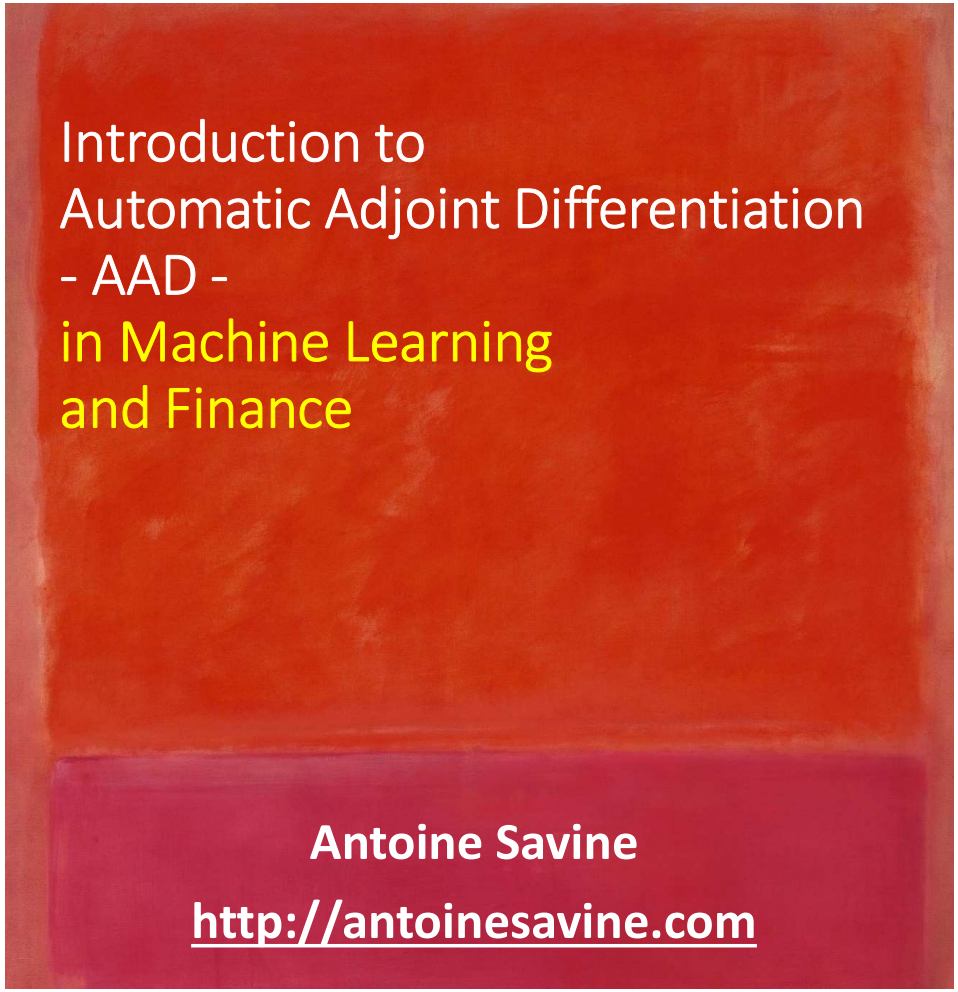
Introduction to
Automatic Adjoint Differentiation
- AAD -
in Machine Learning
and Finance
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http://antoinesavine.com

Introduction

Adjoint Differentiation - AD -

- Algorithm to compute all differentials of a scalar function quickly and accurately
  - Quickly (*constant time*): Compute all differentials in a time similar to one function evaluation
  - Accurately: Analytic differentiation, accurate to machine precision

$$f: \quad \mathbb{R}^D \quad \rightarrow \quad \mathbb{R}$$

$$x = \begin{pmatrix} x_1 \\ \dots \\ x_D \end{pmatrix} \quad \rightarrow \quad y = f(x)$$

$$AD: compute: \frac{\partial f}{\partial x} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \dots \\ \frac{\partial f}{\partial x_D} \end{pmatrix} \text{ in } O(1)$$

- Application: whenever we need to compute many derivatives of one result

Application: model fitting

- Model: $\hat{y} = f(x; \vartheta)$
  - Makes a prediction $\hat{y}$ from a set of inputs $x = (x_1, ..., x_n)^T$
  - Given parameters $\vartheta = (\vartheta_1, ..., \vartheta_D)^T$
- Learns its parameters by minimizing a *cost* function
  - E.g. sum of squared errors: $C(\vartheta) = \sum_{i=1}^{m} \left[f\left(x^{(i)}; \vartheta\right) - y^{(i)} \right]^2 = \sum_{i=1}^{m} c_i(\vartheta)$ (c_i : error or *loss* on training example *i*)
  - Over a training set of *m* labelled examples: $\left(x^{(i)}, y^{(i)}\right)_{1 \le i \le m}$ ($x^{(i)} \in \mathbb{R}^n, y^{(i)} \in \mathbb{R}$)
- Must compute gradient of the cost function for optimization algorithm: $\frac{\partial C}{\partial \vartheta} = \left(\frac{\partial C}{\partial \vartheta_1}, ..., \frac{\partial C}{\partial \vartheta_D} \right)$

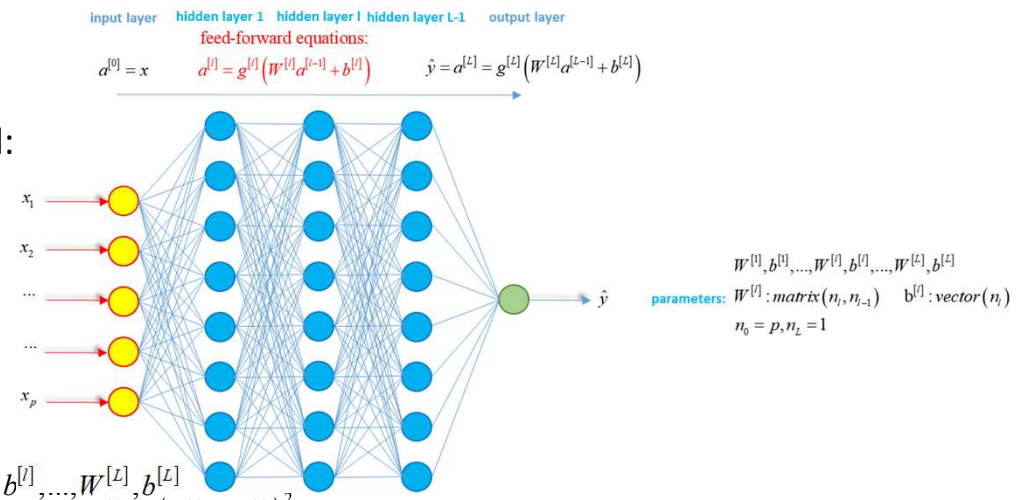
Calibrating a financial pricing model

- Calibration of a pricing model to market data:
  - Prediction: valuation of a financial product $\hat{y} = \text{product value} = f\left(\text{product parameters } x; \text{model parameters } \vartheta\right)$
  - Training set: *m* products, each with *n* known features $x^{(i)}$ and market price $y^{(i)}$
  - Calibration: fit parameters $\vartheta = \left(\vartheta_1, \ldots, \vartheta_D\right)^T$ (e.g. volatilities, correlations, …)
    to minimise cost = sum of errors (losses) on the training set
  - Then apply calibrated model to price other products which prices are unknown
- Minimization algorithms (gradient descent, conjugate gradients, pseudo-Newton methods…)

  require derivatives $\frac{\partial C}{\partial \vartheta} = \left(\frac{\partial C}{\partial \vartheta_1}, \ldots, \frac{\partial C}{\partial \vartheta_D}\right)$ on each iteration, we have as many differentials as we have parameters

Training a deep learning model

- Multi-Layer Perceptron (MLP)
  simplest and most common deep learning model:
  - Prediction: feed-forward equations $a^{[l]} = g^{[l]}\left(W^{[l]}a^{[l-1]} + b^{[l]}\right)$
  - Training set: *m* inputs $x^{(i)}$, each a vector in dimension n_0 with corresponding (scalar) labels $y^{(i)}$



  - Train the network: learn (fit) parameters $W^{[1]}, b^{[1]}, \ldots, W^{[l]}, b^{[l]}, \ldots, W^{[L]}, b^{[L]}$ to minimise cost = sum of errors (losses) on the training set $c^{(i)} = \left(\hat{y}^{(i)} - y^{(i)}\right)^2$
  - Then apply trained model to make predictions on new examples with unknown label

- Minimization (learning) algorithms require derivatives of cost/losses $\frac{\partial c^{(i)}}{\partial W_{j,k}^{[l]}}, \frac{\partial c^{(i)}}{\partial b_j^{[l]}}$ on every iteration

Application: market risk

- Value/risk metric (CVA, xVA…) of a financial product or book of financial products:

  a: vector of *k* market variables (asset prices, rates, spreads, volatilities…)
  b: vector of *n* model parameters (calibrated to market variables so $b = c(a), c : \mathbb{R}^k \to \mathbb{R}^n$)
  g: valuation function of model (generally numerical such as Monte-Carlo simulation) $V = g(b), g : \mathbb{R}^n \to \mathbb{R}$
  f: valuation function of market $V = g(b) = g\left[c(a)\right] = f(a), f : \mathbb{R}^k \to \mathbb{R}$

- Risk report computes model risks $\frac{\partial g}{\partial b}$ and/or market risks $\frac{\partial f}{\partial a}$

- Market risks computed from model risks: $a \in \mathbb{R}^k \xrightarrow[c]{} b \in \mathbb{R}^n \xrightarrow[g]{} v \in \mathbb{R}$ so by the chain rule $\frac{\partial f}{\partial a} = \frac{\partial g}{\partial b}\frac{\partial c}{\partial a}$

  - To compute $\frac{\partial c}{\partial a}$ and market risks $\frac{\partial f}{\partial a} = \frac{\partial g}{\partial b}\frac{\partial c}{\partial a}$ knowing model risks $\frac{\partial g}{\partial b}$, see for instance:
    http://papers.ssrn.com\sol3\papers.cfm?abstract_id=3262571

  - In this presentation, we focus on model risks $\frac{\partial g}{\partial b}$

Differentiation

- In all these applications (and many others)
  - We have a scalar function *f* of many inputs $f:\mathbb{R}^D \to \mathbb{R}$
  - This function is typically expensive to evaluate
    Losses of deep neural nets on large training set or a Monte-Carlo valuation may take several seconds, even on parallel hardware
  - It typically takes a large number *D* of inputs
    Thousands of weights for deep neural nets, or thousands of market/model variables for financial valuation
  - We must compute its sensitivities to all its inputs $\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_D} \right)$

- Conventional differentiation is of linear complexity in the number of inputs/differentials
  - To compute one differential takes time similar to one evaluation of the function
  - For example, with (one-sided) finite differences $\frac{\partial f}{\partial x_i} \approx \frac{f(x+\varepsilon e_i) - f(x)}{\varepsilon}, e_i = (\delta_{ij})_{1 \le j \le n}$
  - We have *(D+1)* function evaluations to compute *D* differentials
  - Illustration: if one function evaluation takes 1sec and we have 1,000 inputs
    It takes 1,001sec (15+ minutes) to evaluate its gradient once
  - This is not viable, a different technology is necessary

Adjoint Differentiation - AD -

- Algorithm to compute analytically all the differentials of *f*: $\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_D} \right)$
  - In a time independent of *D*
  - With an efficient implementation, it takes 4 to 10 times one evaluation of *f* to compute all its differentials
  - So AD can compute the 1,000 differentials of a function that takes 1sec to evaluate in ~4 to 10sec
  - Without loss of accuracy (if anything, AD differentials are *more* accurate)

- Hence the importance of this technology today
  - In finance, AD computes thousands of complex risks accurately and very quickly
  - In machine learning, AD computes the gradient of cost functions to many parameters in constant time
  - The same technology powers banks to estimate financial risks and deep nets to learn their weights
  - AD
    Allows Banks to keep going despite massive amount of regulatory calculations imposed since 2008-2011
    Powers your telephones to learn to recognize you and your friends in reasonable time
    Is largely credited for the recent and spectacular successes in the field of deep learning

A brief history of AD

- Invented in the 1960s (Wengert, 1964)
- Called “holy grail” of sensitivity computation (Griewank, 2012)
- Classified as on the 30 greatest numerical algorithms of the 20th century (Trefethen, 2015)

- Did not take firm hold in the computer science community until 1980
- Applied in deep learning to efficiently compute gradients of cost functions in learning algorithms
- Known under the names
  Back-Propagation (or simply back-prop, in deep learning),
  reverse differentiation, backward differentiation, adjoint accumulation, etc.

- Not adopted in Finance until 2006 (Giles and Glasserman’s “Smoking Adjoints”)
- Large scale implementation in Danske Bank with parallel Monte-Carlo simulations won In-House System of the Year 2015 Risk Award
- Universally adopted today for risk and calibration

- Delays in adoption mainly due to complexity, lack of teaching material and challenges in practical implementation (Andersen, 2018)

Automatic Adjoint Differentiation - AAD -

- Automatic implementation of AD
  - Developers only produce the evaluation code for the function *f*
  - The framework automatically produces (constant time) differentiation code for $\partial f / \partial x$
  - So developers don't need to write (complicated and error prone) AD code
  - And differentiation code is automatically updated when evaluation code changes
- Many commercial and open source AAD frameworks exist
  - Some are generic, some specialize in finance or machine learning
  - Some are free, some as extremely expensive
  - Work in a variety of programming languages: Python, C++, …
  - Work either with source transformation, operator overloading or letting clients build evaluation graphs
- Example: TensorFlow
  - Written in C++/CUDA (GPU)
  - With APIs in Python, JavaScript, Java, Go, Swift…
  - Allow clients to create evaluation graphs
  - And automatically applies AD to compute derivatives through the graphs
  - Popular in the field of machine learning

AAD: challenges

- However it is challenging to develop or even use AAD frameworks:
  - AD is somewhat “mind twisting” and generally poorly understood
  - Memory management: AAD consumes vast amounts of RAM
  - RAM, cache and parallel efficiency are hard to achieve
  - Aspects of practical implementation are topics of advanced research

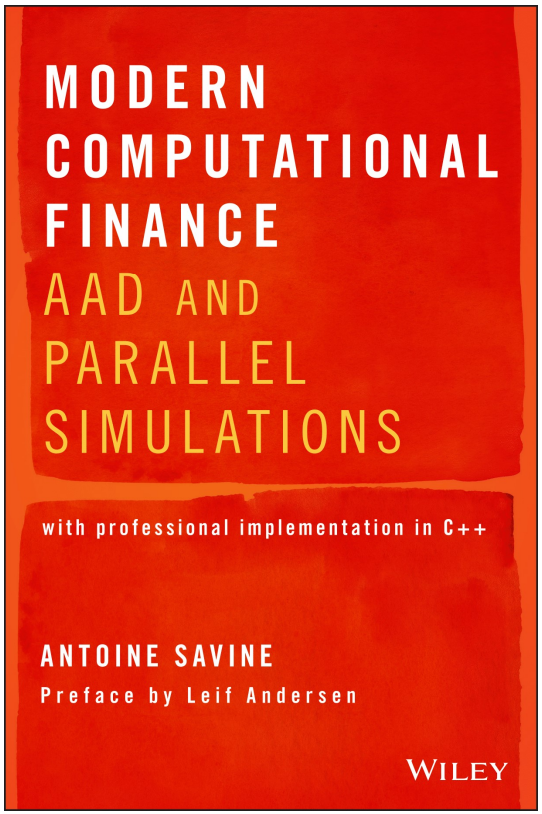
- Blindly applying a framework almost never works
  - Not quite as easy as coding an evaluation and sending it to the framework for differentiation
  - Requires a deep understanding of the theory and implementation
  - Otherwise often results in slow differentiation, incorrect results, crashes, etc.

