Lecture 3. Linear Regression. Optimisation.

COMP90051 Statistical Machine Learning

Semester 2, 2019
Lecturer: Ben Rubinstein

This lecture

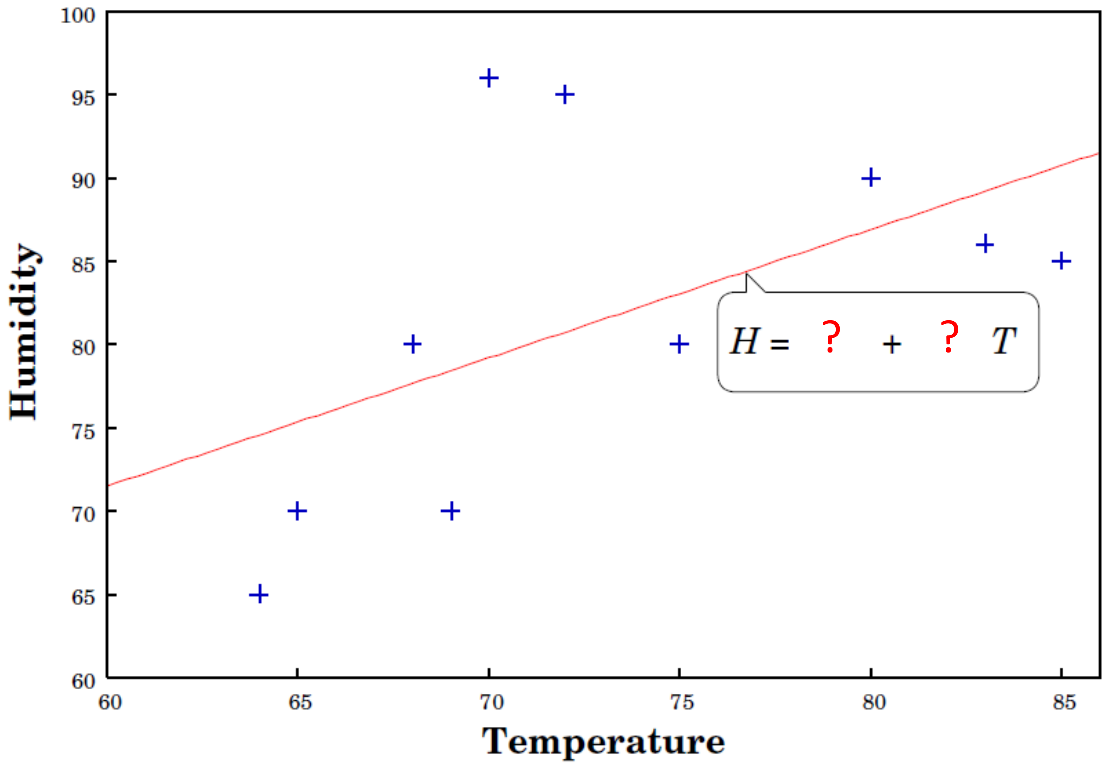
- Linear regression
  - Simple model (convenient maths at expense of flexibility)
  - Often needs less data, “interpretable”, lifts to non-linear
  - Derivable under all Statistical Schools: Lect 2 case study
    - Today: Frequentist + Decision theory derivations
  - Later in semester: Bayesian approach
- Optimisation for ML (first of 2 parts or so)
  - Analytic solutions
  - Gradient descent
  - Convexity
- Later: Lagrangian duality

Linear Regression via Decision Theory

A warm-up example

Example: Predict humidity from temperature

Temperature	Humidity
TRAINING DATA	
85	85
80	90
83	86
70	96
68	80
65	70
64	65
72	95
69	70
75	80
TEST DATA	
75	70



