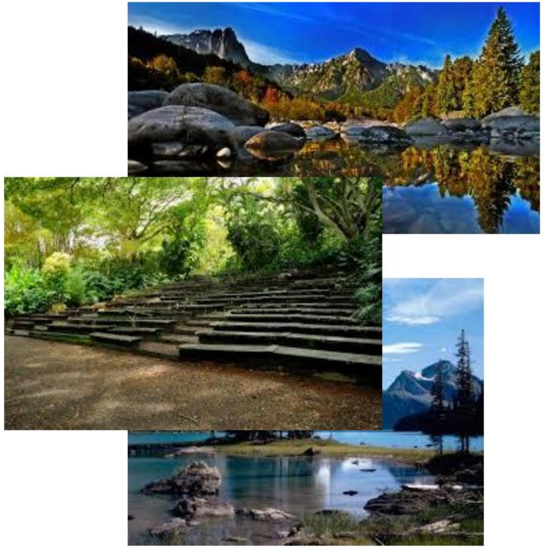
- **Classification:**
  - Learn class labels
  - Example: Digit recognition



Example 1: Image classification



Indoor



outdoor

Example 2: Spam Classification

	#"$"	#"Mr."	#"sale"	…	Spam?
Email 1	2	1	1		Yes
Email 2	0	1	0		No
Email 3	1	1	1		Yes
…					
Email n	0	0	0		No
New email	0	0	1		??

Definition

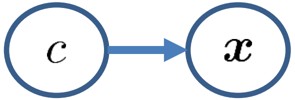
Given the dataset $\mathcal{D} = \{(\boldsymbol{x}_i, c_i)\}_{i=1\ldots N}$, where $\boldsymbol{x}_i \in \mathbb{R}^d$ are the input samples and $c \in \{1 \ldots K\}$ are the class labels, we want to learn a classifier $f(\boldsymbol{x})$ that predicts the class label for unseen samples.

- K = 2: Binary classification
- K > 2: Multi-class classification

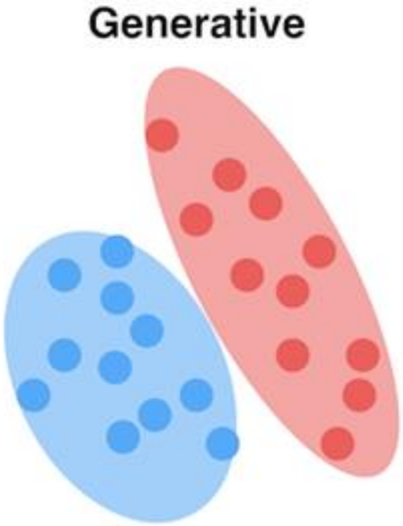
In difference to regression, the output is now discrete!

Generative vs. discriminative modelling

Generative Models:



- Assume some functional form for class prior $p(c)$ and class densities $p(\boldsymbol{x}|c)$
- Learn prior and densities from data
  - This is a "generative" model, as we can create new datapoints ***x*** using $p(\boldsymbol{x}|c)$
- Predict class label by computing posterior $p(c|\boldsymbol{x}) = \dfrac{p(\boldsymbol{x}|c)p(c)}{p(\boldsymbol{x})}$

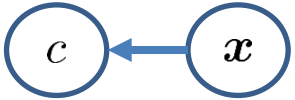


Learn full joint distribution of the data (typically very hard)

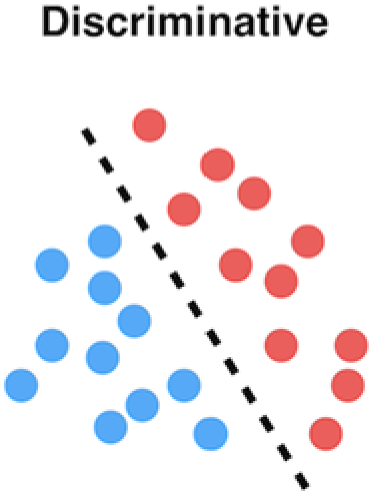
- Our modelling assumptions, e.g. that $p(\boldsymbol{x}|c)$ is Gaussian, might introduce big errors

Generative vs. discriminative modelling

Discriminative Models:



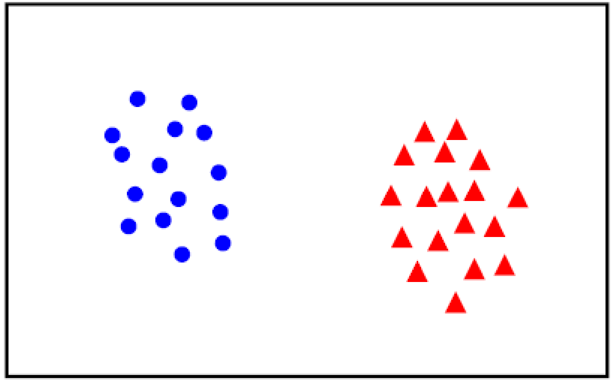
- Directly assume some functional form for $p(c|\boldsymbol{x})$ (or any other predictor $f(\boldsymbol{x})$ that returns the class label).
- This is a 'discriminative' model of the data!
- Estimate parameters of $p(c|\boldsymbol{x})$ directly from training data

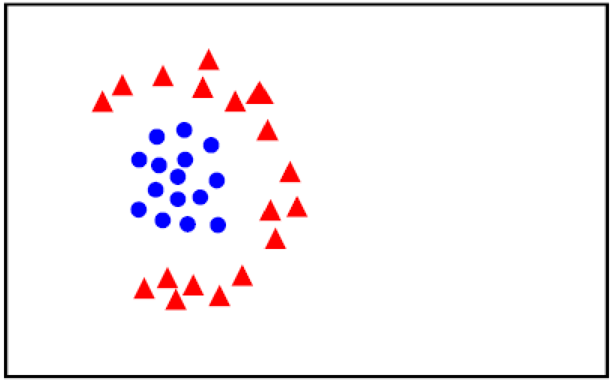


Modelling needs to consider only points on the border

- Typically much simpler than generative modelling
- We therefore concentrate on discriminative models

(Discriminative) Binary Classification





Given the training data $(\boldsymbol{x}_i, y_i)$, i = 1…N, with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$, learn a classifier $f(\boldsymbol{x})$ such that:

$$f(\boldsymbol{x}_i) = \begin{cases} > 0, & \text{if } y_i = 1 \\ < 0, & \text{if } y_i = 0 \end{cases}$$