- This presentation covers the bases of AD and AAD and introduces the book:

Modern Computational Finance: AAD and Parallel Simulations

which explains in deep details all aspects of AAD and its practical implementation

AAD book



- Written by (some of) the people who wrote Danske Bank's award winning systems
- Prefaced by Leif Andersen, read preface on

  researchgate.net/publication/328042479_Modern_Computational_Finance_AAD_and_Parallel_Simulations
- Teaches:
  - The modern design and efficient implementation of financial simulation libraries
  - The implementation of parallel simulation libraries
  - And of course AAD
- AAD is covered in deep detail:
  - Conceptual and mathematical foundations
  - Practical implementation
  - Memory management and check-pointing
  - Application in the context of large Monte-Carlo simulations, including parallel
  - Application to model and market risks
  - Efficient implementation with meta-programming and expression templates
  - And much more
- Ships with complete, professional code in C++
  - Explained in deep detail in the book
  - Freely available on GitHub our repo http://www.github.com\asavine\CompFinance\wiki

Overview

AAD: Demonstration

1. Adjoint Differentiation for Deep Learning
    1. A brief introduction to Artificial Neural Networks (ANN)
    2. Back-Propagation through ANNs

2. Adjoint Differentiation for arbitrary calculation code
    1. Evaluation graphs
    2. Back-Propagation through evaluation graphs

3. Automatic Adjoint Differentiation in C++
    1. AAD with operator overloading
    2. AAD over Monte-Carlo simulations

Demonstration: Dupire's model (1992)

- Extended Black & Scholes dynamics (in the absence of rates, dividends etc.): $\frac{dS}{S} = \sigma(S,t)\,dW$
- Calibrated with Dupire's celebrated formula: $\sigma(K,T) = \frac{2\frac{\partial C}{\partial T}}{\frac{\partial^2 C}{\partial K^2}}$ with *C(K,T)* = call prices of strike *K*, maturity *T*
- Implemented with a (bi-linearly interpolated) local volatility matrix: $\sigma_{ij} = \sigma(S_i, T_j)$
- Volatility matrix: 30 spots (every 5 points 50 to 150) and 36 times (every month from 0 to 3y)
  we have 1,080 volatilities + 1 initial spot (=100) = 1,081 model parameters
- Valuation of a 3y (weekly monitored) barrier option strike *K=120*, barrier *B=150*: $v(S_t,t) = E\left[(S_T - K)^+ 1_{\{\max(S_{T_1},\ldots,S_{T_K})<B\}} \middle| S_t\right]$
- Solved with Monte-Carlo or FDM over the equivalent PDE (from Feynman-Kac's theorem)
- We focus on Monte-Carlo simulations here: 500,000 paths, 156 (weekly) time steps

Demonstration: Results

- Implementation
  - C++ code exported to Excel (see tutorial on http://www.github.com\asavine\CompFinance\wiki)
  - Generic library design with efficient implementation (Chapter 6)
  - Parallel implementation (Chapters 3 and 7)
  - Sobol quasi-random numbers (Chapters 5 and 6)
  - Advanced AAD with expression templates (Chapter 15)

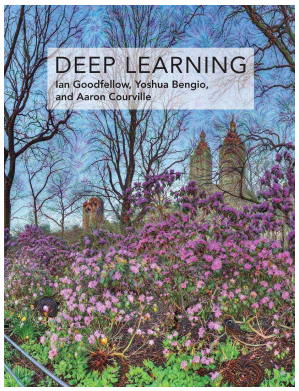
- Hardware: quad-code laptop (surface book 2, 2017)

- Performance:
  - One evaluation with 500,000 paths over 156 time steps take ~0.8sec
  - We have 1,081 risk sensitivities, take about 15 minutes to produces model risk report with linear differentiation
  - With AAD the 1,081 differentials are produced in ~1.5sec

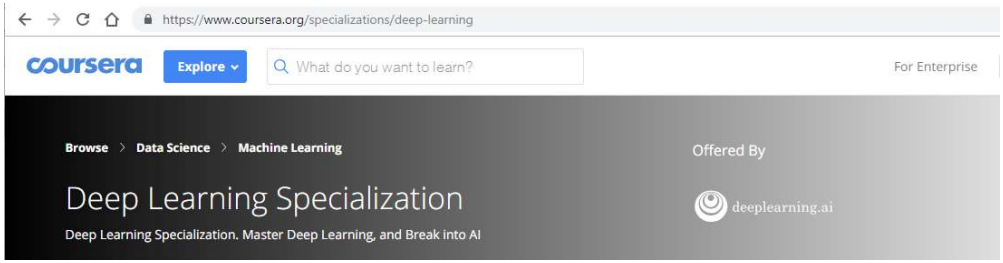
Deep Learning

Neural networks and deep learning

- Adjoint differentiation is best explained in its “natural habitat” of deep learning
- We briefly introduce deep learning to explain AD in this context
- (Much) deeper presentations are found in:



Goodfellow’s book



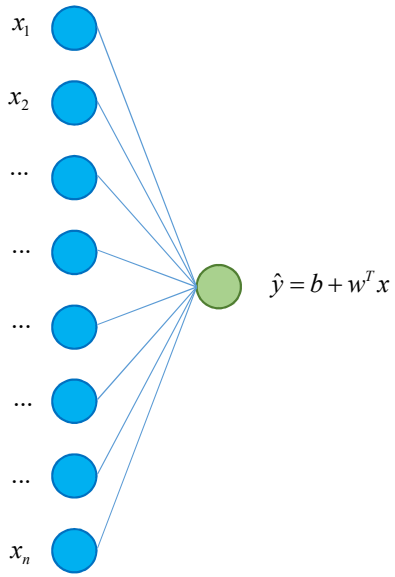
Andrew Ng’s videos on Coursera

…and many other books and resources

Linear regression: prediction

- Linear model (joint Gaussian assumptions): $\hat{y} = E[y|x] = b + \sum_{i=1}^{n} w_i x_i = b + w^T x$

- Parameters: $b \in \mathbb{R}$ and $w \in \mathbb{R}^n$

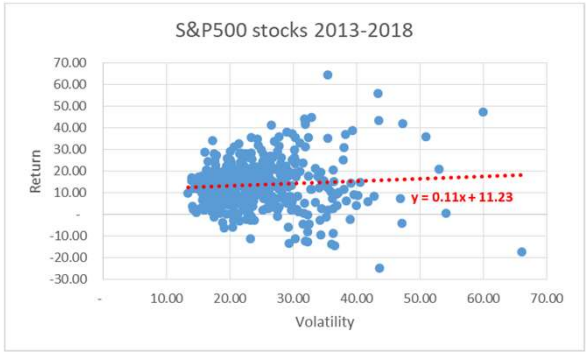


Linear regression and classification (1)

- In *regression* problems we predict real numbers

Example: predict return from volatility

- Each point is a stock in the S&P500
- Horizontal axis is annual volatility
- Vertical axis is annual return
- Estimated with daily data, 2013-2018
- Evidence of (small) risk premium
- Poor regression quality



Linear regression and classification (2)

- Alternatively, *classification* problems predict discrete categories

Example: identify animals in pictures: 0: not an animal, 1: cat, 2: dog, 3: bird, 4: other

picture 1920x1080x24bit color

vector of 1920x1080 pixels

$$\in \left[0, 2^{24}-1\right]$$

$$x = \begin{pmatrix} x_1 \\ \dots \\ x_{2,073,600} \end{pmatrix}$$

softmax regression

$$\hat{y} = s(b + wx) = \begin{bmatrix} \Pr(\text{no animal}) \\ \Pr(\text{cat}) \\ \Pr(\text{dog}) \\ \Pr(\text{bird}) \\ \Pr(\text{other animal}) \end{bmatrix}$$

Parameters:
b: vector of dimension 5
w: matrix 5 x 2,073,600

s: softmax function
$s : \mathbb{R}^5 \to (0,1)^5$ summing to 1

- In this presentation, we stick with regression
- Everything that follows generalises easily to classification and the equations remain essentially identical
- See literature for details, for example Stanford's CS229 on http://cs229.stanford.edu\syllabus.html

Linear regression: training

- Training set of *m* examples $x^{(1)},\ldots,x^{(m)}$ (each a vector in dimension *n*) with corresponding labels $y^{(1)},\ldots,y^{(m)} \in \mathbb{R}$
- Learn parameters: $b \in \mathbb{R}$ and $w \in \mathbb{R}^n$ by minimizing the cost function $C(b,w) = \sum_{i=1}^{m} \left(\underbrace{b + w^T x^{(i)}}_{=\hat{y}^{(i)}} - y^{(i)} \right)^2$
- Note that this is the same as maximizing (log) likelihood under Gaussian assumptions, hence:

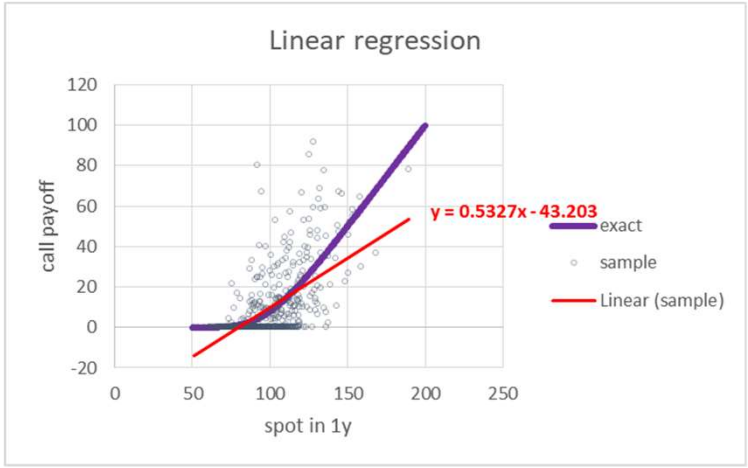
  $b^*, w^* = \arg\min C(b,w)$ are the maximum likelihood estimators (MLE) of the parameters

- *b** and *w** are found analytically, solving for $\frac{\partial C}{\partial b} = 0$ and $\frac{\partial C}{\partial w} = 0$
- Result ("normal equation"): $\begin{pmatrix} b \\ w_1 \\ w_2 \\ \ldots \\ w_n \end{pmatrix} = \left(X^T X\right)^{-1} X^T Y$ where $X = \begin{pmatrix} 1 & x_1^{(1)} & \ldots & x_n^{(1)} \\ 1 & x_1^{(2)} & \ldots & x_n^{(2)} \\ \ldots & x_1^{(i)} & x_j^{(i)} & x_n^{(i)} \\ 1 & x_1^{(m)} & \ldots & x_n^{(m)} \end{pmatrix}$

Lin reg only captures linear functions

- Example:
  - Predict the future price in 1y of a European call strike 100, maturity 2y
  - By regression of the payoff in 2y: $y^{(i)} = \left(S_{2y}{}^{(i)} - K\right)^{+}$
  - Over the underlying asset price in 1y: $x^{(i)} = S_{1y}{}^{(i)}$
  - With a training set of *m* paths $\left(S_{1y}{}^{(i)}, S_{2y}{}^{(i)}\right)_{1 \le i \le m}$

    generated under Black & Scholes' model (spot = 100, volatility of 20%)
  - We know the exact solution is given by Black and Scholes' formula so we can assess the quality of the regression

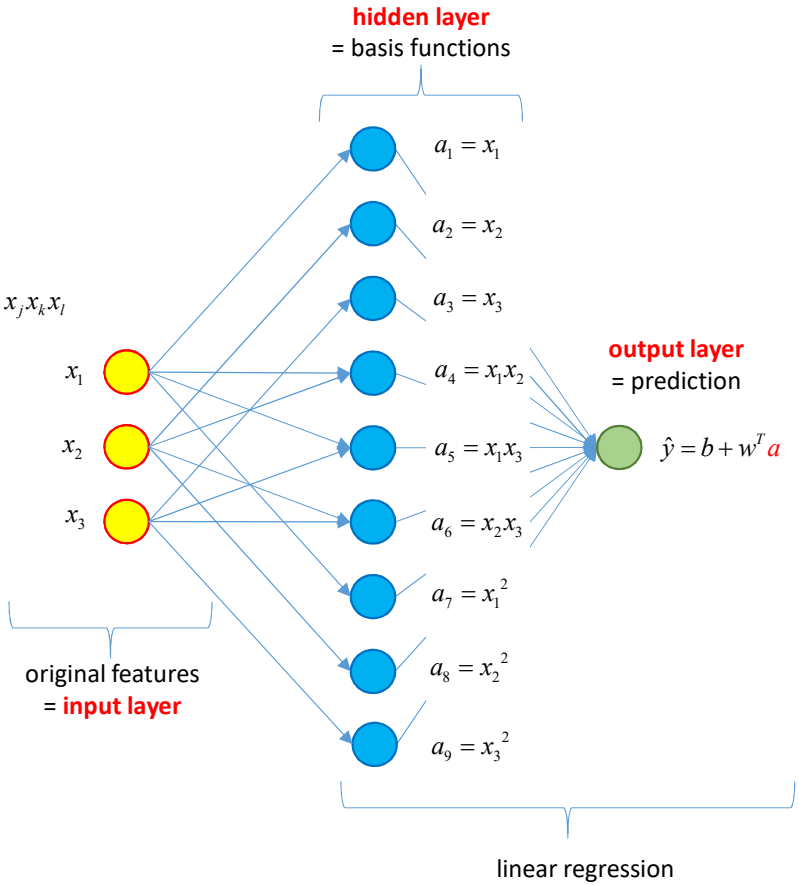


  - Linear regression obviously fails to approximate the correct function because it cannot capture non-linearities