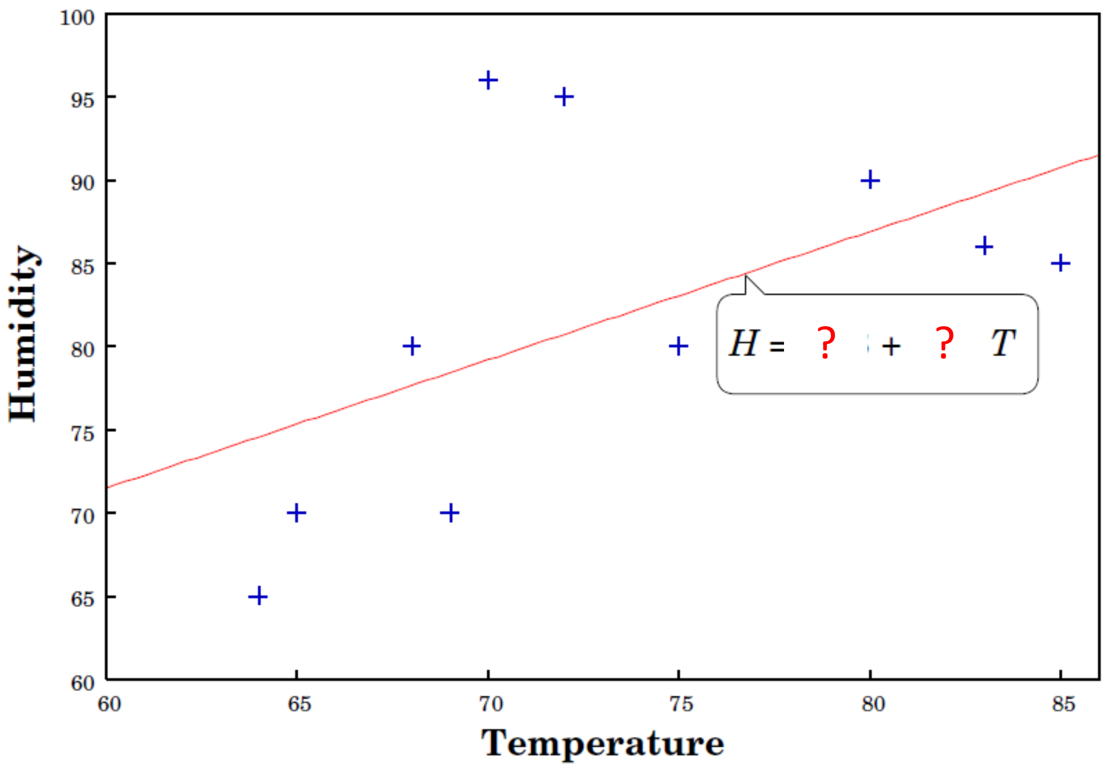
In regression, the task is to predict numeric response (*aka* dependent variable) from features (*aka* predictors or independent variables)

Assume a linear relation: $H = a + bT$

(H – humidity; T – temperature; a, b – parameters)

Example: Problem statement

- The model is
  $H = a + bT$
- Fitting the model = finding "best" a, b values for data at hand
- Popular criterion: minimise the sum of squared errors (*aka* residual sum of squares)



Example: Minimise Sum Squared Errors

To find a, b that minimise $L = \sum_{i=1}^{10}\left(H_i - (a + b\,T_i)\right)^2$

set derivatives to zero:

$$\frac{\partial L}{\partial a} = -2\sum_{i=1}^{10}(H_i - a - b\,T_i) = 0$$

if we know b, then $\hat{a} = \frac{1}{10}\sum_{i=1}^{10}(H_i - b\,T_i)$

$$\frac{\partial L}{\partial b} = -2\sum_{i=1}^{10}T_i(H_i - a - b\,T_i) = 0$$

if we know a, then $\hat{b} = \frac{1}{\sum_{i=1}^{10} T_i^2}\sum_{i=1}^{10} T_i(H_i - a)$

High-school optimisation:
- Write derivative
- Set to zero
- Solve for model
- (Check 2nd derivatives)

Will cover again later

Can we be more systematic?

Example: Analytic solution

- We have two equations and two unknowns a, b
- Rewrite as a system of linear equations

$$\begin{pmatrix} 10 & \sum_{i=1}^{10} T_i \\ \sum_{i=1}^{10} T_i & \sum_{i=1}^{10} {T_i}^2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{10} H_i \\ \sum_{i=1}^{10} T_i H_i \end{pmatrix}$$

- Analytic solution: $a = 25.3, b = 0.77$
- (Solve using `numpy.linalg.solve` or sim.)