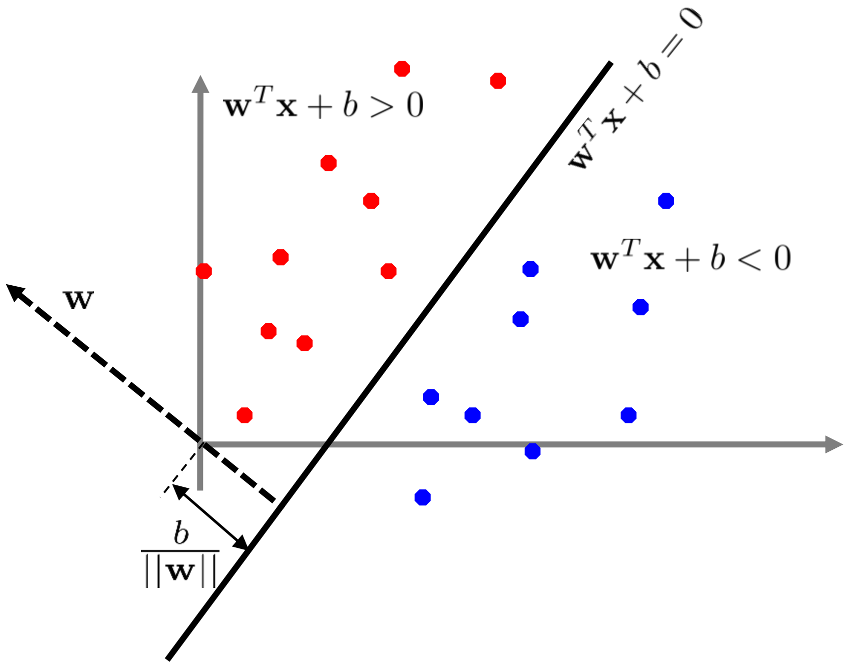
Linear Classifiers

A linear classifier is given in the form:

$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

In 2D, the classifier is a line

- $\mathbf{w}$ is the normal to the line
- b is the bias



Linear Discriminators

A linear discriminator is given in the form:

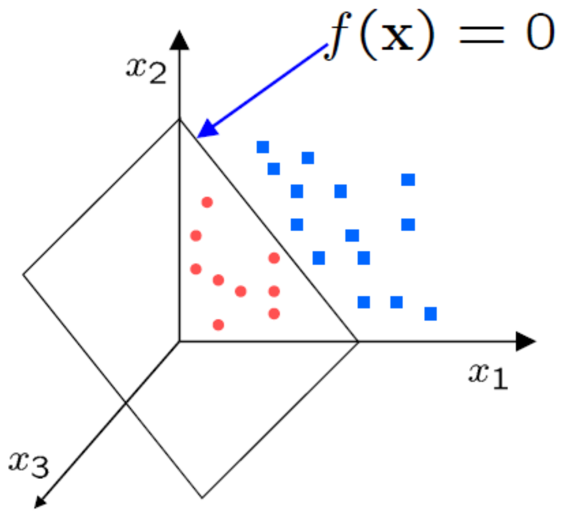
$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$

In 2D, the discriminator is a line

- $\mathbf{w}$ is the normal to the line
- b is the bias

In 3D, it's a **plane**

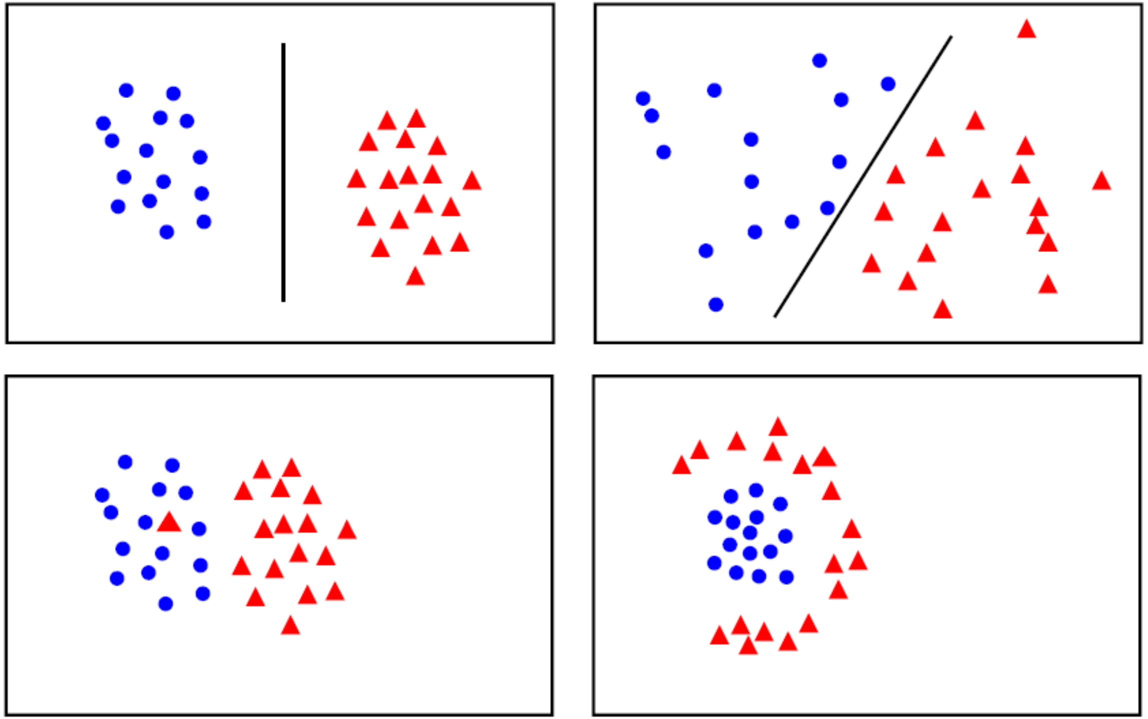
In N-D, it's a **hyper-plane**



Linear Separability

Linear Separable

Non-Linear Separable



Linear Classification: 0-1 loss (1st attempt)

Prediction: $y = \mathrm{step}(f(\boldsymbol{x})) = \mathrm{step}(\boldsymbol{w}^T\boldsymbol{x} + b)$

- Predict class 1 for $f(\boldsymbol{x}) > 0$
- else predict class 0

Optimization: Find $\boldsymbol{w}$ such that

$$L_0(\boldsymbol{w}) = \sum_i \mathbb{I}\left(\mathrm{step}\left(\boldsymbol{w}^T\boldsymbol{x} + b\right) \neq y_i\right)$$