Basis function regression

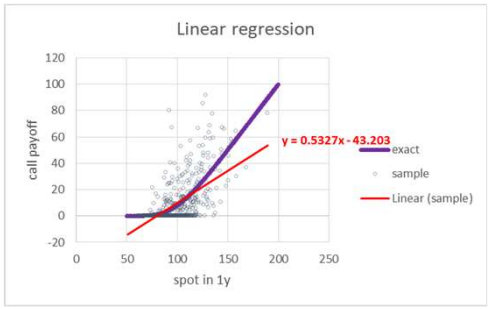
- Solution: regress not on *x* but on basis functions *a* of *x*
- Example: polynomial regression
  - Basis functions (*x* is in dimension n_0):
    - 1st degree: all the xs $a_i = x_i$
    - 2nd degree: all the squares $a_i = x_j^2$ and pair-wise products $a_i = x_i x_j$
    - 3rd degree: all the cubes $a_i = x_j^3$ and pair-wise $a_i = x_j x_k^2$ and triplet-wise $a_i = x_j x_k x_l$
    - Etc.
- Prediction in two steps:
  - Start with the vector *x* of n_0 features
  - Compute vector of n_1 basis functions: $a = \varphi(x)$
  - Predict linearly in the basis functions: $\hat{y} = b + w^T a$
- Training: identical to linear regression on *a* in place of *x*

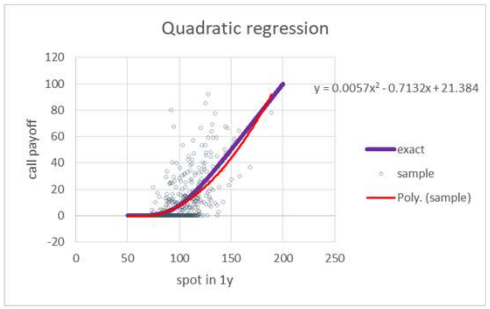
$$\begin{pmatrix} b \\ w_1 \\ w_2 \\ \dots \\ w_{n_1} \end{pmatrix} = \left(A^T A\right)^{-1} A^T Y \quad \text{where} \quad \mathrm{A} = \begin{pmatrix} 1 & a_1^{(1)} & \dots & a_{n_1}^{(1)} \\ 1 & a_1^{(2)} & \dots & a_{n_1}^{(2)} \\ \dots & a_1^{(i)} & a_j^{(i)} & a_{n_1}^{(i)} \\ 1 & a_1^{(m)} & \dots & a_{n_1}^{(m)} \end{pmatrix} \quad \text{and} \quad a^{(i)} = \varphi\left(x^{(i)}\right)$$



Basis function regression: performance

- Works nicely: quadratic regression of $\left(S_{T_2} - K\right)^+$ over S_{T_1} and S_{T_2} approximates Black & Scholes' formula well in simulated example





- Remarkable how the algorithm manages to detect Black & Scholes' pattern in noisy data

- Mathematically:
  - Combinations of polynomials can approximate any smooth function to arbitrary precision
  - Hence, detect any (smooth) non-linear pattern in data
  - *But only with a large number of basis functions / high polynomial degree*

Curse of dimensionality

- How many monomials in a *p*-degree polynomial regression?
  Number n_1 of basis functions (dimension of *a*) grows exponentially in number n_0 of features (dimension of *x*)

  Precisely: $n_1 = \frac{(n_0 + p)!}{n_0!\, p!} - 1$

- Quadratic regression: $n_1 = \frac{(n_0 + 2)(n_0 + 1)}{2} - 1$ dimension grows e.g. from 10 to 65, from 100 to 5,151, from 1,000 to 501,500
- Cubic regression: $n_1 = \frac{(n_0 + 3)(n_0 + 2)(n_0 + 1)}{6} - 1$ dim grows 10 to 286, 100 to 176,851, 1,000 to 167,668,501
- In general, number of basis functions increase exponentially in dimension
- "Rule of ten": to avoid overfitting small data set with many parameters, we need an amount of data (training examples) of approximately ***m > 10n***
- Hence, basis function regression requires amount of data exponential in (original) dimension *p*
- Basis function regression works nicely in low dimension but doesn't scale (think of image processing where *n0* = 1920 x 1080 > 2M)

Overfitting and the rule of ten

- If you fit a linear model with *n* free parameters to *n* data points
  - You will find a perfect fit
  - But the model may not generalize well to new examples
  - Because it captured the noise of the particular training set
  - This is called overfitting

- Solutions exist such as regularization
  See e.g. Stanford's Machine Learning class on Coursera
  Or Bishop's Pattern Recognition and Machine Learning

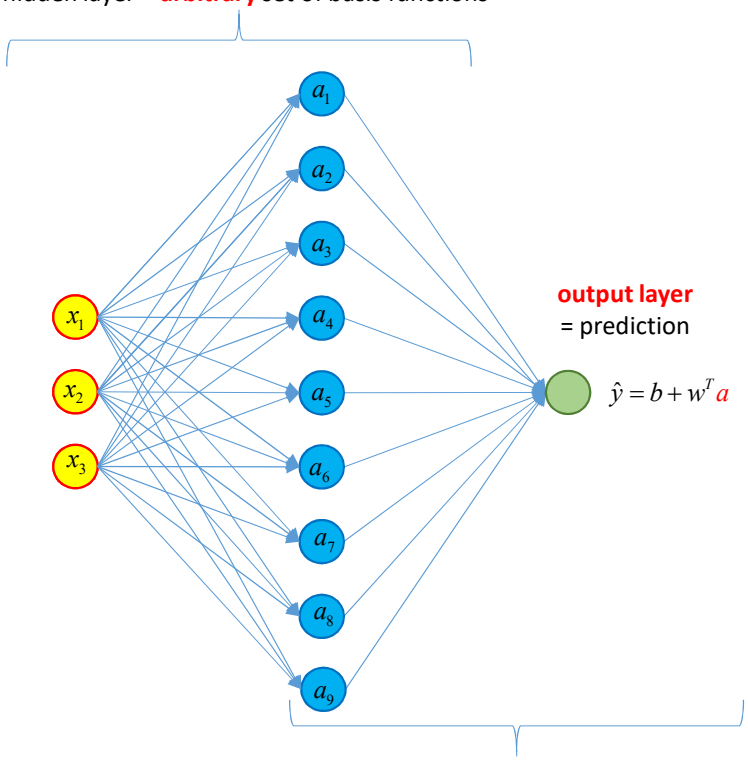
- But the most effective means to avoid overfitting is increase the size of the learning set

- An empirical rule of thumb called "rule of ten"
  recommends a data set of at least 10x the number of fitted parameters

Basis function regression vs ANN

BASIS FUNCTION REGRESSION

hidden layer = **arbitrary** set of basis functions

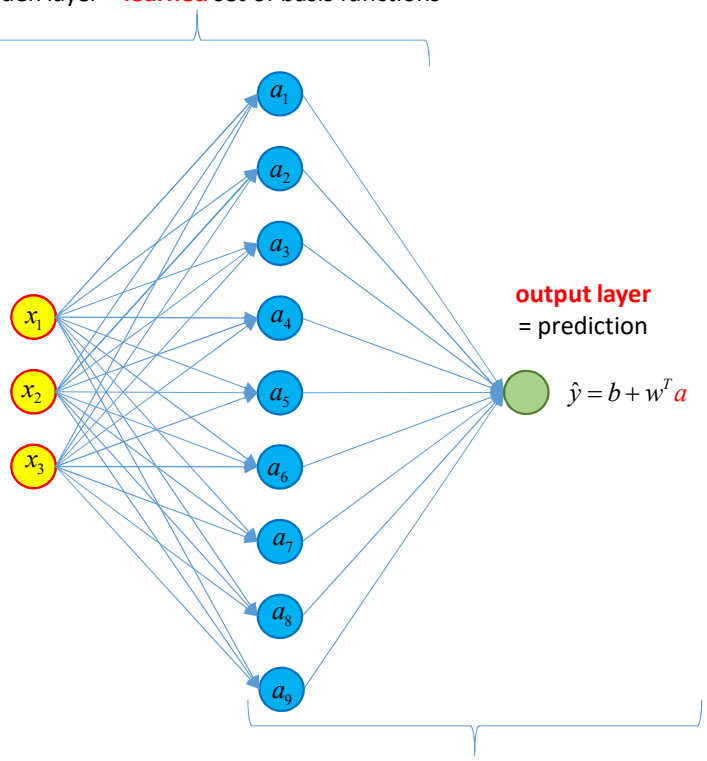


output layer
= prediction

linear regression over basis functions

ANN

hidden layer = **learned** set of basis functions



output layer
= prediction

linear regression over basis functions
identical

ANN basis functions

- How do we learn basis functions *a* from the data?
  - Parametric family of basis functions: $a_i = \varphi(x;\vartheta_i)$
  - Learn parameters ϑ (along with the weights *w* and bias *b* of regression) by minimization of the cost (e.g. sum of squared errors)
- Most common choice of parametric basis functions: "perceptron"
  - Each basis function is a non-linear scalar function *g* of a linear combination of xs (different for each basis function): $a_i = g\left(w^{[1]}{}_i^T x + b^{[1]}{}_i\right)$
  - Where each $w^{[1]}{}_i, 1 \le i \le n_1$ is a vector in dimension n_0 and each $b^{[1]}{}_i, 1 \le i \le n_1$ is a real number
  - Hence, $W^{[1]} = \begin{pmatrix} w^{[1]}{}_1^T \\ \dots \\ w^{[1]}{}_{n_1}^T \end{pmatrix}$ is a $n_1 \times n_0$ matrix and $b^{[1]} = \begin{pmatrix} b^{[1]}{}_1 \\ \dots \\ b^{[1]}{}_{n_1} \end{pmatrix}$ is a n_1 dimensional vector
  - Then the vector of basis functions $a = g\left(W^{[1]}x + b^{[1]}\right)$ where *g* is a scalar function applied element-wise to the n_1-vector $z = W^{[1]}x + b^{[1]}$

ANN: prediction

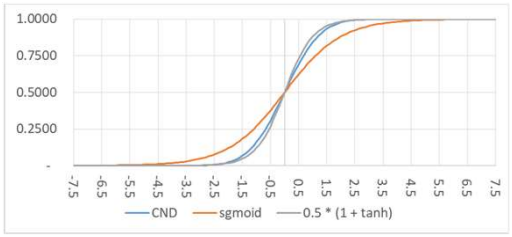
- Prediction in two steps
  - Step 1: hidden layer (basis functions) **inputs *x* → basis functions *a*** $a = g\left(W^{[1]}x + b^{[1]}\right)$
    - Parameters: $W^{[1]}$ matrix in dimension $n_1 \times n_0$ and $b^{[1]}$ vector in dimension n_1
    - The *activation* function *g* is scalar and applied element-wise on the n_1 vector $z^{[1]} = W^{[1]}x + b^{[1]}$
    - *g* must be non-linear or we are back to linear regression
      (linear regression on linear basis functions is identical to linear regression on inputs)
  - Step 2: regression **basis functions *a* → prediction** $\hat{y} = w^{[2]}a + b^{[2]}$
    - Parameters: $w^{[2]}$ column vector in dimension n_1 and $b^{[2]}$ real number
    - $\hat{y}$ is a real number
- Unified notation for both steps = feed-forward equation $a^{[l]} = g^{[l]}\left(W^{[l]}a^{[l-1]} + b^{[l]}\right)$
  - With the notations $a^{[0]} = x$ input layer dim n_0; $g^{[1]} = g, g^{[2]} = id$ hidden and output activations; $\hat{y} = a^{[2]}$ output layer dim $n_2 = 1$ and parameters $W^{[l]}$ of dim $n_l \times n_{l-1}$ and $b^{[l]}$ of dim n_l for $l = 1, 2$

Choice of activation function

- The hidden activation function $g^{[1]}$ must be non-linear – the most common choices are:
  - "Cheap Gaussians"

$$\textit{sigmoid} \quad \sigma(x) = \frac{1}{1+\exp(-x)}$$

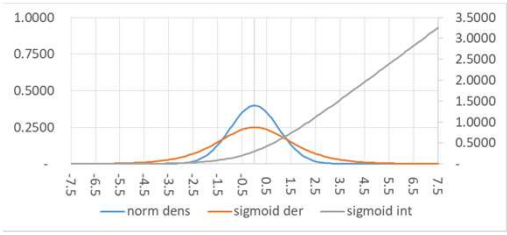
$$\tanh \quad t(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$$



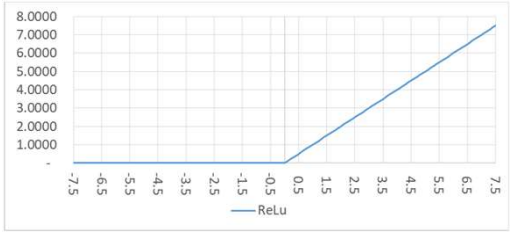
  - Derivatives and integrals of sigmoid

$$\sigma'(x) = \sigma(x)\left(1-\sigma(x)\right)$$

$$\int_{-\infty}^{x} \sigma(x) = \log\left(1+\exp(x)\right) \text{ ("softPlus")}$$

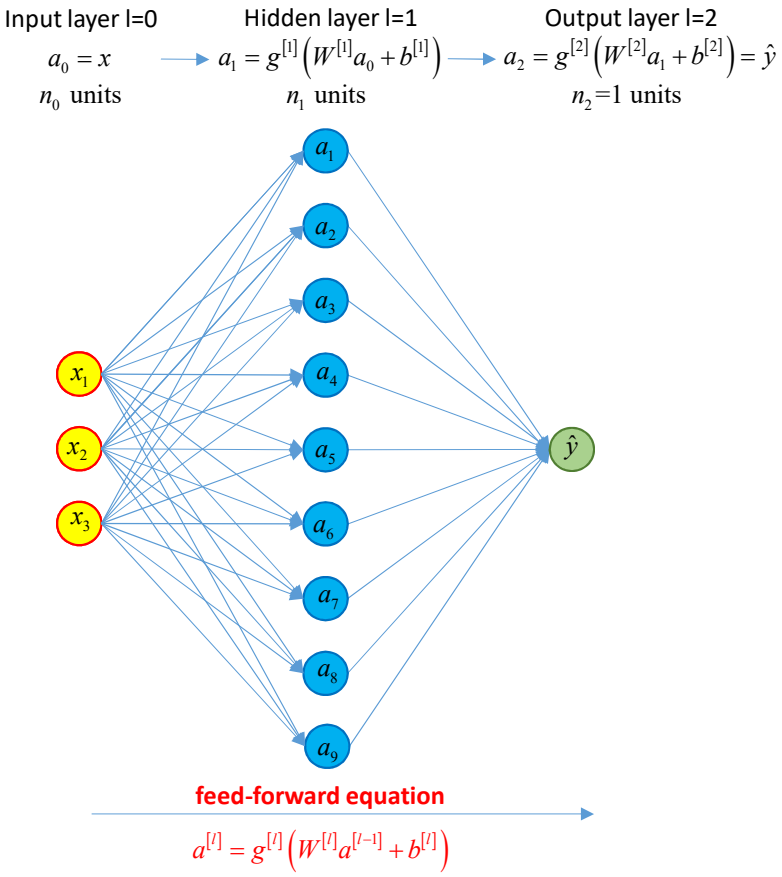


  - **Re**ctified **L**inear **U**nits (ReLu) $r(x) = (x)^{+}$



- The output activation function $g^{[2]}$ is:
  - Identity $g^{[2]}(x) = x$ for regression
  - SoftMax for classification