More general decision rule

- Adopt a linear relationship between response $y \in \mathbb{R}$ and an instance with features $x_1, \dots, x_m \in \mathbb{R}$

$$\hat{y} = w_0 + \sum_{i=1}^{m} x_i w_i$$

Here $w_1, \dots, w_m \in \mathbb{R}$ denote weights (model parameters)

- Trick: add a dummy feature $x_0 = 1$ and use vector notation

$$\hat{y} = \sum_{i=0}^{m} x_i w_i = \boldsymbol{x}'\boldsymbol{w}$$

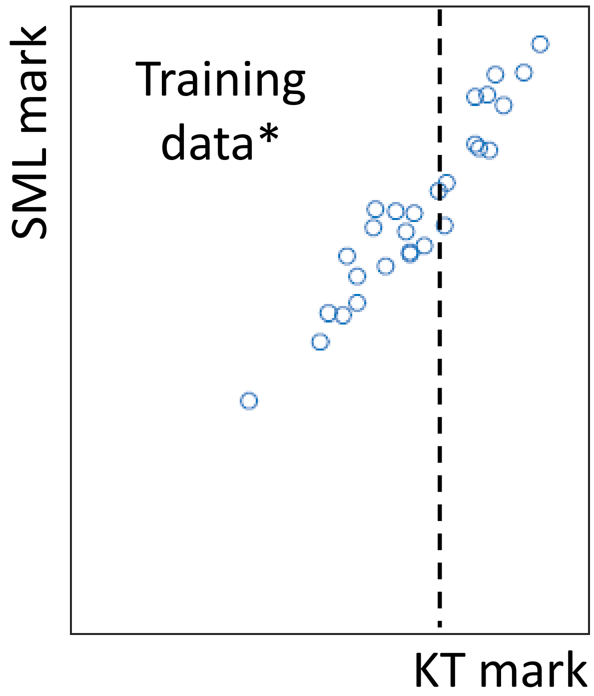
A lowercase symbol in **bold face** indicates a vector; $\boldsymbol{x}'$ denotes transpose

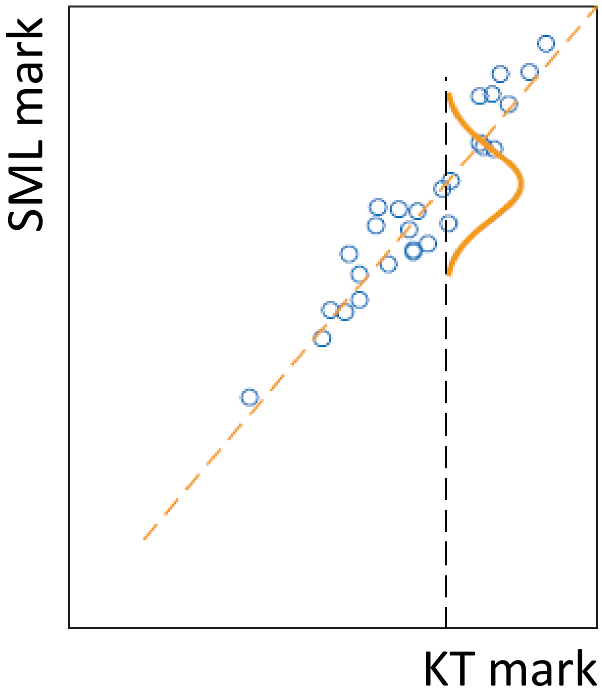
Linear Regression via Frequentist Probabilistic Model

Max Likelihood Estimation

Data is noisy!

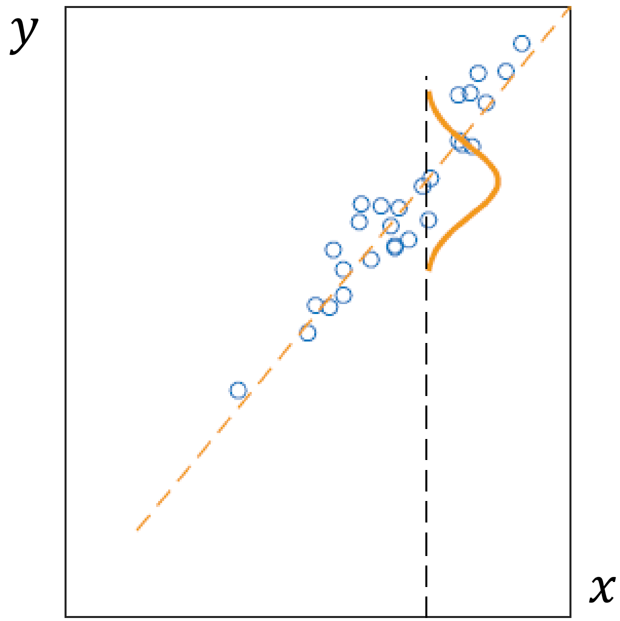
Example: predict mark for Statistical Machine Learning (SML) from mark for Knowledge Technologies (KT)