- where $\mathbb{I}$ returns 1 if the argument is true
- … counts the number of misclassifications

× Very **difficult to optimize**!!! (NP-hard)

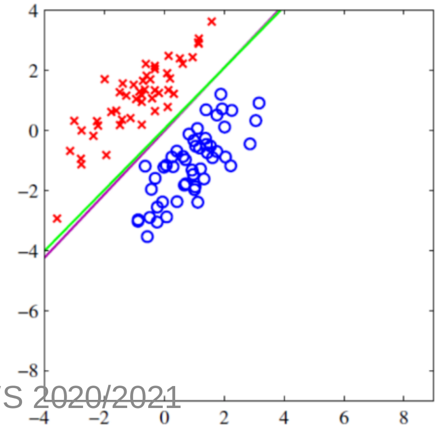
Linear Classification: regression loss (2nd attempt)

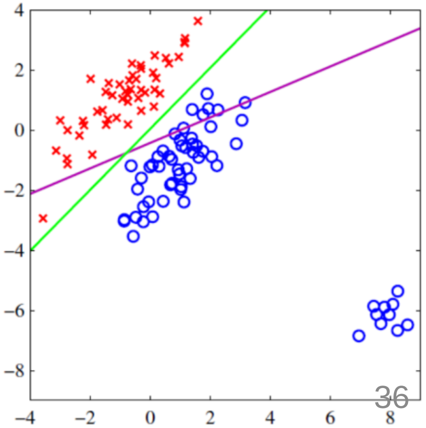
We can use same loss as in regression

$$L_{\text{reg}}(\boldsymbol{w}) = \sum_i \left(f(\boldsymbol{x}_i) - y_i\right)^2$$

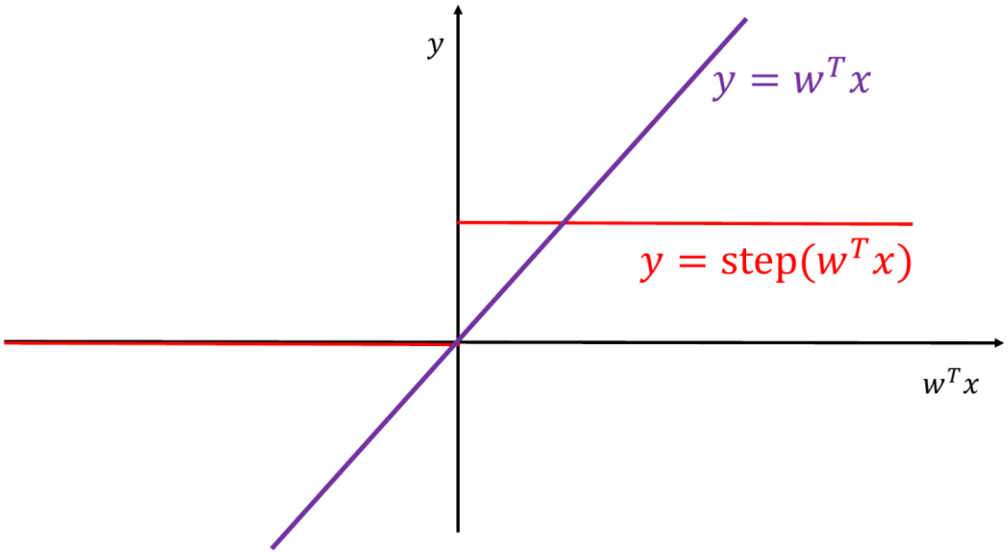
- Minimize the squared error: Easy!
- However: we ignored the fact that y_i is restricted to {0,1}

× **Not robust** to outliers





Compare the two



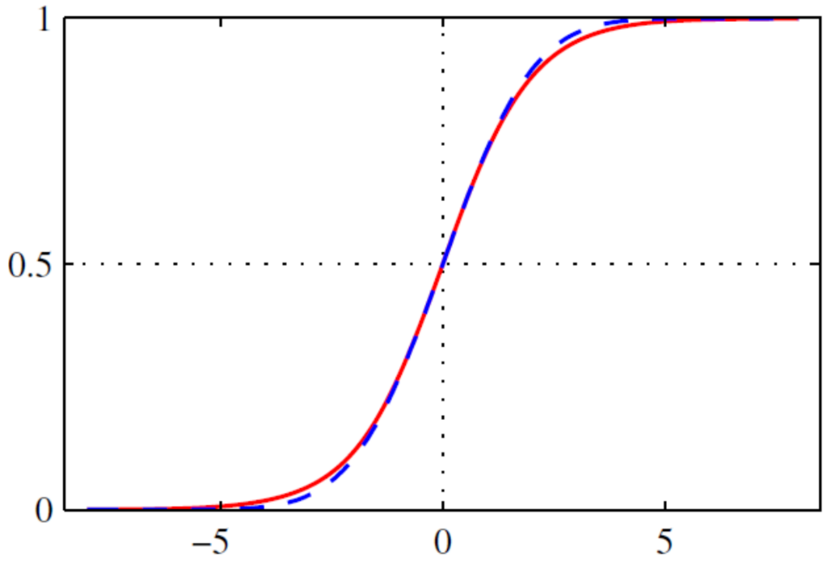
- The output of a linear function is unbounded!
- However, useful output values are only 0 or 1

Logistic sigmoid function

Sigmoid function:

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

- Output is bounded between 0 and 1
- Smooth



For linear classification:

- Squash the output of the linear function
- Minimize the loss

$$L(\boldsymbol{w}) = \sum_i \left(\sigma\left(f(\boldsymbol{x}_i)\right) - y_i\right)^2 = \sum_i \left(\sigma\left(\boldsymbol{w}^T\boldsymbol{x} + b\right) - y_i\right)^2$$

Better: Probabilistic View

Define conditional probability distribution of the class label

$$p(c=1|\boldsymbol{x}) = \sigma(\boldsymbol{w}^T\boldsymbol{x}+b), \quad p(c=0|\boldsymbol{x}) = 1-\sigma(\boldsymbol{w}^T\boldsymbol{x}+b)$$

- This is now a conditional Bernoulli distribution. I.e. the outcome of the event c depends on **x**
- We can use the same "exponential trick" to select the correct probability depending on the value of c, i.e.