ANN: computation graph



Computation complexity (time)

To the leading order (ignoring activations and additions)

We have 2 matrix by vector products $\underbrace{W^{[1]}}_{n_1 \times n_0}\underbrace{a_0}_{n_0}$ and $\underbrace{W^{[2]}}_{n_2 \times n_1}\underbrace{a_1}_{n_1}$

Hence quadratic complexity $n_1 n_0 + n_2 n_1$

To simplify when all layers have *n* units, complexity ~$2n^2$

More generally, with *L* hidden layers, complexity ~Ln^2

Examples:

- With 1,000 features/basis functions and 2 layers
  complexity = 2M, fraction of a second on modern CPU
- With 1M features/basis functions and 100 layers
  (not unrealistic in computer vision)
  complexity = 200 trillion, many seconds even on best GPU

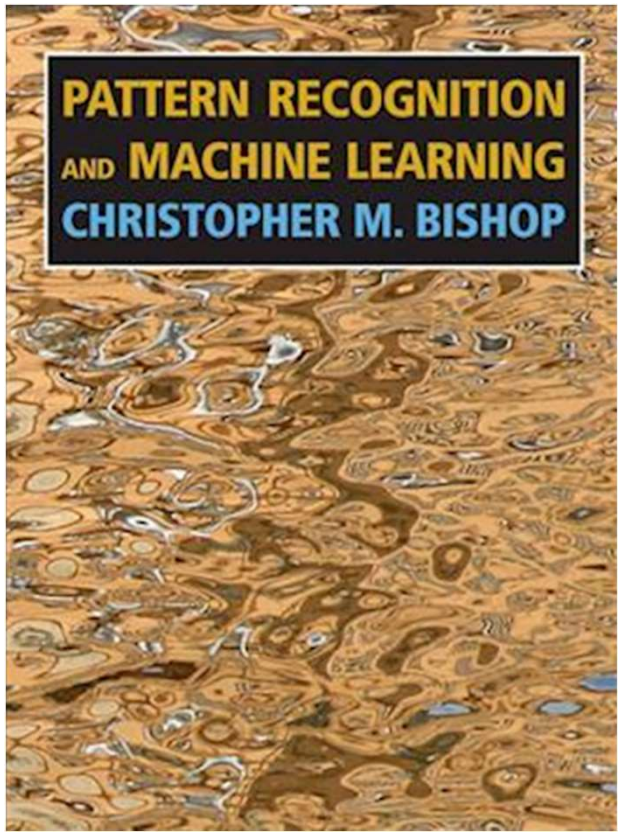
ANN: training

- Training set of *m* examples $x^{(1)},\ldots,x^{(m)}$ (each a vector in dimension n_0) with corresponding labels $y^{(1)},\ldots,y^{(m)} \in \mathbb{R}$
- Learn parameters: $b^{[1]} \in \mathbb{R}^{n_1}, b^{[2]} \in \mathbb{R}^{n_2=1}$ and $\mathrm{W}^{[1]} \in \mathbb{R}^{n_1 \times n_0}, W^{[2]} \in \mathbb{R}^{(n_2=1)\times n_1}$ that is $D = n_1 + n_2 + n_1 n_0 + n_2 n_1$ parameters
- By minimizing the cost function $C\left(b^{[1]}, b^{[2]}, W^{[1]}, W^{[2]}\right) = \sum_{i=1}^{m} c_i\left(b^{[1]}, b^{[2]}, W^{[1]}, W^{[2]}\right)$ with loss $c_i\left(b^{[1]}, b^{[2]}, W^{[1]}, W^{[2]}\right) = \left(\underbrace{a^{[2](i)}}_{=\hat{y}^{(i)}} - y^{(i)}\right)^2$
- No more analytic solution (*C* is not even convex in the *D* parameter space…)
- We must apply a numerical minimization algorithm
- Many iterative algorithms exist in literature and standard libraries
  - Gradient descent and variants
  - Pseudo-Newton methods based on an estimation of the hessian (second order derivatives) matrix
  - Levenberg and Marquard's algorithm
  - And many others, see **Numerical Recipes**
- Most algorithms (and all efficient ones) require differentials of cost function to all the parameters
- On each iteration, we must compute not only the cost function but also its *D* derivatives where we recall that $D \sim O(n_1 n_0)$

Universal representation theorem

- Polynomial regression offers mathematical guarantees
  - Combinations of monomials can approximate all smooth functions to arbitrary accuracy
  - Hence, polynomial regression can capture (with max degree *p* high enough) can capture any (smooth) relation in the data
  - (At the cost of a high number of basis functions and the requirement of ten times that much data)
- Similarly, feed-forward ANNs with "perceptron" basis functions offer mathematical guarantees
  - Known as Universal Representation Theorem
  - States that a feed-forward ANN may represent, and therefore capture, any smooth function
  - (Provided technical assumptions on activation functions, sigmoidal and variants all pass)
  - With a sufficient number of hidden units
- In conclusion
  - ANNs are superior to basis function regression in what they learn basis functions from the data
  - ANNs offer the same guarantees as basis function regression
  - But they lose analytic solution for training and require iterative cost minimization
  - Iterative minimization procedures require gradients (all differentials) of the cost function on every iteration
  - Therefore a quick computation of derivatives is key to training in reasonable time

More on regression, basis functions and ANNs



Deep learning: composing basis functions

- Shallow (one hidden layer) ANN:
  - Prediction is a linear combination of hidden layer activations: $\hat{y} = W^{[2]} a_1 + b^{[2]}$
  - Hidden layer activations are basis functions of the input layer: $a_1 = g^{[1]}\left(W^{[1]} x + b^{[1]}\right)$
  - So we linearly regress on (learnt) basis functions of inputs

- ANN with two hidden layers:
  - Prediction is a linear combination of the **second** hidden layer: $\hat{y} = W^{[3]} a_2 + b^{[3]}$
  - Second layer activations are basis functions of the first hidden layer: $a_2 = g^{[2]}\left(W^{[2]} a_1 + b^{[2]}\right)$
  - First hidden layer activations are basis functions of the input layer: $a_1 = g^{[1]}\left(W^{[1]} x + b^{[1]}\right)$
  - So we regress on **basis functions of basis functions**

- Deep ANN with L layers (L-1 hidden layers)
  - Prediction is a linear combination of the **last** hidden layer: $\hat{y} = W^{[L]} a_{L-1} + b^{[L]}$
  - Last hidden layer contains basis functions of basis functions of basis functions … of basis functions of the inputs from the feed-forward equation: $a_l = g^{[l]}\left(W^{[l]} a_{l-1} + b^{[l]}\right)$
  - So we regress on many **layers of composition** of basis functions $a_0 = x$

Why deep learning?

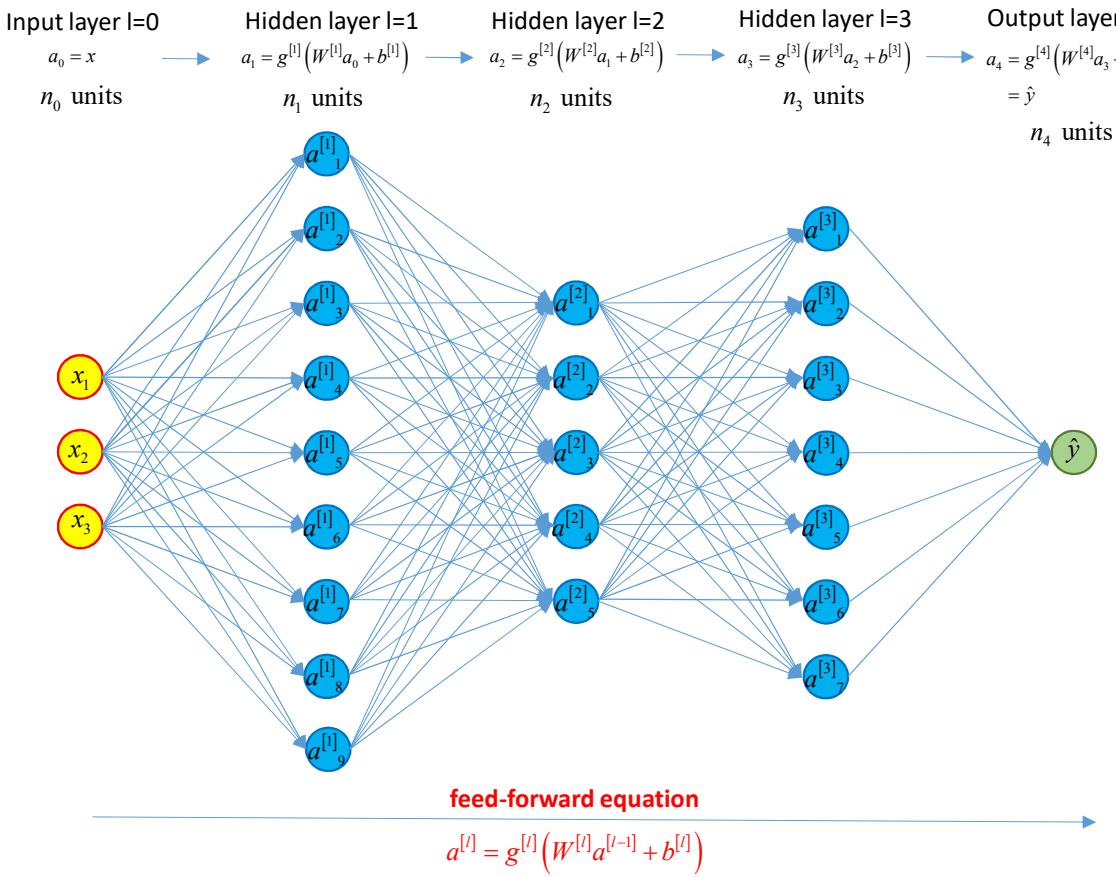
- We know from the Universal Representation Theorem that:
  - An ANN with a single hidden layer can approximate any (smooth) function given enough units
  - So what is the point of multiple layers?

- Composition of basis function offers (exponentially) better function representation abilities
  - With a limited number of units, a single layer ANN only correctly approximates a limited sub-space of functions
  - But if we allow basis functions to compose, we can represent an exponentially wider variety of functions
  - This result should be intuitive, it was demonstrated in particular cases and widely illustrated and empirically validated in a vast number of contexts
  - In short, 2 layers of 10 units each approximate a (much) wider sup-space of functions than 1 layer with 10 units

- This is the basis for deep learning

- Deep ANNs are otherwise a trivial generalization of shallow ANNs

Deep feed-forward networks



- Prediction: feed-forward equations

$$a_0 = x\ ,\ a^{[l]} = g^{[l]}\left(W^{[1]}a^{[l-1]} + b^{[1]}\right)\ ,\ y = a^{[L]}$$

- Parameters: $\text{for } 1 \le l \le L\ :\ \mathrm{W}^{[l]}\left(n_l \times n_{l-1}\right), b^{[l]}\left(n_l\right)$

- Number of parameters: $D = \sum_{l=1}^{L} n_l\left(1 + n_{l-1}\right)$

- Complexity $\sim D = \sum_{l=1}^{L} n_l n_{l-1}$

- Training: find all $\mathrm{W}^{[l]}$ and $b^{[l]}$ to minimise cost

$$C = \sum_{i=1}^{m} c_i\ ,\ c_i = \left(\hat{y}^{(i)} - y^{(i)}\right)^2$$

- Use iterative algorithms
  compute all D differentials on each iteration

- Key: quickly compute
  large number *D* of differentials

Back-Propagation in deep neural nets

Differentials of the cost function

- Mutli-layer perceptrons (MLPs) predict with the feed-forward equations:
  - Recall: $a_0 = x$, $a^{[l]} = g^{[l]}\left(W^{[l]}a^{[l-1]} + b^{[l]}\right)$, $y = a^{[L]}$
  - Parameters: $\text{for } 1 \le l \le L$: $\mathrm{W}^{[l]}\left(n_l \times n_{l-1}\right), b^{[l]}\left(n_l\right)$, $D = \sum_{l=1}^{L} n_l\left(1 + n_{l-1}\right) \sim Ln^2$ parameters
  - Cost: $C = \sum_{i=1}^{m} c_i$, $c_i = \left(\hat{y}^{(i)} - y^{(i)}\right)^2$
  - Must compute *D* differentials $\frac{\partial C}{\partial W^{[l]}_{i,j}}, \frac{\partial C}{\partial b^{[l]}_{i}}$ on each iteration
- Feed-forward complexity:
  - For a “reasonable” network with 10 layers of 100 units, D=100,000
  - To make one prediction: complexity ~ D ~ 100,000
  - We need at least m=10D training examples to avoid overfitting, so to compute one cost, complexity $> 10D^2 \sim 10^{11}$
  - With linear differentials algorithms, we compute the cost D times to calculate D differentials, complexity $> 10D^3 \sim 10^{16}$
  - Not viable, even on parallel on most powerful GPUs

Differentials by finite differences

- Finite difference (FD) algorithm:
  - First compute the cost C_0
  - To compute the sensitivity of the cost to each (scalar) parameter $P_d, 1 \le d \le D$:
    - Bump the parameter by a small amount ε
    - Re-compute the cost C_1 , repeating feed-forward equations for all training examples
    - $\partial C / \partial P_i \approx (C_1 - C_0) / \varepsilon$
- FD is (obviously) linear in *D*, therefore not viable
- But it has very desirable properties

FD and automatic differentiation

- Implementation is straightforward with little scope for error
- Importantly, FD differentiation is **automatic**
  - Developers only write prediction (feed-forward) code
  - FD computes differentials automatically by calling the feed-forward code repeatedly
  - Developers don't need to write any differentiation code
- More importantly, FD automatically **synchronises** with modifications to feed-forward code
  - Tricks of the trade (see e.g. Coursera's Deep Learning Spec) to train deep nets faster and better:
    - Regularization: add a regularization term to cost function
    - Dropout: randomly drop connections between units
    - Batch Norm: normalize the mean and variance on all layers
    - And many more
  - All these modify feed-forward equations and code, and affect differentials
  - With manual differentiation, developers must ensure consistency of evaluation and differentiation code
  - This is painful and prone to error
  - With automatic differentiation, differentiation always remains consistent with evaluation
- This being said, FD and other linear algorithms are not viable for training deep nets