* synthetic data :)

Regression as a probabilistic model



- Assume a probabilistic model: $Y = \boldsymbol{X}'\boldsymbol{w} + \varepsilon$
  - Here $\boldsymbol{X}, Y$ and ε are r.v.'s
  - Variable ε encodes noise
- Next, assume Gaussian noise (indep. of $\boldsymbol{X}$): $\varepsilon \sim \mathcal{N}(0, \sigma^2)$

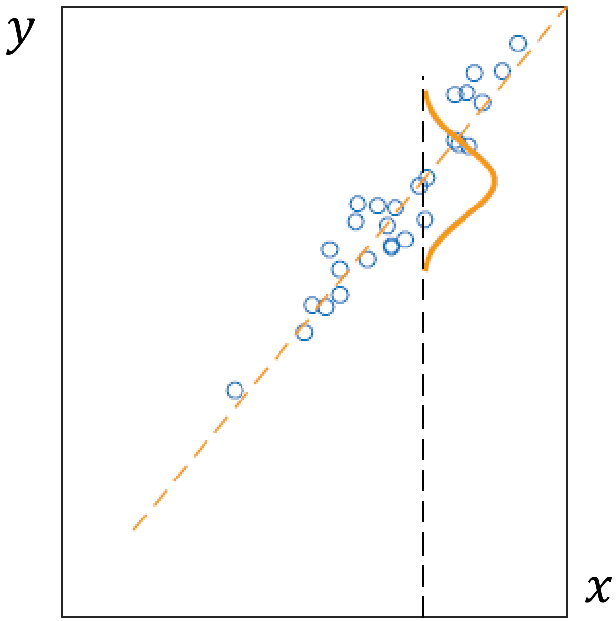
$Y \sim \mathcal{N}(w'X, \sigma^2)$

this is a squared error!

- Recall that $\mathcal{N}(x; \mu, \sigma^2) \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
- Therefore

$$p_{\boldsymbol{w},\sigma^2}(y|\boldsymbol{x}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{\boxed{(y - \boldsymbol{x}'\boldsymbol{w})^2}}{2\sigma^2}\right)$$

Parametric probabilistic model



- Using simplified notation, discriminative model is:

$$p(y|\boldsymbol{x}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \boldsymbol{x}'\boldsymbol{w})^2}{2\sigma^2}\right)$$

- Unknown parameters: $\boldsymbol{w}, \cancel{\sigma^2}$

- Given observed data $\{(\boldsymbol{X}_1, Y_1), \dots, (\boldsymbol{X}_n, Y_n)\}$, we want to find parameter values that "best" explain the data
- Maximum likelihood estimation: choose parameter values that maximise the probability of observed data

Maximum likelihood estimation

- Assuming independence of data points, the probability of data is

$$p(y_1, \dots, y_n | \boldsymbol{x}_1, \dots, \boldsymbol{x}_n) = \prod_{i=1}^{n} p(y_i | \boldsymbol{x_i})$$

- For $p(y_i|\boldsymbol{x}_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \boldsymbol{x}_i{}'\boldsymbol{w})^2}{2\sigma^2}\right)$

- "Log trick": Instead of maximising this quantity, we can maximise its logarithm (why?)

$$\sum_{i=1}^{n} \log p(y_i|\boldsymbol{x_i}) = -\frac{1}{2\sigma^2} \boxed{\sum_{i=1}^{n} (y_i - \boldsymbol{x}_i{}'\boldsymbol{w})^2} + C$$

the sum of squared errors!

here C doesn't depend on $\boldsymbol{w}$ (it's a constant)

- Under this model, maximising log-likelihood as a function of $\boldsymbol{w}$ is equivalent to minimising the sum of squared errors