$$p(c|\boldsymbol{x}) = p(c=1|\boldsymbol{x})^c p(c=0|\boldsymbol{x})^{1-c} = \sigma(\boldsymbol{w}^T\boldsymbol{x}+b)^c\big(1-\sigma(\boldsymbol{w}^T\boldsymbol{x}+b)\big)^{1-c}$$

Log-Likelihood

We can now directly optimize the conditional Bernoulli log-likelihood

$$\begin{aligned}\mathrm{loglik}(\tilde{\boldsymbol{w}}, D) &= \sum_i \log p(c_i|\boldsymbol{x}_i) = \sum_i \log\left(p(c=1|\boldsymbol{x}_i)^{c_i} p(c=0|\boldsymbol{x}_i)^{1-c_i}\right) \\ &= \sum_i c_i \log p(c=1|\boldsymbol{x}_i) + (1-c_i)\log p(c=0|\boldsymbol{x}_i) \\ &= \sum_i c_i \log \sigma(\tilde{\boldsymbol{w}}^T\tilde{\boldsymbol{x}}_i) + (1-c_i)\log\left(1-\sigma(\tilde{\boldsymbol{w}}^T\tilde{\boldsymbol{x}}_i)\right)\end{aligned}$$

– Negative likelihood is also often referred to as **cross-entropy loss**

Logistic Regression

Optimizing the log-likelihood of a sigmoid is called **logistic regression**

$$\mathrm{argmax}_{\tilde{\boldsymbol{w}}}\ \mathrm{loglik}(\tilde{\boldsymbol{w}}, D) = \mathrm{argmax}_{\tilde{\boldsymbol{w}}} \sum_i c_i \log \sigma(\tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{x}}_i) + (1 - c_i) \log \left(1 - \sigma(\tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{x}}_i)\right)$$

- … even though we solve a classification problem
- One can show that the function is still convex (only one maximum exists)
- However, there is **no closed form solution** as in linear regression

How can we find the maximum? **-> Gradient Descent!**

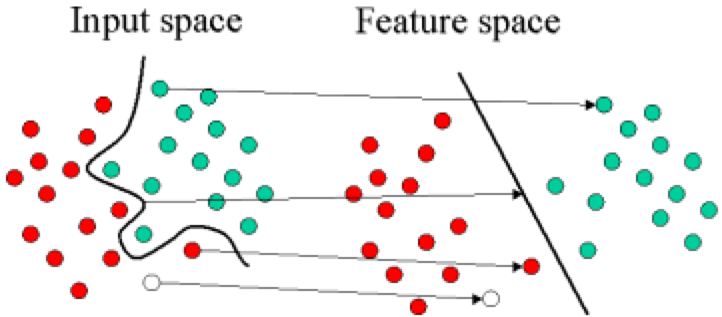
Generalized logistic models

We can fit a **linear discriminator** in a **non-linear feature** space

- Similar to generalized linear regression models

$$\mathrm{argmax}_{\boldsymbol{w}}\, \mathrm{loglik}(\boldsymbol{w}, D) = \mathrm{argmax}_{\boldsymbol{w}} \sum_i c_i \log \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)) + (1 - c_i) \log \left(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))\right)$$

- Problems that are not linear separable in input space can be linear separable in feature space



Regularization

Similar as in linear regression, we can again add a **regularization penalty**

$$L(\tilde{\boldsymbol{w}}, D) = \mathrm{loglik}(\tilde{\boldsymbol{w}}, D) - \lambda \, \mathrm{penalty}(\tilde{\boldsymbol{w}})$$

Most common: L2 regularization loss

$$\mathrm{penalty}(\tilde{\boldsymbol{w}}) = ||\tilde{\boldsymbol{w}}||^2$$

- L is still convex for most penalty terms

Today‘s Agenda!

Basics: Probability Theory

- Probabilistic Models
- Expectations and Monte Carlo Methods
- Maximum Likelihood

Linear Classification:

- Linear Classifiers
- Logistic Regression

Basics: Gradient Descent

Optimization

For most ML algorithms, we want to find the best model to fit the data.

Two examples we already know:

- **Least squares solution:**

  $$\operatorname{argmin}_{\boldsymbol{w}} \mathrm{SSE}(\boldsymbol{w}, D)$$

- **Maximum likelihood solution:**

  $$\operatorname{argmax}_{\boldsymbol{w}} \mathrm{loglik}(\boldsymbol{w}, D)$$

Optimization

For most ML algorithms, we want to find the best model to fit the data.

Two examples we already know:

- **Least squares solution:**

$$\operatorname{argmin}_{\boldsymbol{w}} \operatorname{SSE}(\boldsymbol{w}, D) + \lambda \operatorname{penalty}(\boldsymbol{w})$$

- **Maximum likelihood solution:**

$$\operatorname{argmax}_{\boldsymbol{w}} \operatorname{loglik}(\boldsymbol{w}, D) - \lambda \operatorname{penalty}(\boldsymbol{w})$$

… plus regularization penalty

Note that:

$$\arg\min_{\boldsymbol{x}} f(\boldsymbol{x}) = \arg\max_{\boldsymbol{x}} -f(\boldsymbol{x})$$

Hence, the role of the penalty is the same

Optimization

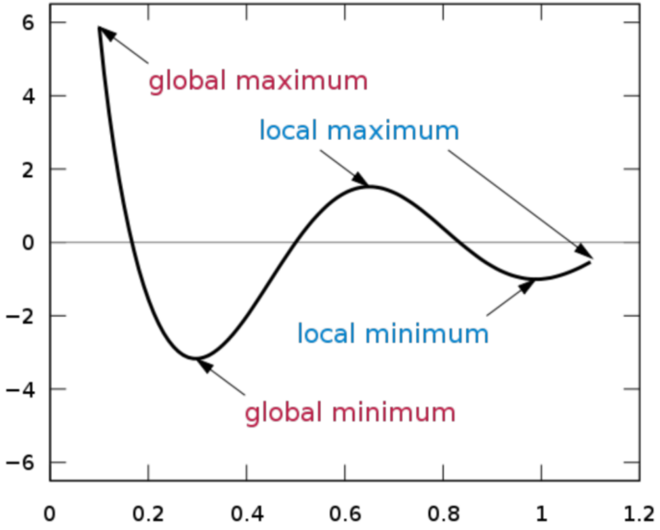
General form of optimization for ML: loss + penalty

$$\underset{\text{parameters } \boldsymbol{\theta}}{\arg\min} \sum_{i=1}^{N} l(\boldsymbol{x}_i, \boldsymbol{\theta}) + \lambda \,\text{penalty}(\boldsymbol{\theta})$$

- Summed sample-loss plus regularization penalty

How to do that? **Optimization**

When can we do that?