Computing cost differentials

- First notice: $C = \sum_{i=1}^{m} c_i$ so $\frac{\partial C}{\partial -} = \sum_{i=1}^{m} \frac{\partial c_i}{\partial -}$
- Then: $c = (\hat{y} - y)^2 = \left(a^{[L]} - y\right)^2$ (dropping the example index *i* to simplify notations) so $\frac{\partial c}{\partial \hat{y}} = \frac{\partial c}{\partial a^{[L]}} = 2\left(a^{[L]} - y\right) = \text{"2 prediction errors"}$ (**eq1**)
- From the feed-forward equation: $a^{[l]} = g^{[l]}\left(\underbrace{W^{[l]} a^{[l-1]} + b^{[l]}}_{z^{[l]}}\right)$
  - We get the Jacobian matrix of $a^{[l]}$ to $a^{[l-1]}$ (**eq2**): $\underbrace{\frac{\partial a^{[l]}}{\partial a^{[l-1]}}}_{n_l \times n_{l-1}} = \frac{\partial a^{[l]}}{\partial z^{[l]}} \frac{\partial z^{[l]}}{\partial a^{[l-1]}} = \underbrace{diag\left[\underbrace{g^{[l]\prime}\left(z^{[l]}\right)}_{n_l \times 1}\right]}_{n_l \times n_l} \underbrace{W^{[l]}}_{n_l \times n_{l-1}}$
  - And from the chain rule we have **eq3**: $\frac{\partial c}{\partial W^{[l]}_{ij}} = \frac{\partial c}{\partial a^{[l]}_{i}} \frac{\partial a^{[l]}_{i}}{\partial W^{[l]}_{ij}} = \frac{\partial c}{\partial a^{[l]}_{i}} g^{[l]\prime}\left(z^{[l]}_{i}\right) a^{[l-1]}_{j}$ and $\frac{\partial c}{\partial b^{[l]}_{i}} = \frac{\partial c}{\partial a^{[l]}_{i}} \frac{\partial a^{[l]}_{i}}{\partial b^{[l]}_{i}} = \frac{\partial c}{\partial a^{[l]}_{i}} g^{[l]\prime}\left(z^{[l]}_{i}\right)$
- Don't worry too much about the equations or their derivation -- The take away here is:
  - **Eq 1 and 2 give us $\partial c / \partial a^{[L]}$ and all the Jacobians $\partial a^{[l]} / \partial a^{[l-1]}$ so we can recursively compute the $\partial c / \partial a^{[l]}$ for all layers *l***
  - **Eq 3 gives us the desired differentials to parameters $\partial c / \partial W^{[l]}_{ij}$ and $\partial c / \partial b^{[l]}_{i}$ from the $\partial c / \partial a^{[l]}$**

Differentials by forward Jacobian propagation

- We must compute $\frac{\partial c}{\partial a^{[l]}}$ for all layers *l*, then eq 3 gives us $\frac{\partial c}{\partial W^{[l]}_{ij}}$ and $\frac{\partial c}{\partial b^{[l]}_{i}}$
- Let us start with $\frac{\partial c}{\partial a^{[1]}}$
- We know all the $\frac{\partial a^{[l]}}{\partial a^{[l-1]}}$ from eq 2, so we have the Jacobian of $a^{[2]}$ to $a^{[1]}$: $\frac{\partial a^{[2]}}{\partial a^{[1]}}$
- Which we propagate forward one layer to get the Jacobian of $a^{[3]}$ to $a^{[1]}$: $\frac{\partial a^{[3]}}{\partial a^{[1]}} = \underbrace{\frac{\partial a^{[3]}}{\partial a^{[2]}}}_{\text{from eq 2}} \underbrace{\frac{\partial a^{[2]}}{\partial a^{[1]}}}_{\text{from previous step}}$
- We repeat, iterating towards layer *L*, computing the Jacobian $a^{[l]}$ to $a^{[1]}$: $\frac{\partial a^{[l]}}{\partial a^{[1]}} = \underbrace{\frac{\partial a^{[l]}}{\partial a^{[l-1]}}}_{\text{from eq 2}} \underbrace{\frac{\partial a^{[l-1]}}{\partial a^{[1]}}}_{\text{from previous step}}$
- Finally, we get the Jacobian of the output layer $a^{[L]}$ to $a^{[1]}$: $\frac{\partial a^{[L]}}{\partial a^{[1]}}$ and multiply it by $\frac{\partial c}{\partial a^{[L]}}$ (given by eq 1) to get the result: $\frac{\partial c}{\partial a^{[1]}} = \frac{\partial c}{\partial a^{[L]}} \frac{\partial a^{[L]}}{\partial a^{[1]}}$
- We followed the order of the feed-forward equations, propagating the Jacobians $a^{[l]}$ to $a^{[1]}$ forward through the network:

$$\frac{\partial a^{[2]}}{\partial a^{[1]}} \rightarrow \frac{\partial a^{[3]}}{\partial a^{[1]}} \rightarrow \frac{\partial a^{[4]}}{\partial a^{[1]}} \rightarrow \frac{\partial a^{[l]}}{\partial a^{[1]}} \rightarrow \frac{\partial a^{[L]}}{\partial a^{[1]}} \rightarrow \frac{\partial c}{\partial a^{[1]}}$$

Jacobian propagation: performance

- Cubic complexity
  - The Jacobians $\frac{\partial a^{[l]}}{\partial a^{[1]}}$ that we sequentially compute are matrices with dimension $n_l \times n_1$
  - The propagation equation $\frac{\partial a^{[l]}}{\partial a^{[1]}} = \frac{\partial a^{[l]}}{\partial a^{[l-1]}} \frac{\partial a^{[l-1]}}{\partial a^{[1]}}$ multiplies these Jacobians by $\frac{\partial a^{[l]}}{\partial a^{[l-1]}}$, which are matrices of dimension $n_l \times n_{l-1}$
  - So we repeatedly perform matrix products, of cubic complexity $n_l n_{l-1} n_1$
  - Besides, once we computed $\frac{\partial c}{\partial a^{[1]}}$, we must repeat the process for $\frac{\partial c}{\partial a^{[2]}}$, propagating Jacobians $a^{[l]}$ to $a^{[2]}$, and so on for all layers
- Reverse computation $\frac{\partial c}{\partial a^{[1]}} \leftarrow \frac{\partial c}{\partial a^{[2]}} \leftarrow \frac{\partial c}{\partial a^{[3]}} \overset{n_l}{\leftarrow} \frac{\partial c}{\partial a^{[1]}} \leftarrow \frac{\partial c}{\partial a^{[L-1]}} \leftarrow \frac{\partial c}{\partial a^{[L]}}$
  - Alternatively, note that $\frac{\partial c}{\partial a^{[l-1]}} = \frac{\partial c}{\partial a^{[l]}} \frac{\partial a^{[l]}}{\partial a^{[l-1]}}$ and we know $\frac{\partial c}{\partial a^{[L]}}$ from eq 1
  - So we can compute the $\frac{\partial c}{\partial a^{[l]}}$ in the **reverse** order, starting with layer *L* and ending with layer 1
  - Since the cost is scalar, $\frac{\partial c}{\partial a^{[l]}}$ is a **vector** of dimension n_l (not a matrix) called the **adjoint** of $a^{[l]}$

Adjoint propagation: performance

- Quadratic complexity
  - The adjoints $\frac{\partial c}{\partial a^{[l]}}$ that we sequentially compute in the reverse propagation are **vectors** of dimension n_l
  - The propagation equation $\frac{\partial c}{\partial a^{[l-1]}} = \frac{\partial c}{\partial a^{[l]}} \frac{\partial a^{[l]}}{\partial a^{[l-1]}}$ multiplies them by matrices of dimension $n_l \times n_{l-1}$, resulting in a vector of dimension n_{l-1}
  - So we repeatedly perform matrix by vector products, of quadratic complexity $n_l n_{l-1}$, one order of magnitude faster than Jacob. Prop.
- Constant time differentiation
  - In addition, we compute all the adjoints $\frac{\partial c}{\partial a^{[l]}}$ in one reverse sweep, from one another:
  - Notice, the overall complexity is $O\left(\sum_{l=1}^{L} n_l n_{l-1}\right)$, same as feed-forward prediction
  - As promised, we compute a large number *D* of differentials in a time similar to one evaluation
  - This procedure is called back-propagation, or simply back-prop in the context of deep learning
    In general, it is called (reverse) adjoint propagation (RAP) or simply adjoint differentiation (AD)

$$\frac{\partial c}{\partial a^{[1]}} = \underbrace{\underbrace{\underbrace{\underbrace{\frac{\partial c}{\partial a^{[L]}} \frac{\partial a^{[L]}}{\partial a^{[L-1]}}}_{\frac{\partial c}{\partial a^{[L-1]}}} \frac{\partial a^{[L-1]}}{\partial a^{[L-2]}}}_{\frac{\partial c}{\partial a^{[L-2]}}} \cdots \frac{\partial a^{[l]}}{\partial a^{[l-1]}}}_{\frac{\partial c}{\partial a^{[l-1]}}} \cdots \frac{\partial a^{[3]}}{\partial a^{[2]}}}_{\frac{\partial c}{\partial a^{[2]}}} \frac{\partial a^{[2]}}{\partial a^{[1]}}$$

Back-Propagation

- Reverse adjoint propagation
  - Computes all differentials of the cost to the many parameters in deep net in a time similar to one evaluation of the cost
  - Achieves this remarkable result by reversing the order of the calculations
  - Is the only viable means to train deep nets in reasonable time
  - Is the reason why deep learning achieved such spectacular success and why your phone quickly learns to recognise you
- However manual AD code is
  - Complicated and prone to error
  - Painful to maintain and synchronize as we modify feed-forwards code
- However manual AD code is
  - Next, we learn to automate AD
  - Since AD propagate adjoints in the reverse order through evaluation graphs
  - We will learn to automatically generate graphs
  - Not only for deep nets, but for any calculation
  - Including a large Monte-Carlo simulation

AD through evaluation graphs

Evaluation graphs and adjoint propagation

- Evaluation graph
  - We have seen evaluation graphs for neural nets
  - Evaluation graphs express the order and dependencies of “atomic” computations involved in a calculation
  - Any calculation defines an evaluation graph
  - To some extent, every calculation defines a sequence of feed-forward operations, similarly to a neural net
  - Chapter 9 of the AAD book teaches to build evaluation graphs in memory with operator overloading in C++

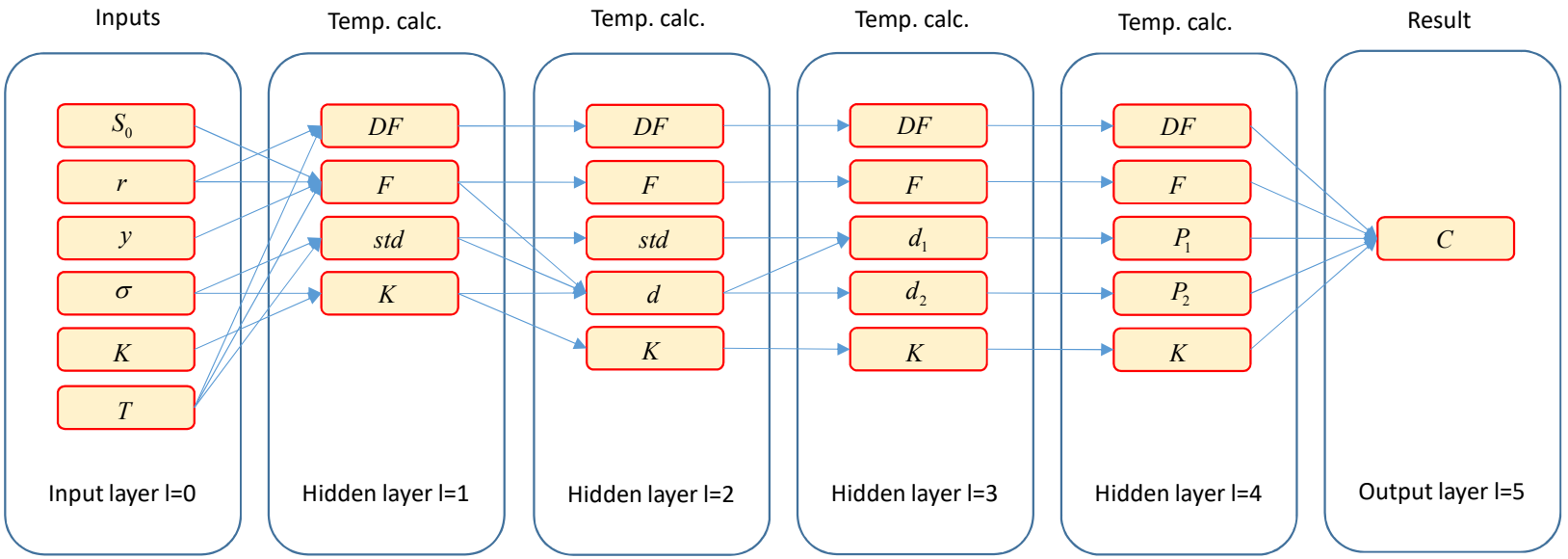
- Adjoint Differentiation
  - Is not limited to neural nets
  - Is applicable to any calculation
  - Propagates adjoints through the evaluation graph
  - Offers constant time efficiency (all differentials for an expense similar to one evaluation) for scalar calculations
  - A scalar calculation is one where the final result (output layer) is scalar

- Once we have an evaluation graph, AD may be automated

Example: Black & Scholes

- Black & Scholes' formula: $C(S_0, r, y, \sigma, K, T) = DF\left[FN(d_1) - KN(d_2)\right]$ with
  - Discount factor to maturity: $DF = \exp(-rT)$
  - Forward: $F = S_0 \exp\left[(r-y)T\right]$
  - Standard deviation: $std = \sigma\sqrt{T}$
  - Log-moneyness: $d = \dfrac{\log\left(\dfrac{F}{K}\right)}{std}$
  - D's: $d_1 = d + \dfrac{std}{2}$, $d_2 = d - \dfrac{std}{2}$
  - Probabilities to end in the money, resp. under spot and risk-neutral measures: $P_1 = N(d_1)$, $P_2 = N(d_2)$
  - Call price: $C = DF\left[FP_1 - KP_2\right]$