Non-linear Continuous Optimisation

Brief summary of a few basic optimisation methods vital for ML

Optimisation formulations in ML

- Training = Fitting = Parameter estimation
- Typical formulation

$$\hat{\boldsymbol{\theta}} \in \underset{\boldsymbol{\theta} \in \Theta}{\operatorname{argmin}} \, L(data, \boldsymbol{\theta})$$

  - argmin because we want a minimiser not the minimum
    - Note: argmin can return a set (minimiser not always unique!)
  - Θ denotes a model family (including constraints)
  - L denotes some objective function to be optimised
    - E.g. MLE: (conditional) likelihood
    - E.g. Decision theory: (regularised) empirical risk

Two solution approaches

- Analytic (*aka* closed form) solution
  - Known only in limited number of cases
  - Use 1st-order necessary condition for optimality*:

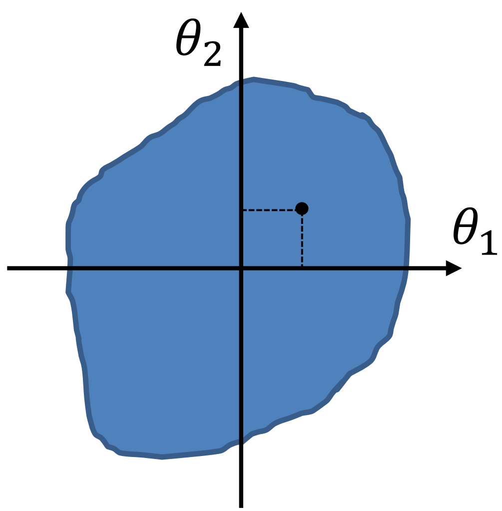
$$\frac{\partial L}{\partial \theta_1} = \cdots = \frac{\partial L}{\partial \theta_p} = 0$$

Assuming unconstrained, differentiable *L*

- Approximate iterative solution
  1. Initialisation: choose starting guess $\boldsymbol{\theta}^{(1)}$, set $i = 1$
  2. Update: $\boldsymbol{\theta}^{(i+1)} \leftarrow SomeRule\left[\boldsymbol{\theta}^{(i)}\right]$, set $i \leftarrow i + 1$
  3. Termination: decide whether to Stop
  4. Go to Step 2
  5. Stop: return $\widehat{\boldsymbol{\theta}} \approx \boldsymbol{\theta}^{(i)}$

* Note: to check for local minimum, need positive 2nd derivative (or Hessian positive definite); this assumes unconstrained – in general need to also check boundaries. See also Lagrangian techniques later in subject.