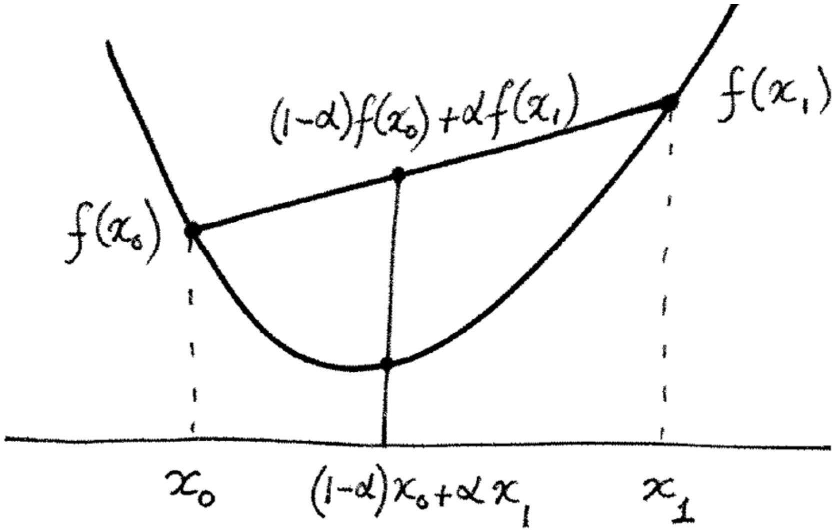
- The global minimum/maximum can only be found for convex functions!
- For non-convex functions we are limited to finding a local minimum / maximum

Convex functions

A convex function $f : \mathbb{R}^d \to \mathbb{R}$ satisfies for any $\boldsymbol{x}_0, \boldsymbol{x}_1 \in \mathbb{R}^d$

$$f\big((1-\alpha)\boldsymbol{x}_0 + \alpha \boldsymbol{x}_1\big) \leq (1-\alpha) f(\boldsymbol{x}_0) + \alpha f(\boldsymbol{x}_1), \quad \alpha \in [0,1]$$

- Line joining $\big(\boldsymbol{x}_0, f(\boldsymbol{x}_0)\big)$ and $\big(\boldsymbol{x}_1, f(\boldsymbol{x}_1)\big)$ is always above the function value
- There is only one minimum!



Example: Linear Regression Objective

$$L_{\text{ridge}} = (\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{w})^T(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{w}) + \lambda \boldsymbol{w}^T\boldsymbol{w}$$

- Convex
- Quadratic function in w
- Minimum can be obtained analytically
- One of the very rare cases!

In most other cases, we have to resort to incremental methods: **Gradient descent**

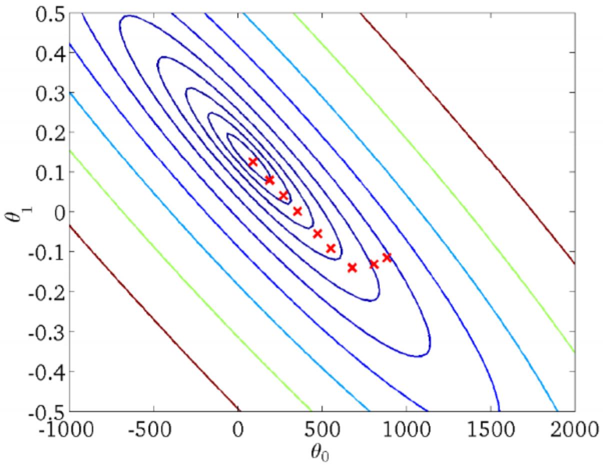
Gradient Descent

- Is good for finding **global minima** if function is **convex**
- Is good for finding **local minima** if function is **non-convex**
- Has many applications in ML:
  - Logistic Regression
  - Linear Regression (for large input dimensions)
  - Neural Networks
  - Mixture Models
  - …

Gradient Descent

Start at some point, follow the gradient towards (a) minimum

$$
\begin{aligned}
&\boldsymbol{x}_0 \leftarrow \text{init},\ t = 0\\
&\textbf{while } \text{termination condition does not hold } \textbf{do}\\
&\quad \boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \eta \nabla f(\boldsymbol{x}_t), \qquad t = t + 1\\
&\textbf{end while}
\end{aligned}
$$

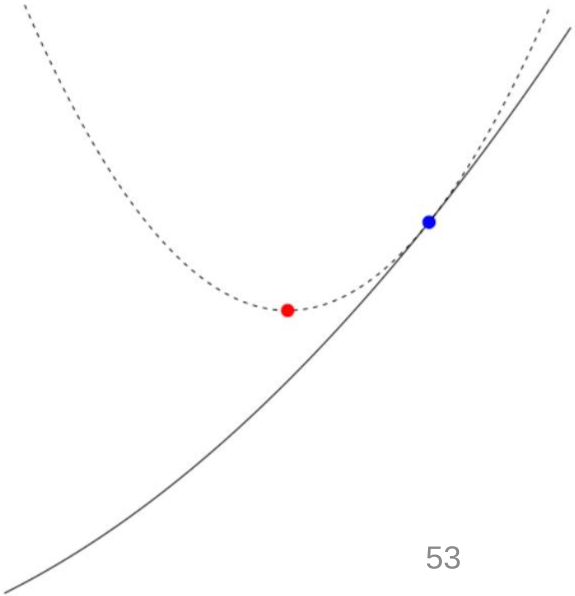


- $\eta \ldots$ learning rate or step size
- Gradient always points in the direction of **steepest ascen.**

Gradient Descent Interpretation

Approximate the function as quadratic function:

$$\hat{f}(\boldsymbol{x}) = \underbrace{f(\boldsymbol{x}_t) + \nabla f(\boldsymbol{x}_t)^T(\boldsymbol{x} - \boldsymbol{x}_t)}_{\text{linear approximation}} + \underbrace{\frac{1}{2\eta}||\boldsymbol{x}_t - \boldsymbol{x}||^2}_{\text{proximity of } \boldsymbol{x}_t} \approx f(\boldsymbol{x})$$