Black & Scholes: evaluation graph



$a^{[0]} = (S_0, r, y, \sigma, K, T)^T$

$n_0 = 6$

$a^{[1]} = (DF, F, std, K)^T$

$= g^{[1]}(a^{[0]})$

$n_1 = 4$

$a^{[2]} = (DF, F, std, d, K)^T$

$= g^{[2]}(a^{[1]})$

$n_2 = 5$

$a^{[3]} = (DF, F, d_1, d_2, K)^T$

$= g^{[3]}(a^{[2]})$

$n_3 = 5$

$a^{[4]} = (DF, F, P_1, P_2, K)^T$

$= g^{[4]}(a^{[3]})$

$n_4 = 5$

$a^{[5]} = C$

$= g^{[5]}(a^{[4]})$

$n_5 = 1$

Feed-forward equations

- As in deep nets, for **any** calculation, we have the feed-forward equation defining the evaluation graph:

inputs: $a^{[0]} = x$

feed-forward: $a^{[l]} = g^{[l]}\left(a^{[l-1]}\right)$

result: $\mathrm{y} = a^{[L]}$

- In Black & Scholes, we have

$$g^{[1]}(x) = \begin{pmatrix} \exp(-x_2 x_6) \\ x_1 \exp\left[(x_2 - x_3)x_6\right] \\ x_4\sqrt{x_6} \\ x_5 \end{pmatrix} \quad g^{[2]}(x) = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \log(x_2/x_4) \\ x_3 \\ x_4 \end{pmatrix} \quad g^{[3]}(x) = \begin{pmatrix} x_1 \\ x_2 \\ x_4 + \frac{x_3}{2} \\ x_4 - \frac{x_3}{2} \\ x_5 \end{pmatrix} \quad g^{[4]}(x) = \begin{pmatrix} x_1 \\ x_2 \\ N(x_3) \\ N(x_4) \\ x_5 \end{pmatrix} \quad g^{[5]}(x) = x_1(x_2 x_3 - x_5 x_4)$$

Differentiation equations

- For **any** calculation, where we compute the differentials of the result to the inputs: $\frac{\partial a^{[L]}}{\partial a^{[0]}}$
- If we split the calculation into small enough pieces, we can easily compute the Jacobians of activations: $g^{[l]\prime} = \frac{\partial a^{[l]}}{\partial a^{[l-1]}}$
- In Black & Scholes, we have, for instance

$$g^{[1]\prime}(x) = \begin{pmatrix} 0 & -x_6\exp(-x_2x_6) & 0 & 0 & 0 & -x_2\exp(-x_2x_6) \\ \exp\left[(x_2-x_3)x_6\right] & x_1x_6\exp\left[(x_2-x_3)x_6\right] & -x_1x_6\exp\left[(x_2-x_3)x_6\right] & 0 & 0 & x_1(x_2-x_3)\exp\left[(x_2-x_3)x_6\right] \\ 0 & 0 & 0 & \sqrt{x_6} & 0 & \frac{x_4}{2\sqrt{x_6}} \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad g^{[2]}(x) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & \frac{1}{x_2x_3} & -\frac{\log(x_2/x_4)}{x_3^2} & -\frac{1}{x_3x_4} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$g^{[3]}(x) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 1 & 0 \\ 0 & 0 & -\frac{1}{2} & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad g^{[4]\prime}(x) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & n(x_3) & 0 & 0 \\ 0 & 0 & 0 & n(x_4) & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad g^{[5]\prime}(x) = \left((x_2x_3 - x_5x_4), x_1x_3, x_1x_2, -x_1x_5, -x_1x_1x_4\right)$$

- Note that the Jacobian of the output layer is a vector, as with any scalar calculation

Forward and backward differentiation

- For **any** calculation, we have: $\frac{\partial a^{[L]}}{\partial a^{[0]}} = \frac{\partial a^{[L]}}{\partial a^{[L-1]}} \frac{\partial a^{[L-1]}}{\partial a^{[L-2]}} \cdots \frac{\partial a^{[l]}}{\partial a^{[l-1]}} \cdots \frac{\partial a^{[2]}}{\partial a^{[1]}} \frac{\partial a^{[1]}}{\partial a^{[0]}}$

- If we compute this product right to left:
  - We follow the order of the calculation
  - We propagate Jacobians to the inputs up from layer 2 to the output layer
  - We repeatedly multiply matrices, with cubic complexity

- If we compute this product left to right:
  - We follow the reverse order of the calculation
  - We propagate adjoints of the result down from layer *L-1* to the input layer
  - Provided the final result is scalar, we repeatedly multiply matrices by vectors, with quadratic complexity

- To Black & Scholes' Jacobians of the previous slide and find its well known derivatives (or "Greeks) is left as an exercise

Evaluation graphs: conclusion

- All calculations define a graph
- Like deep nets, evaluation graphs may be organized in successive layers function of one another: $a^{[l]} = g^{[l]}\left(a^{[l-1]}\right)$
- Once the evaluation graph is known down to elementary operations:
  - The Jacobians $g^{[l]\prime} = \frac{\partial a^{[l]}}{\partial a^{[l-1]}}$ are found trivially
  - Adjoint differentiation may be conducted an order of magnitude faster than Jacobian propagation (provided the calculation is scalar):

adjoint propagation, quadratic

$$\frac{\partial a^{[L]}}{\partial a^{[0]}} = \frac{\partial a^{[L]}}{\partial a^{[L-1]}} \frac{\partial a^{[L-1]}}{\partial a^{[L-2]}} \cdots \frac{\partial a^{[l]}}{\partial a^{[l-1]}} \cdots \frac{\partial a^{[2]}}{\partial a^{[1]}} \frac{\partial a^{[1]}}{\partial a^{[0]}}$$

Jacobian propagation, cubic

- Next, we show how evaluation graphs may be automatically generated

Recording calculations on tape

Automatic differentiation

- Finite Differences
  - Computes derivatives by running evaluation repeatedly
  - Only requires executable evaluation code
  - Linear complexity in the number of differentials
- AAD
  - Computes derivatives by running AD in reverse order over an evaluation graph
  - Requires a graph to traverse
  - Constant complexity in the number of differentials : fast differentiation of scalar code
  - To implement AAD we must extract an evaluation graph: sequence of calculations (nodes) and their dependencies (edges)

Building evaluation graphs

- Explicit evaluation graphs
  - Solution implemented in TensorFlow
  - Lets users explicitly build graphs by calling node/edge creation functions exported to many languages
  - Then call TensorFlow API to evaluate or differentiate the graphs efficiently: AD, parallel CPU, GPU
  - Smart and efficient
  - But forces developers to explicitly build charts in place of calculation code
  - (TensorFlow has a nice API that makes building graphs similar to coding calculations)
  - What we want here is take some calculation code and automatically extract its graph
- Source transformation
  - Code that reads and understand evaluation code, extracts graph and writes backward differentiation code automatically
  - Complex, specialized work similar to writing compilers
  - Variant: template meta-programming and introspection (introduced in chapter 15)

Operator overloading

- Alternative: operator overloading (in languages that support it like C++)
- When code applies operators (like + or *) or math functions (like log or sqrt) to real numbers (*double* type) the corresponding operations are evaluated immediately (or *eagerly*):

```
double x = 1, y = 2;      //  x and y are doubles
double z = x + y;         //  evaluates x + y and stores result in z
double t = log(x);        //  evaluates log(x) and stores result in t
```

- When the same operators are applied to **custom types** (our own type to store real numbers) developers decide what exactly is executed:

```
class myNumberType
{
    //  class definition here
};

myNumberType operator+(const myNumberType& lhs, const myNumberType& rhs)
{
    //  this code is executed anytime two numbers of type myNumberType are added
}

myNumberType log(const myNumberType& arg)
{
    //  this code is executed anytime log is called on a number of type myNumberType
}

myNumberType x, y;          //  x and y are of type myNumberType
myNumberType z = x + y;     //  executes code in operator+
myNumberType t = log(x);    //  executes code in log
```

Recording operations

- We apply operator overloading to **record** all operations on tape:

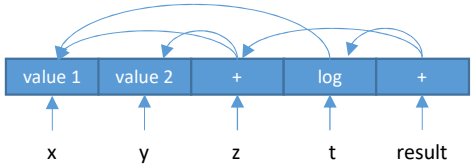
```
class myNumberType
{
    myNumberType(const double x)
    {
        //  constructor initilizes value to x and record node
    }
};

myNumberType operator+(const myNumberType& lhs, const myNumberType& rhs)
{
    recordAddition(lhs, rhs);   //  records addition with dependency on lhs and rhs
}

myNumberType log(const myNumberType& arg)
{
    recordLog(arg);             //  records log with dependency on arg
}

myNumberType x = 1, y = 2;      //  initializes x to 1 and y to 2 and records them
myNumberType z = x + y;         //  records addition
myNumberType t = log(x);        //  records log
myNumberType result = t + z;    //  records addition
```

Lazy evaluation

- When this code is executed:

```
myNumberType x = 1, y = 2;      //  initializes x to 1 and y to 2 and records them
myNumberType z = x + y;         //  records addition
myNumberType t = log(x);        //  records log
myNumberType result = t + z;    //  records addition
```

- Nothing is calculated, instead the following sequence is recorded in memory:



- This sequence can be evaluated later (*lazy evaluation*) or differentiated (applying AD from back to front)

- This is how we build the evaluation graph at run time, by executing calculation code with a custom type for which operators are overloaded to perform recording

Conventional implementation

- We introduce the conventional implementation of AAD
  - Where every math operation: +, -, *, /, pow, log, exp, sqrt, … is recorded on a data structure called **tape**
  - (It is really an evaluation graph but we call it tape in AAD lingo)

- Cutting-edge implementation records whole expressions
  - With template meta-programming and expression templates
  - Resulting in 2x to 5x faster code
  - Sometimes called “tape compression”
  - Extreme instance: “tapeless AD” where we don’t record anything!
  - All implemented in professional code on GitHub and explained in detail in chapter 15
  - In this presentation, we stick with conventional implementation

- We record every mathematical operation involved in a calculation
  - Every calculation, up to complex Monte-Carlo simulations, is a sequence of +, -, *, /, pow, log, exp, sqrt, … !
  - We record every single one
  - Note that all operations have either 0, 1 or 2 arguments

Simplistic implementation

- In this presentation, we focus on the simplicity of the code
  - We use basic C++ code and disregard efficiency, scalability and best practice
  - Our aim is to explain the key ideas with simplistic code
  - This code works, just not efficiently
- In the book, on the contrary, we build professional, scalable, efficient code in modern C++
- This is particularly important for AAD because of:
  - Recording overhead
    - Every addition, multiplication, etc. produces a record
    - Recording necessarily involves an overhead
    - An efficient implementation must minimize overhead and make recording as efficient as possible
  - Vast memory consumption
    - We store in memory all the operations involved in a large calculation, this is a very large number of records
    - Estimated RAM consumption around 5GB per second
    - Efficient memory and cache management are key to an efficient implementation
- An efficient implementation of AAD is given and explained in chapter 10
  - Effective, custom memory management
  - Recording with minimum overhead, cache efficiency and so on

Record and tape data structures

- A record
  - Stores one operation $y = f(x)$ where $f = +, *, -, /, \log, \sqrt{}, \ldots$
  - Knows the number of location of the 0, 1 or 2 arguments x_i
  - Stores the 0, 1 or 2 partial derivatives to its arguments $\partial f / \partial x_i$ so we can apply AD

- The tape stores the sequence of records

```
struct Record
{
    int     numArg;       //  number of arguments: 0, 1 or 2
    int     idx1;         //  index of first argument on tape
    int     idx2;         //  index of second argument on tape
    double  der1;         //  partial derivative to first argument
    double  der2;         //  partial derivative to second argument
};

//  The tape, declared as a global variable
vector<Record> tape;
```

Custom real number

- Our custom number
  - Stores its value and
  - Knows the index of the corresponding operation on tape
  - May be initialized with a value
    to create a record (without arguments) on tape

```
struct Number
{
    double  value;
    int     idx;

    //  default constructor does nothing
    Number() {}

    //  constructs with a value and record
    Number(const double& x) : value(x)
    {
        //  create a new record on tape
        tape.push_back(Record());
        Record& rec = tape.back();

        //  reference record on tape
        idx = tape.size() - 1;

        //  populate record on tape
        rec.numArg = 0;
    }
};
```

- We overload all mathematical operators and functions to:
  - Evaluate and store result as usual
  - Additionally, record the operation and its derivatives on tape
  - So code is evaluated and recorded at the same time

```
Number operator+(const Number& lhs, const Number&rhs)
{
    //  create a new record on tape
    tape.push_back(Record());
    Record& rec = tape.back();

    //  compute result
    Number result;
    result.value = lhs.value + rhs.value; //  calling double overload

    //  reference record on tape
    result.idx = tape.size() - 1;

    //  populate record on tape
    rec.numArg = 2;
    rec.idx1 = lhs.idx;
    rec.idx2 = rhs.idx;

    //  compute derivatives, both derivatives of addition are 1
    rec.der1 = 1;
    rec.der2 = 1;

    return result;
}
```

Operator overloading

- Similarly, we overload -, *, and /
- Same code exactly, only values and derivatives change

```
Number operator-(const Number& lhs, const Number&rhs)
{
 //  ...

 //  compute value
     result.value = lhs.value - rhs.value;

 //  ...

 //  compute derivatives
    rec.der1 = 1;
    rec.der2 = -1;

 //  ...
}
```

```
 Number operator*(const Number& lhs, const Number&rhs)
{
 //  ...

 //  compute value
     result.value = lhs.value * rhs.value;

 //  ...

 //  compute derivatives
    rec.der1 = rhs.value;
    rec.der2 = lhs.value;

 //  ...
}
```

```
 Number operator/(const Number& lhs, const Number&rhs)
{
 //  ...

 //  compute value
     result.value = lhs.value / rhs.value;

 //  ...

 //  compute derivatives
    rec.der1 = 1.0 / rhs.value;
    rec.der2 = - lhs.value / (rhs.value * rhs.value);
 //  ...
}
```

On-class operator overloading

- We must also overload +=, -=, *- and /=, as well as unary + and -, on class

The final Number class is therefore:

```
struct Number
{
    double  value;
    int     idx;

    //  default constructor does nothing
    Number() {}

    //  constructs with a value and record
    Number(const double& x) : value(x)
    {
        //  create a new record on tape
        tape.push_back(Record());
        Record& rec = tape.back();

        //  reference record on tape
        idx = tape.size() - 1;

        //  populate record on tape
        rec.numArg = 0;
    }

    Number operator +() const { return *this; }
    Number operator -() const { return Number(0.0) - *this; }

    Number& operator +=(const Number& rhs) { *this = *this + rhs; return *this; }
    Number& operator -=(const Number& rhs) { *this = *this - rhs; return *this; }
    Number& operator *=(const Number& rhs) { *this = *this * rhs; return *this; }
    Number& operator /=(const Number& rhs) { *this = *this / rhs; return *this; }
};
```