Finding the deepest point

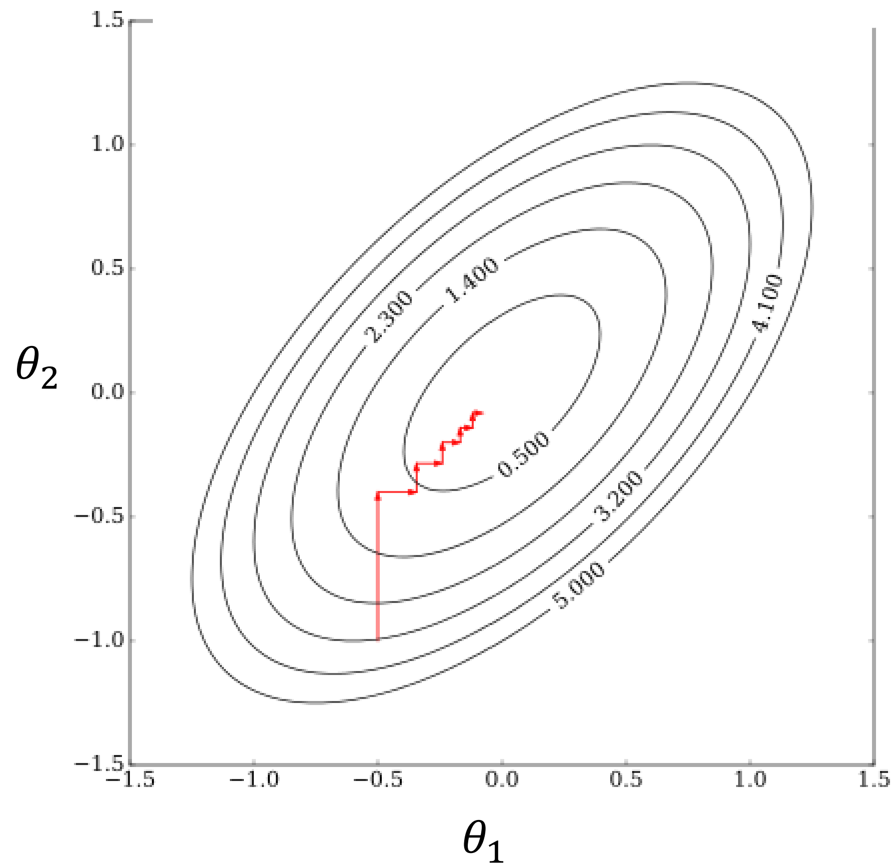


- In this example, a model has 2 parameters
- Each location corresponds to a particular combination of parameter values
- Depth indicates objective value (e.g. loss) of that candidate model on data

Coordinate descent

- Suppose $\boldsymbol{\theta} = [\theta_1, \dots, \theta_K]'$

1. Choose $\boldsymbol{\theta}^{(1)}$ and some T
2. For i from 1 to T (*)
   1. $\boldsymbol{\theta}^{(i+1)} \leftarrow \boldsymbol{\theta}^{(i)}$
   2. For j from 1 to K
      1. Fix components of $\boldsymbol{\theta}^{(i+1)}$, except j-th component
      2. Find $\hat{\theta}_j^{(i+1)}$ that minimises $L\left(\theta_j^{(i+1)}\right)$
      3. Update j-th component of $\boldsymbol{\theta}^{(i+1)}$
3. Return $\widehat{\boldsymbol{\theta}} \approx \boldsymbol{\theta}^{(i)}$



*Other stopping criteria can be used

Reminder: The gradient

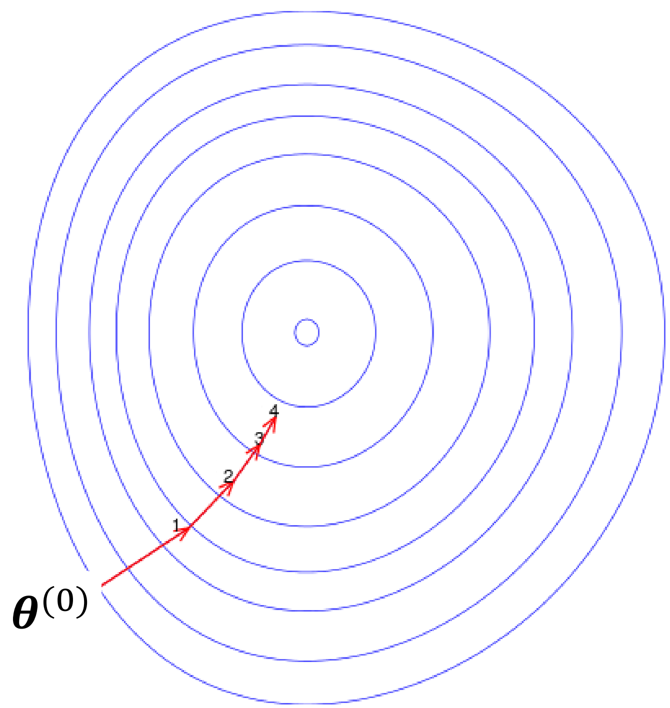
- Gradient at $\boldsymbol{\theta}$ defined as $\left[\frac{\partial L}{\partial \theta_1}, \dots, \frac{\partial L}{\partial \theta_p}\right]'$ evaluated at $\boldsymbol{\theta}$
- The gradient points to the direction of maximal change of $L(\boldsymbol{\theta})$ when departing from point $\boldsymbol{\theta}$
- Shorthand notation
  - $\boldsymbol{\nabla} L \stackrel{\text{def}}{=} \left[\frac{\partial L}{\partial \theta_1}, \dots, \frac{\partial L}{\partial \theta_p}\right]'$ computed at point $\boldsymbol{\theta}$
  - Here $\boldsymbol{\nabla}$ is the “nabla” symbol


Harps, p. 984.