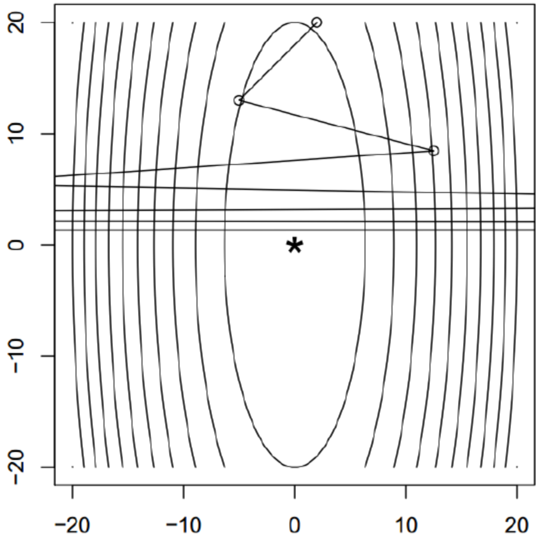


- Finding the minimum of $\hat{f}(\boldsymbol{x})$ yields the gradient descent rule

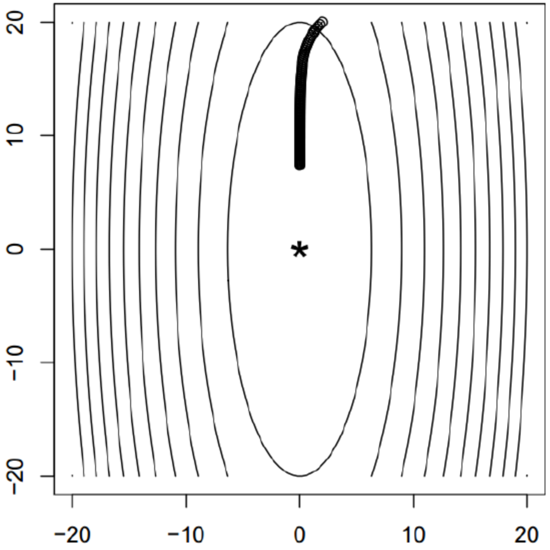
$$\boldsymbol{x}_{t+1} = \arg\min_{\boldsymbol{x}} \hat{f}(\boldsymbol{x}), \qquad \boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \eta \nabla f(\boldsymbol{x}_t)$$

Choosing the step-size

$\eta_t = t$, it is too big



too small η_t, after 100 iterations



How to terminate

When change in iterates is small

- When gradient is small
- When change in function value is small

Or after a fixed time step or budget

Stochastic Gradient Descent

- Usually we are minimizing the empirical loss (**batch gradient descent**)

$$\frac{1}{n}\sum_i l(\boldsymbol{x}_i;\boldsymbol{\theta})$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \frac{\eta}{n}\sum_i \nabla_{\boldsymbol{\theta}} l(\boldsymbol{x}_i;\boldsymbol{\theta}_t)$$

- We do this to approximate the expected loss

$$\mathbb{E}_{\boldsymbol{x}}\left[l(\boldsymbol{x};\boldsymbol{\theta})\right]$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta\mathbb{E}_{\boldsymbol{x}}\left[\nabla_{\boldsymbol{\theta}} l(\boldsymbol{x};\boldsymbol{\theta}_t)\right]$$

- Use a rougher, cheaper approximation: **stochastic gradient descent**

$$l(\boldsymbol{x}_i;\boldsymbol{\theta})$$

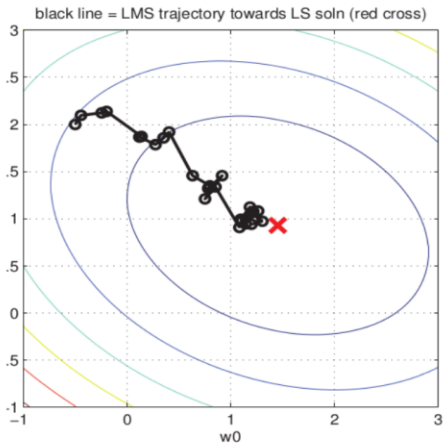
$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta\nabla_{\boldsymbol{\theta}} l(\boldsymbol{x}_i;\boldsymbol{\theta}_t)$$

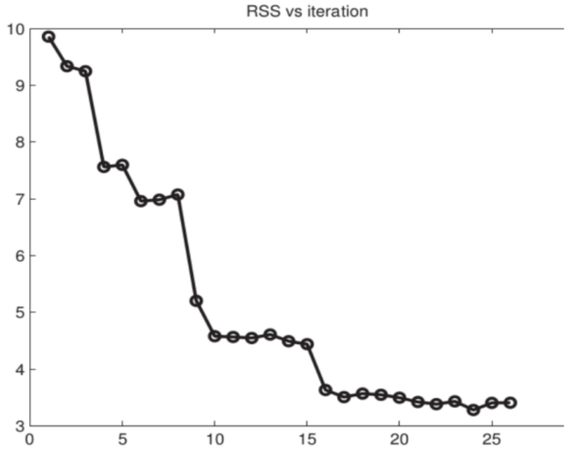
  - for random sample i

Stochastic Gradient Descent (SGD)

Use only one sample to compute the update

- Does NOT always “descent”
- Iterations are much cheaper
- Requires more iterations
- … and smaller step sizes



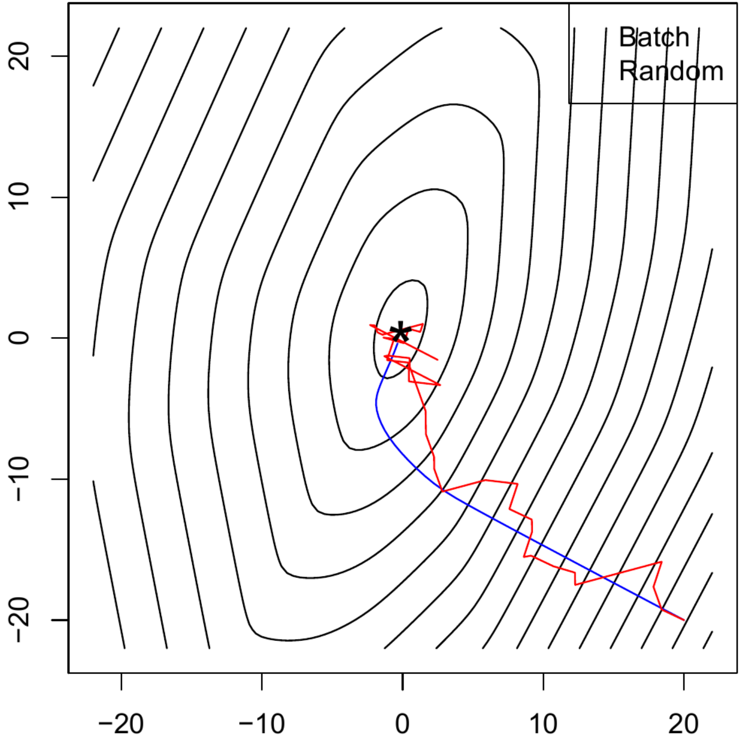


Stochastic vs. Batch Gradients

- Blue: Batch Gradients
- Red: Stochastic Gradients

Rule of thumb:

- Stochastic methods work well far away from optimum
- But struggle to find the exact optimum



Step-sizes

Standard in SGD is to use diminishing step sizes, e.g., $\eta_t = \frac{1}{t}$

- Assymptotically approach the optimum
- instead of "wiggling" around optimum

In general, it can be shown that SGD **converges to the optimum** for strictly convex functions if (**stochastic approximation theory**)

$$\sum_t \eta_t = \infty \quad \text{and} \quad \sum_t \eta_t^2 < \infty$$

Stochastic vs. Batch Gradients

Why are stochastic gradients often better than batch?

- Typically, our data-set will contain redundancy
- Hence, some computation in the batch gradients are redundant
  - compute the gradients for similar samples
  - using the same parameter vector
- This does not happen if we update immediately after one sample

As a consequence, **SGD requires less computation** (in most cases)

Mini-Batches

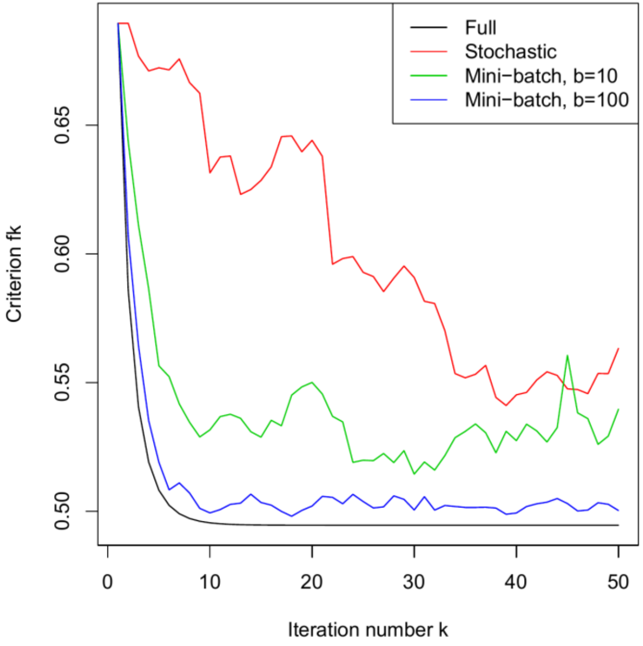
Take **subset of samples** $I_t \subset \{1, \ldots, n\}, \ |I_t| = b, \ b \ll n$ to approximate real gradient:

$$\frac{1}{b} \sum_{i \in I_t} l(\boldsymbol{x}_i; \boldsymbol{\theta}) \qquad\qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \frac{\eta}{b} \sum_{i \in I_t} \nabla_{\boldsymbol{\theta}} l(\boldsymbol{x}_i; \boldsymbol{\theta}_t)$$

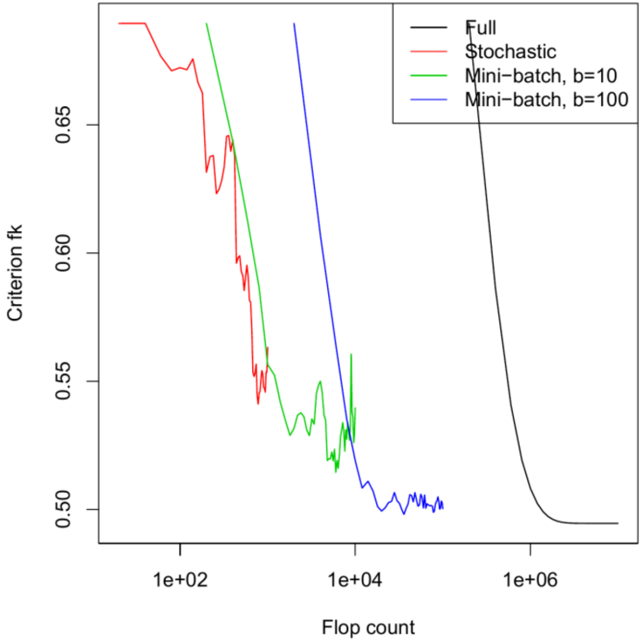
- Intermediate version of stochastic and batch gradient descent
- Less noisy estimates
- Achieves “descent” more often
- Preferable for GPU implementations

Example

10000 samples, loglikelihood logistic regression:



per iteration



per flop

Gradient Descent for Logistic Regression

Properties of the sigmoid function:

- Bounded: $$\sigma(a) = \frac{1}{1+\exp(-a)} \in (0,1)$$
- Symmetric: $$1 - \sigma(a) = \frac{\exp(-a)}{1+\exp(-a)} = \frac{1}{1+\exp(a)} = \sigma(-a)$$
- Gradient: $$\sigma'(a) = \frac{\exp(-a)}{(1+\exp(-a))^2} = \sigma(a)(1-\sigma(a))$$

Classification loss

Data log-likelihood:

$$\mathrm{loglik}(\mathcal{D}, \boldsymbol{w}) = \sum_{i=1}^{N} p(c_i|\boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{w}) = \sum_{i=1}^{N} \underbrace{c_i \log \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)) + (1 - c_i) \log\left(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))\right)}_{\mathrm{loss}_i \ldots \text{ loss of the ith sample}}$$

$$\begin{aligned}\frac{\partial \mathrm{loss}_i}{\partial \boldsymbol{w}} &= \frac{\partial}{\partial \boldsymbol{w}} \left(c_i \log \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)) + (1 - c_i) \log\left(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))\right)\right) \\ &= ?\end{aligned}$$