Function overloading

- Similarly, we overload log, exp, sqrt
- We should really overload all standard math functions
- Code is identical for all functions, only value and derivatives change

```
Number log(const Number& arg)
{
    //  create a new record on tape
    tape.push_back(Record());
    Record& rec = tape.back();

    //  compute result
    Number result;
    result.value = log(arg.value);

    //  reference record on tape
    result.idx = tape.size() - 1;

    //  populate record on tape
    rec.numArg = 1;
    rec.idx1 = arg.idx;

    //  compute derivative
    rec.der1 = 1.0 / arg.value;

    return result;
}
```

```
Number exp(const Number& arg)
{
    //  create a new record on tape
    tape.push_back(Record());
    Record& rec = tape.back();

    //  compute result
    Number result;
    result.value = exp(arg.value);

    //  reference record on tape
    result.idx = tape.size() - 1;

    //  populate record on tape
    rec.numArg = 1;
    rec.idx1 = arg.idx;

    //  compute derivative
    rec.der1 = result.value;

    return result;
}
```

```
Number sqrt(const Number& arg)
{
    //  create a new record on tape
    tape.push_back(Record());
    Record& rec = tape.back();

    //  compute result
    Number result;
    result.value = sqrt(arg.value); //  calling double overload

    //  reference record on tape
    result.idx = tape.size() - 1;

    //  populate record on tape
    rec.numArg = 1;
    rec.idx1 = arg.idx;

    //  compute derivative
    rec.der1 = 0.5 / result.value;

    return result;
}
```

Custom function overloading

- Also overload building blocks that are not standard to C++ but frequently applied in applications
- In financial application, we use cumulative normal distributions and normal densities all the time
- The functions are defined in the file gaussians.h in the repo
- We overload here (once again, only change is in value and derivatives):

```
Number normalDens(const Number& arg)
{
    //  create a new record on tape
    tape.push_back(Record());
    Record& rec = tape.back();

    //  compute result
    Number result;
    result.value = normalDens(arg.value);

    //  reference record on tape
    result.idx = tape.size() - 1;

    //  populate record on tape
    rec.numArg = 1;
    rec.idx1 = arg.idx;

    //  compute derivative
    rec.der1 = - result.value * arg.value;

    return result;
}
```

```
Number normalCdf(const Number& arg)
{
    //  create a new record on tape
    tape.push_back(Record());
    Record& rec = tape.back();

    //  compute result
    Number result;
    result.value = normalCdf(arg.value); //  calling double overload in gaussians.h

    //  reference record on tape
    result.idx = tape.size() - 1;

    //  populate record on tape
    rec.numArg = 1;
    rec.idx1 = arg.idx;

    //  compute derivative
    rec.der1 = normalDens(arg.value);

    return result;
}
```

Avoiding code duplication

- The code for all binary operators and for all unary function is identical
- Only values and derivatives are different
- This is poor design:
  If we change something in the logic, we must consistently modify many different functions
- In the professional code of chapters 10 and 15
  we structure code and apply “policy design” (Alexandresku, 2001) to avoid duplication without overhead
- Here, we stick with duplicated code

Comparison operator overloading

- Our custom number must do everything a double does
- In particular, we must be able to compare two Numbers
- Hence, to complete our simple framework, we must also overload comparison operators:

```
bool operator==(const Number& lhs, const Number& rhs) { return lhs.value == rhs.value; }
bool operator!=(const Number& lhs, const Number& rhs) { return lhs.value != rhs.value; }
bool operator>(const Number& lhs, const Number& rhs) { return lhs.value > rhs.value; }
bool operator>=(const Number& lhs, const Number& rhs) { return lhs.value >= rhs.value; }
bool operator<(const Number& lhs, const Number& rhs) { return lhs.value < rhs.value; }
bool operator<=(const Number& lhs, const Number& rhs) { return lhs.value <= rhs.value; }
```

Applying the recording framework

- Our simple recording framework is complete, the complete code in the repo, file toyCode.h
- We may use it to record calculations
- Example: Black and Scholes

```
inline double blackScholes(
    //  input layer 0
    const double spot, const double rate, const double yield, const double vol, const double strike, const double mat)
{
/* layer 1 */        double df = exp(-rate * mat), fwd = spot * exp((rate - yield) * mat), std = vol * sqrt(mat);
/* layer 2 */        double d = log(fwd / strike) / std;
/* layer 3 */        double d1 = d + 0.5 * std, d2 = d - 0.5 * std;
/* layer 4 */        double p1 = normalCdf(d1), p2 = normalCdf(d2);
/* output layer 5 */ return df * (fwd * p1 - strike * p2);
}
```

Instrumenting computation code

- To record a Black & Scholes calculation, we must call it with our number type
- This is called *instrumentation*
- We can replace all doubles by Numbers:

```
inline Number blackScholes(
    //  input layer 0
    const Number spot, const Number rate, const Number yield, const Number vol, const Number strike, const Number mat)
{
/* layer 1 */        Number df = exp(-rate * mat), fwd = spot * exp((rate - yield) * mat), std = vol * sqrt(mat);
/* layer 2 */        Number d = log(fwd / strike) / std;
/* layer 3 */        Number d1 = d + 0.5 * std, d2 = d - 0.5 * std;
/* layer 4 */        Number p1 = normalCdf(d1), p2 = normalCdf(d2);
/* output layer 5 */ return df * (fwd * p1 - strike * p2);
}
```

Instrumenting computation code

- Better solution: template code on number representation type

```
template <class T> inline T blackScholes(
    //  input layer 0
    const T spot, const T rate, const T yield, const T vol, const T strike, const T mat)
{
/* layer 1 */        T df = exp(-rate * mat), fwd = spot * exp((rate - yield) * mat), std = vol * sqrt(mat);
/* layer 2 */        T d = log(fwd / strike) / std;
/* layer 3 */        T d1 = d + 0.5 * std, d2 = d - 0.5 * std;
/* layer 4 */        T p1 = normalCdf(d1), p2 = normalCdf(d2);
/* output layer 5 */ return df * (fwd * p1 - strike * p2);
}
```

- Best practice: produce templated code in the first place

- To evaluate and record code, call with Numbers as arguments:

AAD

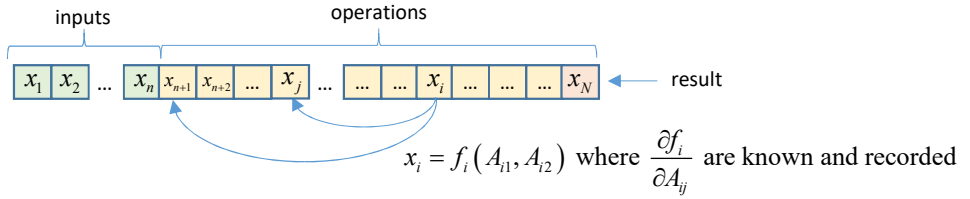
State of the tape after recording

- We call the instrumented instance of our code:

```
Number spot = 100, rate = 0.02, yield = 0.05, vol = 0.2, strike = 110, mat = 2; // initializes and records inputs
auto result = blackScholes(spot, rate, yield, vol, strike, mat);                // evaluates and records operations
cout << result.value;   //  5.03705
```

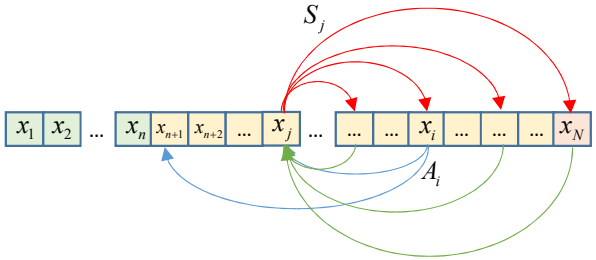
- Which evaluates the calculation and records all operations on tape
  - Denote f_i the operation number i, this is a function of 0, 1 or 2 arguments
  - The arguments must also be on tape, with indices < i
  - Denote A_i the set of indices of the arguments to f_i - this is a set of 0, 1 or 2 indices, all < i
  - Denote *n* the number of inputs and *N* the number of operations on tape, including inputs
  - Denote x_i the result of operation i and $y = x_N$ the final result
  - Note that all the local derivatives $\frac{\partial f_i}{\partial x_j}$ for all $j \in A_i$ have been computed and recorded on tape during evaluation

- Our tape therefore looks like:



Successors and adjoints

- Successors
  - Denote S_j the set of indices of the successors of x_j on tape
  - This is the indices *i* of all functions f_i , calculated **after** x_j that use x_j as an argument
  - Formally: $S_j = \{i > j, j \in A_i\}$
  - Note that S_i may contain many indices
  - Whereas an empty S_i reveals an unused input or intermediate result



- Adjoints
  - Denote $\bar{x}_i \equiv \frac{\partial y}{\partial x_i} = \frac{\partial x_N}{\partial x_i}$ the adjoint of x_i
  - Then (evidently): $\bar{x}_N = 1$
  - And in a direct application of the chain rule: $\bar{x}_j = \sum_{i \in S_j} \frac{\partial f_i}{\partial x_j} \bar{x}_i$ because $\frac{\partial y}{\partial x_j} = \sum_{i \in S_j} \frac{\partial y}{\partial x_i} \frac{\partial x_i}{\partial x_j}$ and we recall that all the $\frac{\partial x_i}{\partial x_j}$ are on tape

Adjoint propagation

- Adjoints therefore satisfy a backward recursion
  - The last adjoint $\bar{x}_N = 1$ is given
  - All other adjoints are a function of future adjoints: for all j $\bar{x}_j = f\left(\bar{x}_i, i \in S_j, i > j\right)$
- Therefore the following algorithm is guaranteed to correctly accumulate all adjoints
  - Initialize all adjoints to 0 and the last adjoint to 1 (this is called *seeding* the tape): $\bar{x}_j = \delta_{N-j}$
  - Repeat for *i* iterating backwards from *N* to *0:* $\text{for all } j \in A_i : \bar{x}_j \leftarrow \bar{x}_j + \frac{\partial f_i}{\partial x_j}\bar{x}_i$
  - The differentials of the calculation to its inputs $x_1, x_2, \ldots, x_n$ are, by definition, $\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n$
- This algorithm is called (reverse) adjoint propagation
- AAD is the sum of a recording framework and adjoint propagation

Complexity

- One *evaluation* of the calculation
  - Sweeps forward through the sequence of its operations
  - Executes every operation exactly once
  - Therefore its complexity is *N*, the number of records that end up on tape

- Adjoint propagation
  - Also sweeps through the sequence of operations, backward
  - Executes 0, 1 or 2 operations on every record, depending on the number of arguments
  - Therefore, as advertised, AAD computes **all n** differentials in **constant time**
  - In theory, all differentials are propagated in less than 2x one evaluation
  - In addition, the calculation must evaluated (and recorded) first so the theoretical upper bound is 3x one evaluation
  - Due to recording and tape traversal overhead, a good implementation generally produces many differentials in 4x to 10x

- Our professional code from chapters 10, 12 and 15 beat the theoretical bound!
  - Remember from the demonstration, one evaluation = 0.8sec, 1,081 differentials = 1.5sec, less than 2x one evaluation
  - Due to “selective instrumentation”, a strong optimization, explained, along many others, in chapter 12

Adjoint propagation code

- After we record a tape by calling the instrumented instance of our code:

```
Number spot = 100, rate = 0.02, yield = 0.05, vol = 0.2, strike = 110, mat = 2; // initializes and records inputs
auto result = blackScholes(spot, rate, yield, vol, strike, mat);               // evaluates and records operations
cout << result.value;   //  5.03705
```

- We proceed with adjoint propagation:

```
//  initialization
vector<double> adjoints(tape.size(), 0.0);  //  initialize all to 0
int N = result.idx;                         //  find N
adjoints[N] = 1.0;                          //  seed aN = 1

//  backward propagation
for(int j=N; j>0; --j)  //  iterate backwards over tape
{
    if (tape[j].numArg > 0)
    {
        adjoints[tape[j].idx1] += adjoints[j] * tape[j].der1;       //  propagate first argument

        if (tape[j].numArg > 1)
        {
            adjoints[tape[j].idx2] += adjoints[j] * tape[j].der2;   //  propagate second argument
        }
    }
}

//  show derivatives
cout << "Derivative to spot (delta) = " << adjoints[spot.idx] << endl;          //  0.309
cout << "Derivative to rate (rho) = " << adjoints[rate.idx] << endl;            //  51.772
cout << "Derivative to dividend yield = " << adjoints[yield.idx] << endl;       //  -61.846
cout << "Derivative to volatility (vega) = " << adjoints[vol.idx] << endl;      //  46.980
cout << "Derivative to strike (-digital) = " << adjoints[strike.idx] << endl;   //  -0.235
cout << "Derivative to maturity (-theta) = " << adjoints[mat.idx] << endl;      //  1.321
```

- The code works nicely and produces correct values
- Not very interesting for Black & Scholes
  - Fast, analytic evaluation
  - Only 6 differentials to compute
- Next, we apply AAD to a barrier option in

Conclusion

- We implemented AAD in the simplest possible manner, scratching the surface of possibilities
- Part III (Chapters 8 to 15) gives the details of a complete, professional, efficient implementation
  - How to minimize recording overhead
  - Efficient memory management constructs
  - Apply check-pointed AAD to differentiate a calculation piece by piece to mitigate RAM footprint and cache inefficiency
  - Efficiently differentiate non-scalar calculations that return multiple results
  - Cutting-edge implementation with template meta-programming and expression templates, faster by 2x to 5x
  - Parallel implementation
  - Advise for debugging and optimization
  - And much more
- Still the simplistic code works and produces the correct values
- Not very interesting for Black & Scholes
  - Fast, analytic evaluation
  - Only 6 differentials to compute
- Next, we apply the framework to a barrier option in Dupire Monte-Carlo
  - Long, complex evaluation
  - 1,081 differentials to compute

AAD for financial simulations

Simple simulation code

- We implement a simplistic simulation code for a barrier option in Dupire's model
  - Recall local volatility is given in a matrix and bi-linearly interpolated in spot and time
- We need the following pieces, which we assume are given here
  - A matrix class to hold local volatilities (matrix.h in the repo, chapters 1 and 2 in the book)
  - A bi-linear interpolation function (interp.h in the repo, chapter 6, section 6.4 in the book)
  - Random number generators to produce independent Gaussian increments (chapters 5 and 6)
- The code is templated on the real number representation type