Gradient descent

1. Choose $\boldsymbol{\theta}^{(1)}$ and some T
2. For i from 1 to T*
    1. $\boldsymbol{\theta}^{(i+1)} = \boldsymbol{\theta}^{(i)} - \eta \nabla L(\boldsymbol{\theta}^{(i)})$
3. Return $\widehat{\boldsymbol{\theta}} \approx \boldsymbol{\theta}^{(i)}$

Assuming L is differentiable



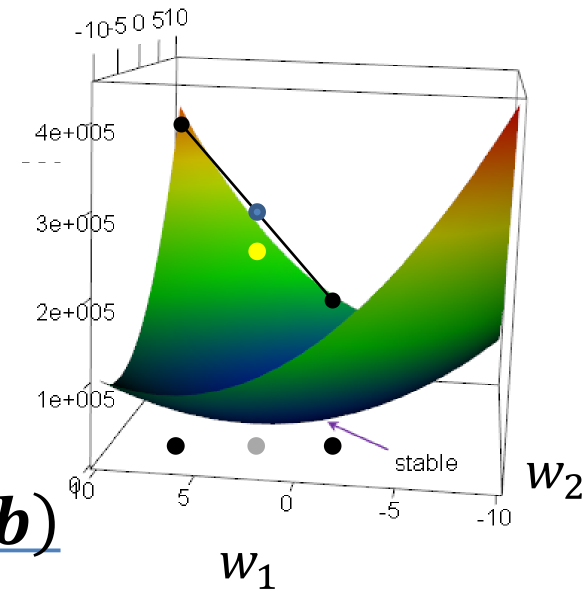
- Note: η is dynamically updated in each step
- Variants: Stochastic GD, Mini batches, Momentum, AdaGrad, ….

*Other stopping criteria can be used

Wikimedia Commons. Authors: Olegalexandrov, Zerodamage

Convex objective functions

- 'Bowl shaped' functions
- Informally: if line segment between any two points on graph of function lies above or on graph
- Formally* $f : D \rightarrow \mathbf{R}$ is convex if $\forall \boldsymbol{a}, \boldsymbol{b} \in D, t \in [0,1]$:
  $f(t\boldsymbol{a} + (1-t)\boldsymbol{b}) \leq tf(\boldsymbol{a}) + (1-t)f(\boldsymbol{b})$
  Strictly convex if inequality is strict (<)
- Gradient descent on (strictly) convex function guaranteed to find a (unique) global minimum!



* Aside: Equivalently we can look to the second derivative. For *f* defined on scalars, it should be non-negative; for multivariate f, the Hessian matrix should be positive semi-definite (see linear algebra supplemental deck).

L_1 and L_2 norms

- Throughout the course we will often encounter norms that are functions $\mathbb{R}^n \to \mathbb{R}$ of a particular form
  - Intuitively, norms measure lengths of vectors in some sense
  - Often component of objectives or stopping criteria in optimisation-for-ML
- More specifically, we will often use the L_2 norm (*aka* Euclidean distance)

$$\|\boldsymbol{a}\| = \|\boldsymbol{a}\|_2 \equiv \sqrt{a_1^2 + \cdots + a_n^2}$$

- And also the L_1 norm (*aka* absolute norm or Manhattan distance)