Gradient for Logistic Regression

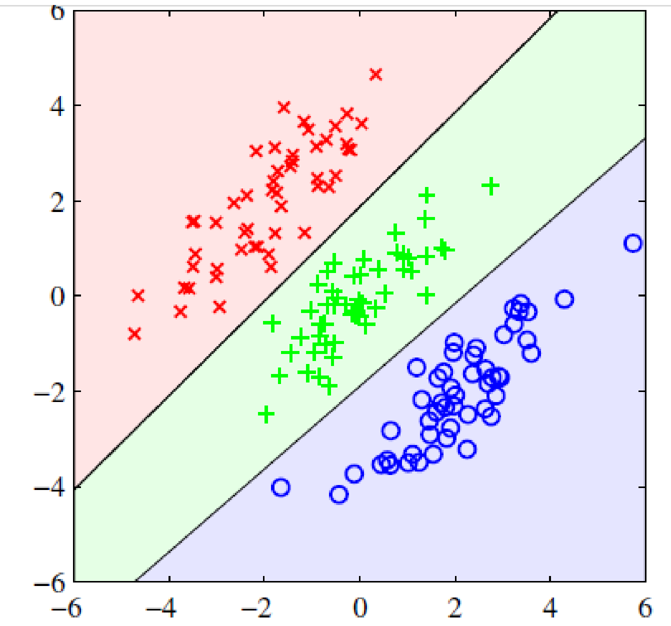
$$
\begin{aligned}
\frac{\partial \mathrm{loss}_i}{\partial \boldsymbol{w}} &= \frac{\partial}{\partial \boldsymbol{w}} \Big(c_i \log \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)) + (1 - c_i) \log \big(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))\big) \Big) \\
&= c_i \frac{1}{\sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))} \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)))\phi(\boldsymbol{x}_i) \\
&\quad + (1 - c_i) \frac{1}{1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))} (-) \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)))\phi(\boldsymbol{x}_i) \\
&= c_i(1 - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i)))\phi(\boldsymbol{x}_i) - (1 - c_i)\sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))\phi(\boldsymbol{x}_i) \\
&= \big(c_i - \sigma(\boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))\big)\phi(\boldsymbol{x}_i)
\end{aligned}
$$

Multiclass Classification

Softmax Likelihood function:

$$p(c = i|\boldsymbol{x}) = \frac{\exp\left(\boldsymbol{w}_i^T \boldsymbol{\phi}(\boldsymbol{x})\right)}{\sum_{k=1}^{K} \exp\left(\boldsymbol{w}_k^T \boldsymbol{\phi}(\boldsymbol{x})\right)}$$

- Each class gets a weight vector
- Higher probability for class i if $\boldsymbol{w}_i^T \boldsymbol{\phi}(\boldsymbol{x})$ is high
- For K = 2, $\boldsymbol{w}_2$ is redundant -> better to use sigmoid



Recap: Multinomial distribution

Multinomial / Categorical Distribution:

- K different events: $C \in \{1, \ldots, K\}$
- Directly specifies probabilities: $p(C = k) = \mu_k, \quad \mu_k \geq 0, \quad \sum_{k=1}^{K} \mu_k = 1$
- Or written with 1-hot-encoding (without an “if” clause)

$$p(c) = \prod_{k=1}^{K} \mu_k^{\boldsymbol{h}_{c,k}}$$

Depending on the class label of x, selects the correct μ_k

  - where $\boldsymbol{h}_x$ is the K-dimensional 1-hot encoding vector, which is one for the dimension c = k and 0 elsewhere. $\boldsymbol{h}_{x,k}$ is the k-th element of this vector.

- Think of it as tossing a die

Multiclass Classification

The multi-class classification problem can expressed as a conditional multinomial distribution:

- I.e. the probability of the event *c* depends on the input ***x***
- We can again use the “exponential trick” to select the correct probability depending on c

$$p(c|\boldsymbol{x}) = \prod_{k=1}^{K} p(c = k|\boldsymbol{x})^{\boldsymbol{h}_{c,k}}$$

$$= \prod_{k=1}^{K} \left(\frac{\exp(\boldsymbol{w}_k^T \boldsymbol{\phi}(\boldsymbol{x}_i))}{\sum_{k'=1}^{K} \exp(\boldsymbol{w}_{k'}^T \boldsymbol{\phi}(\boldsymbol{x}_i))} \right)^{\boldsymbol{h}_{c,k}}$$

Multiclass Classification

Data log-likelihood: $\mathrm{loglik}(\mathcal{D}, \boldsymbol{w}_{1:K}) = \sum_{i=1}^{N} \log p(c_i|\boldsymbol{x}_i) = \sum_{i=1}^{N} \underbrace{\sum_{k=1}^{K} \boldsymbol{h}_{c_i,k} \log p(k|\boldsymbol{x}_i)}_{\mathrm{loss}_i \ldots \text{ loss of the ith sample}}$

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} \boldsymbol{h}_{c_i,k} \left[\boldsymbol{w}_k^T \boldsymbol{\phi}(\boldsymbol{x}_i) - \log \left(\sum_{j=1}^{K} \exp\left(\boldsymbol{w}_j^T \boldsymbol{\phi}(\boldsymbol{x}_i)\right) \right) \right]$$

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} \boldsymbol{h}_{c_i,k} \boldsymbol{w}_k^T \boldsymbol{\phi}(\boldsymbol{x}_i) - \underbrace{\log \left(\sum_{j=1}^{K} \exp\left(\boldsymbol{w}_j^T \boldsymbol{\phi}(\boldsymbol{x}_i)\right) \right)}_{\text{independet from k}} \underbrace{\sum_{k} \boldsymbol{h}_{c_i,k}}_{=1}$$

- Can again be optimized by gradient ascent

Multiclass Classification

Gradient:

$$\frac{\partial \text{loss}_i}{\partial \boldsymbol{w}_k} = \frac{\partial}{\partial \boldsymbol{w}_k} \left(\sum_{k=1}^{K} \boldsymbol{h}_{c_i,k} \boldsymbol{w}_k^T \boldsymbol{\phi}(\boldsymbol{x}_i) - \log \left(\sum_{j=1}^{K} \exp\left(\boldsymbol{w}_j^T \boldsymbol{\phi}(\boldsymbol{x}_i) \right) \right) \right)$$

$$= ?$$

Takeaway messages

What have we learned today?

- Refresher on probability theory and maximum likelihood
- Relation between maximum likelihood and least squares
- What is a linear classification problem …
- … and how to formalize it as likelihood maximization problem
  - Sigmoid likelihood for binary classification
  - Soft-max likelihood for multi-class
- What is gradient descent, stochastic gradient descent and mini-batches?
- How to apply gradient descent to logistic regression