Simulation code, version 1

```
//  Signature

template <class T>
inline T toyDupireBarrierMc(
    //  Spot
    const T            S0,
    //  Local volatility
    const vector<T>    spots,
    const vector<T>    times,
    const matrix<T>    vols,
    //  Product parameters
    const T            maturity,
    const T            strike,
    const T            barrier,
    //  Number of paths and time steps
    const int          Np,
    const int          Nt,
    //  Initialized random number generator
    RNG&               random)
```

```
//  implementation

//  Initialize
T result = 0;
// double because the RNG is not templated (and doesn't need to be, see chapter 12)
vector<double> gaussianIncrements(Nt);
const T dt = maturity / Nt, sdt = sqrt(dt);

//  Loop over paths
for (int i = 0; i < Np; ++i)
{
    //  Generate Nt Gaussian Numbers
    random.nextG(gaussianIncrements);
    //  Euler's scheme, step by step
    T spot = S0, time = 0;
    bool alive = true;
    for (size_t j = 0; j < Nt; ++j)
    {
        //  Interpolate volatility
        const T vol = interp2D(spots, times, vols, spot, time);
        time += dt;
        //  Simulate return
        spot *= exp(-0.5 * vol * vol * dt + vol * sdt * gaussianIncrements[j]);
        //  Monitor barrier
        if (spot > barrier)
        {
            alive = false;
            break;
        }
    }
    //  Payoff
    if (alive && spot > strike) result += spot - strike;
}   //  paths

return result / Np;
```

A simplistic code

- This code “does the job” but is not acceptable by professional standards

- The code is specific to Dupire’s model and an up & out call, therefore not scalable
  - To price another product (Asian option, Ratchet option, …) copy the code and change the lines that evaluate payoffs
  - To price in another model (Heston, …) copy the code and change the lines that generate the scenarios
  - End up with many different functions implementing the same simulation logic for different couples of models and products
  - To modify the simulation logic, consistently change all the function! This is obviously not viable

- Chapter 6 teaches a professional architecture for generic simulation libraries
  - Encapsulate scenario generation in Model objects
  - Encapsulate payoff evaluation in Product objects
  - Encapsulate simulation logic in a generic Monte-Carlo engine
  - Code every model and every product exactly once, mix and match at run time

- We stick with the simplistic code for demonstration purposes

An inefficient code

- The code does too much work repeatedly during simulations
  - Key to efficient Monte-Carlo code:
    Do as much work as possible once, on initialization, and as little as possible repeatedly, during simulations
  - Example: we perform an expensive bi-linear interpolation in the innermost loop, for every path, on every time step
  - We interpolate in spot and time, spot is stochastic (scenario dependent), time is not
  - Therefore we can (and should) pre-interpolate in time on initialization
    And perform only 1D interpolations in the innermost loop
- Chapter 6 teaches and builds fully optimized code

- The code is serial, it executes sequentially on one core
  - Since even phones are multi-core today, professional code is always parallel
  - With Monte-Carlo simulations, it is relatively easy to obtain a speed-up by the number of physical cores
- Chapter 3 teaches modern parallel C++, chapter 7 builds a professional *parallel* simulation library
  And section 12.5 instruments it with AAD in parallel

- For the purpose of demonstration, we stick with the not so efficient, serial version

Smoothing barrier options

- Discretely monitored barrier options are discontinuous, their value jumps to 0 at the barrier
  - Therefore, our code is not differentiable
  - AAD does not help: it cannot perform the impossible task of differentiating a discontinuous functions
  - With finite differences, barrier risks are unstable, with AAD they are all zero
  - Find the reason why as an exercise!

- Therefore traders always smooth discontinuous transactions (barriers, digitals etc.)
- Smoothing = applying a close, continuous approximation in place of the discontinuous function

- Smoothing in finance, and its connection to fuzzy logic, are explained in the presentation:

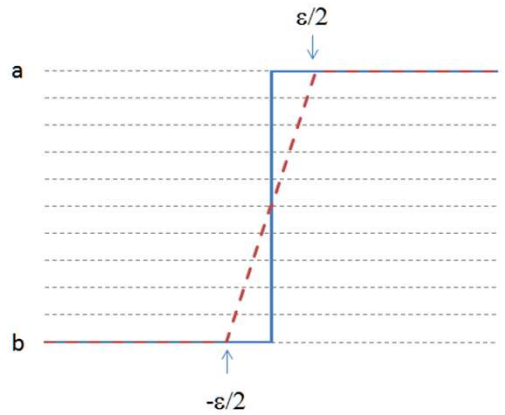
  http://www.slideshare.net\AntoineSavine\stabilise-risks-of-discontinuous-payoffs-with-fuzzy-logic

Freely available on slideShare

- Here, we briefly explain the “smooth barrier” algorithm, universally applied on derivatives desks

Smooth barrier

- Hard barrier
  - 100% dead above the barrier, 100% alive below the barrier
  - Hence, discontinuous



- Soft barrier
  - 100% dead above the barrier **plus epsilon**, 100% alive below the barrier **minus epsilon**
  - In between, lose a fraction of notional interpolated between (barrier-epsilon,0) and (barrier+epsilon,1)
  - And continue with the remaining notional
  - Hence, continuous

- Smoothing and fuzzy logic
  - Like Schrodinger's cat, the transaction is in a superposition of dead and alive states
  - Smoothing is achieved by replacing sharp logic (dead or alive?) by fuzzy logic (how much alive?)
  - More in the presentation

Simulation code with smooth barrier

```
template <class T>
inline T toyDupireBarrierMc(
    //  Spot
    const T            S0,
    //  Local volatility
    const vector<T>    spots,
    const vector<T>    times,
    const matrix<T>    vols,
    //  Product parameters
    const T            maturity,
    const T            strike,
    const T            barrier,
    //  Number of paths and time steps
    const int          Np,
    const int          Nt,
    //  Smoothing
    const T            epsilon,
    //  initialized random number generator
    RNG&               random)
```

```
//  Initialize
T result = 0;
// double because the RNG is not templated (and doesn't need to be, see chapter 12)
vector<double> gaussianIncrements(Nt);
const T dt = maturity / Nt, sdt = sqrt(dt);

//  Loop over paths
for (int i = 0; i < Np; ++i)
{
    //  Generate Nt Gaussian Numbers
    random.nextG(gaussianIncrements);
    //  Step by step
    T spot = S0, time = 0;
    /*  bool alive = true; */ T alive = 1.0; // alive is a real number in (0,1)
    for (size_t j = 0; j < Nt; ++j)
    {
        //  Interpolate volatility
        const T vol = interp2D(spots, times, vols, spot, time);
        time += dt;
        //  Simulate return
        spot *= exp(-0.5 * vol * vol * dt + vol * sdt * gaussianIncrements[j]);
        //  Monitor barrier
        /* if (spot > barrier) { alive = false; break; } */
        if (spot > barrier + epsilon) { alive = 0.0; break; }       //   definitely dead
        else if (spot < barrier - epsilon) { /* do nothing */ };    //   definitely alive
        else /* in between, interpolate */ alive *= 1.0 - (spot - barrier + epsilon) / (2 * epsilon);

    }
    //  Payoff paid on surviving notional
    /* if (alive && spot > strike) result += spot - strike; */ if (spot > strike) result += alive * (spot - strike);
}   //  paths
return result / Np;
```

Simulation code

- The toy simulation code is found on the file ToyCode.h in the repo
- To be compared with professional code in the files with names prefixed by “mc”
- Our simple code returns the same result as the professional code
- It is twice slower than the serial version of the professional code
- On a quad-code computer, it is 8x slower than the parallel version
- Next, we differentiate it with our simple AAD framework

Differentiation steps

Just like we did for Black & Scholes, to compute differentials, we:

1. Initialize the inputs as Numbers, which records them on tape

2. Call our templated evaluation code, instantiated with the Number type
   Which performs the evaluation *and* records operations on tape

3. Propagate adjoints backwards through the tape

4. Pick differentials as the adjoints of the parameters

Differentiation code

Just like we did for Black & Scholes, to compute differentials, we:

1. Initialize the inputs as Numbers
   Which also records them on tape

2. Call our templated evaluation code, instantiated with the Number type
   Which performs the evaluation *and* records operations on tape

3. Propagate adjoints backwards through the tape

4. Pick differentials as the adjoints of the parameters

Initialization

```
void toyDupireBarrierMcRisks(
const double S0, const vector<double> spots, const vector<double> times, const matrix<double> vols,
const double maturity, const double strike, const double barrier,
const int Np, const int Nt, const double epsilon, RNG& random,
/* results: value and dV/dS, dV/d(local vols) */ double& price, double& delta, matrix<double>& vegas)
{

//  1. Initialize inputs

ToyNumber nS0(S0), nMaturity(maturity), nStrike(strike), nBarrier(barrier), nEpsilon(epsilon);
vector<ToyNumber> nSpots(spots.size()), nTimes(times.size());
matrix<ToyNumber> nVols(vols.rows(), vols.cols());

for (int i = 0; i < spots.size(); ++i) nSpots[i] = ToyNumber(spots[i]);
for (int i = 0; i < times.size(); ++i) nTimes[i] = ToyNumber(times[i]);
for (int i = 0; i < vols.rows(); ++i) for (int j = 0; j < vols.cols(); ++j) nVols[i][j] = ToyNumber(vols[i][j]);
```

Record evaluation, propagate adjoints

```
//  2. Call instrumented evaluation code, which evaluates the barrier option price and records all operations

ToyNumber nPrice = toyDupireBarrierMc(nS0, nSpots, nTimes, nVols, nMaturity, nStrike, nBarrier, Np, Nt, nEpsilon, random);

//  3. Adjoint propagation, the exact same code as before, should be encapsulated in a dedicated function

//  initialization
vector<double> adjoints(tape.size(), 0.0);  //  initialize all to 0
int N = nPrice.idx;                         //  find N
adjoints[N] = 1.0;                          //  seed aN = 1

//  backward propagation
for (int j = N; j > 0; --j)  //  iterate backwards over tape
{
    if (tape[j].numArg > 0)
    {
        adjoints[tape[j].idx1] += adjoints[j] * tape[j].der1;       //  propagate first argument

        if (tape[j].numArg > 1)
        {
            adjoints[tape[j].idx2] += adjoints[j] * tape[j].der2;   //  propagate second argument
        }
    }
}
```

Pick and return results

```
    //  4. Pick results

    price = nPrice.value;
    delta = adjoints[nS0.idx];
    for (int i = 0; i < vols.rows(); ++i) for (int j = 0; j < vols.cols(); ++j) vegas[i][j] = adjoints[nVols[i][j].idx];
}
```

Testing the code

- We run the code in the same context as the initial demonstration but with 100,000 paths instead of 500,000
- The computer runs out of memory and crashes!
- Running AAD on a simulation with 100,000 paths consumes an insane amount of RAM
- Even on a computer with enough memory, such large tape is cache inefficient

Solution in principle

- Run a series of risks on mini-batches of say, 1024 paths and average in the end
- Wipe the tape in between mini-batches
- The average of differentials is the differential of the average
- So we get the same results while reducing memory footprint to operations recorded over 1,024 paths
- Note with mini-batches of size 1, this is known as “path-wise differentiation”
- This is also a particular, and simple case of the general check-pointing algorithm explained in chapter 13

Solution in code

- Rename our function DupureRisksMiniBatch(), call it sequentially from a wrapper function

```
void toyDupireBarrierMcRisks(
    const double S0, const vector<double> spots, const vector<double> times, const matrix<double> vols,
    const double maturity, const double strike, const double barrier,
    const int Np, const int Nt, const double epsilon, RNG& random,
    /* results: value and dV/dS, dV/d(local vols) */ double& price, double& delta, matrix<double>& vegas)
{
    price = delta = 0;
    for (int i = 0; i < vegas.rows(); ++i) for (int j = 0; j < vegas.cols(); ++j) vegas[i][j] = 0;
    double batchPrice, batchDelta; matrix<double> batchVegas(vegas.rows(), vegas.cols());
    int pathsToGo = Np, pathsPerBatch = 1024;
    //  calculate btach sensitivities sequentially
    while (pathsToGo > 0)
    {
        //  wipe tape
        tape.clear();

        //  do mini batch
        int paths = min(pathsToGo, pathsPerBatch);
        dupireRisksMiniBatch(S0, spots, times, vols, maturity, strike, barrier, paths, Nt, epsilon, random, batchPrice, batchDelta, batchVegas);

        //  update results
        price += batchPrice * paths / Np;
        delta += batchDelta * paths / Np;
        for (int i = 0; i < vegas.rows(); ++i) for (int j = 0; j < vegas.cols(); ++j) vegas[i][j] += batchVegas[i][j] * paths / Np;

        pathsToGo -= paths;
    }
}
```

Performance

- With 100,000 paths, 156 steps, we compute the 1,081 differentials in around 7 seconds
- This is 1,081 differentials in the time of around 6 evaluations
- This is a very remarkable result, especially with such simplistic code
- Try it yourself with the code in the repo!
- This being said, the professional code is around 8 times faster in serial mode,
  32 times faster in parallel mode on a quad-core laptop

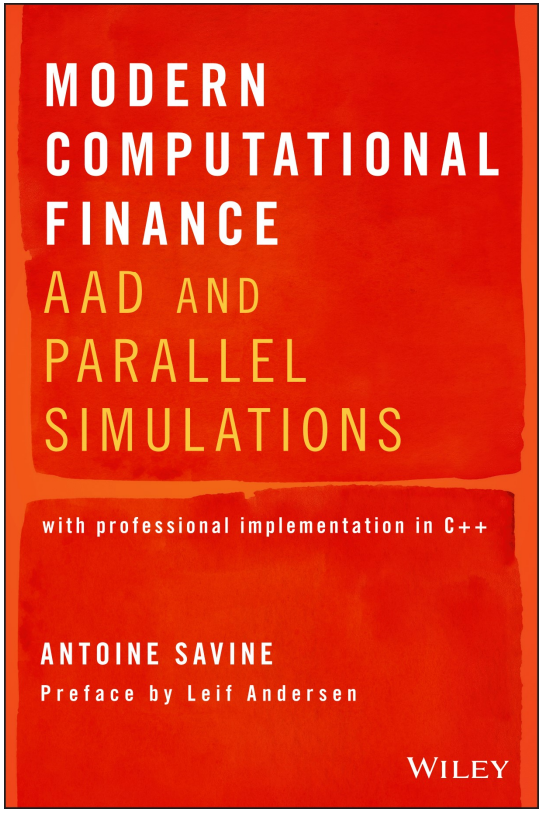
Conclusion

- We learned AAD in principle and in code
  And applied it to machine learning and finance

- But we really just scratched the surface

- For example:
  - How to efficiently differentiate the multiple results of non-scalar functions?
  - How to compute risks not on model parameters like local volatilities
    But on tradable market variables like implied volatilities?
  - How to implement AAD in modern C++ and manage memory efficiently?
  - How to implement AAD over parallel simulations and run it at least 32x faster?

- The answers, and much more, are in the book



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Thank you for your attention.

The slides are available on http://antoinesavine.com/lectures

The code is available on http://www.github.com/asavine/CompFinance/wiki , follow the repo to get update notifications

The book is available on http://www.amazon.com/author/antoinesavine