$$\|\boldsymbol{a}\|_1 \equiv |a_1| + \cdots + |a_n|$$

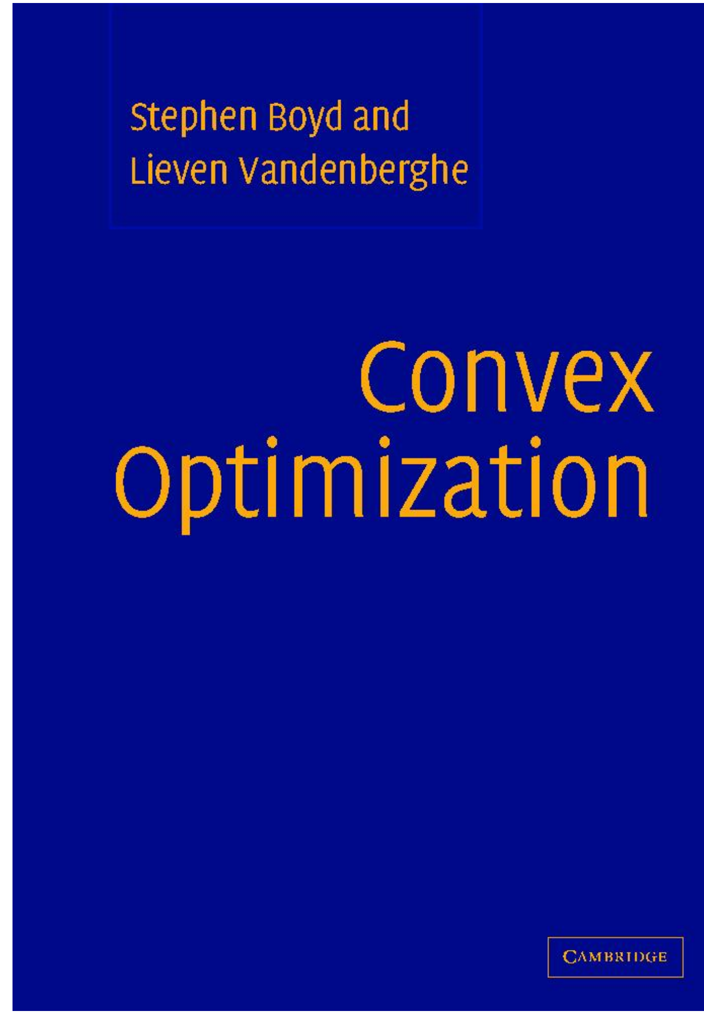
- For example, the sum of squared errors is a squared norm

$$L = \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{m} X_{ij} w_j \right)^2 = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|^2$$

…And much much more

- What if you have constraints?
- What about speed of convergence?
- Is there anything faster than gradient descent (yes, but can be expensive)
- Do you really need differentiable objectives? (no)
- Are there more tricks? (hell yeah!)

We'll see Lagrangian duality later on



Free at http://web.stanford.edu/~boyd/cvxbook/

One we've seen: Log trick

- Instead of optimising $L(\theta)$, try convenient $\log L(\theta)$
- Why are we allowed to do this?
- Strictly monotonic function: a $> b \Longrightarrow f(a) > f(b)$
  - Example: log function!
- **Lemma**: Consider any objective function $L(\theta)$ and any strictly monotonic f. θ^* is an optimiser of $L(\theta)$ if and only if it is an optimiser of $f(L(\theta))$.
  - Proof: Try it at home for fun!

Linear Regression Optimisation

For either MLE/decision-theoretic derivations

Method of least squares

Analytic solution:
- Write derivative
- Set to zero
- Solve for model

- Training data: $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n)\}$. Note bold face in $\boldsymbol{x}_i$
- For convenience, place instances in rows (so attributes go in columns), representing training data as an $n \times (m+1)$ matrix $\boldsymbol{X}$, and n vector $\boldsymbol{y}$
- Probabilistic model/decision rule assumes $\boldsymbol{y} \approx \boldsymbol{X}\boldsymbol{w}$
- To find $\boldsymbol{w}$, minimise the sum of squared errors

$$L = \sum_{i=1}^{n}\left(y_i - \sum_{j=0}^{m} X_{ij} w_j\right)^2$$

- Setting derivative to zero and solving for $\boldsymbol{w}$ yields

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

  * This system of equations called the normal equations
  * System is well defined only if the inverse exists

$L = \|y - Xw\|_2^2$

$\frac{\partial L}{\partial w} = 2X'(y - X\hat{w}) = 0$

$X'y = X'X\hat{w}$

In this slide: UPPERCASE symbol in bold face means matrix; $\boldsymbol{X}'$ denotes transpose; $\boldsymbol{X}^{-1}$ denotes matrix inverse

Wherefore art thou: Bayesian derivation?

- Later in the semester: return of linear regression
- Fully Bayesian, with a posterior:
  * Bayesian linear regression
- Bayesian (MAP) point estimate of weight vector:
  * Adds a penalty term to sum of squared losses
  * Equivalent to L_2 "regularisation" to be covered soon!
  * Called: ridge regression

Summary

- Linear regression
  - Probabilistic frequentist derivation
  - Decision-theoretic frequentist derivation
  - Later in semester: Bayesian approaches
- Optimisation for ML

Next time:

logistic regression - linear probabilistic model for classification; basis expansion for non-linear extensions