Deep Learning (CS324)

2. Mathematical background*

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Linear algebra

THIS IS YOUR MACHINE LEARNING SYSTEM?

YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.

WHAT IF THE ANSWERS ARE WRONG?



Scalars and vectors

- A scalar is a single number
- Integers, real numbers, rational numbers, etc.
- We denote it with italic font: a, n, x
- A vector is a 1-D array of numbers:

$$oldsymbol{x} = \left[egin{array}{c} x_1 \ x_2 \ dots \ x_n \end{array}
ight]$$

Matrices and tensors

• A matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ is a 2-D array of numbers

$$\left[egin{array}{cc} A_{1,1} & A_{1,2} \ A_{2,1} & A_{2,2} \end{array}
ight]$$

- A tensor is an array of numbers, that may have
 - zero dimensions, and be a scalar
 - one dimension, and be a vector
 - two dimensions, and be a matrix
 - or more dimensions.

Matrix transpose

$$(\boldsymbol{A}^{\top})_{i,j} = A_{j,i}.$$

$$(\boldsymbol{A}\boldsymbol{B})^{ op} = \boldsymbol{B}^{ op} \boldsymbol{A}^{ op}$$

$$oldsymbol{A} = egin{bmatrix} A_{1,1} & A_{1,2} \ A_{2,1} & A_{2,2} \ A_{3,1} & A_{3,2} \end{bmatrix} \Rightarrow oldsymbol{A}^ op = \left[egin{array}{ccc} A_{1,1} & A_{2,1} & A_{3,1} \ A_{1,2} & A_{2,2} & A_{3,2} \end{array}
ight]$$

Figure 2.1: The transpose of the matrix can be thought of as a mirror image across the main diagonal.

Matrix addition and subtraction

• We can add or subtract two matrices \mathbf{A} and \mathbf{B} only if these have the same size, and the result (for addition) is a matrix $\mathbf{C} = \mathbf{A} + \mathbf{B}$ with elements $c_{ij} = a_{ij} + b_{ij}$ for each $1 \le i \le m$ and $1 \le j \le n$

$$\mathbf{A} + \mathbf{B} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} + \begin{bmatrix} -1 & 2 \\ 4 & -8 \\ -16 & 32 \end{bmatrix} = \begin{bmatrix} 0 & 4 \\ 7 & -4 \\ -11 & 38 \end{bmatrix} = \mathbf{C}$$

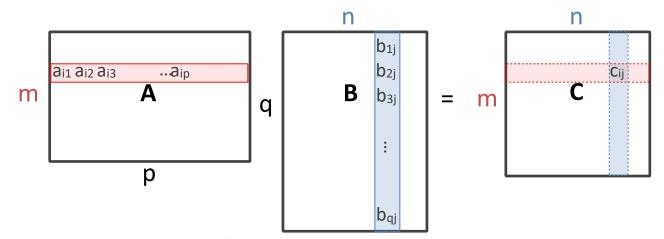
Scalar multiplication

 The multiplication of a matrix by a scalar t produces as a result a matrix of the same size whose entries are each multiplied by t

$$\mathbf{B} = t\mathbf{A} = t \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} = \begin{bmatrix} 1t & 2t \\ 3t & 3t \\ 5t & 6t \end{bmatrix} = \mathbf{C}$$

Matrix multiplication

• Let **A** be a m by p matrix and **B** a q by n matrix: the product **AB** is defined only when p = q



The elements of C are

$$c_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj} = a_{i1} b_{ij} + a_{i2} b_{2j} + \dots + a_{ip} b_{pj}$$

Identity matrix

 The identity matrix is the diagonal matrix with ones on the diagonal and zero everywhere else

$$\left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right]$$

Figure 2.2: Example identity matrix: This is I_3 .

If A is m x n then

$$\mathbf{AI}_n = \mathbf{A} \quad \mathbf{I}_m \mathbf{A} = \mathbf{A}$$

Trace of a matrix

 The trace of a matrix is equal to then sum of its diagonal elements

$$\operatorname{Tr}(oldsymbol{A}) = \sum_i oldsymbol{A}_{i,i}$$

$$\operatorname{Tr}(\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}) = \operatorname{Tr}(\boldsymbol{C}\boldsymbol{A}\boldsymbol{B}) = \operatorname{Tr}(\boldsymbol{B}\boldsymbol{C}\boldsymbol{A})$$

Linear systems of equations

- A linear system of equations Ax = b can have:
 - No solution
 - Many solutions
 - Exactly one solution: if A is invertible

$$\boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}_n$$

Linear systems of equations

- A linear system of equations Ax = b can have:
 - No solution
 - Many solutions
 - Exactly one solution: if A is invertible

$$oldsymbol{A}oldsymbol{x} = oldsymbol{b}$$
 $oldsymbol{A}^{-1}oldsymbol{A}oldsymbol{x} = oldsymbol{A}^{-1}oldsymbol{b}$ $oldsymbol{I}_noldsymbol{x} = oldsymbol{A}^{-1}oldsymbol{b}$

Linear systems of equations

- A linear system of equations Ax = b can have:
 - No solution
 - Many solutions
 - Exactly one solution: if A is invertible
 - Matrix can't be inverted if...
 - More rows/columns than columns/rows
 - Redundant rows/columns ("linearly dependent", "low rank")

Norms

- Functions that measure how "large" a vector is
- Similar to a distance between zero and the point represented by the vector

- $\bullet \ f(\boldsymbol{x}) = 0 \Rightarrow \boldsymbol{x} = \boldsymbol{0}$
- $f(x + y) \le f(x) + f(y)$ (the triangle inequality)
- $\forall \alpha \in \mathbb{R}, f(\alpha \boldsymbol{x}) = |\alpha| f(\boldsymbol{x})$

Norms

• L_p norms

$$||oldsymbol{x}||_p = \left(\sum_i |x_i|^p
ight)^{rac{1}{p}}$$

- Most popular norm: L₂ norm
- *L*₁ norm:

$$||\boldsymbol{x}||_1 = \sum_i |x_i|$$

Max norm, infinite p:

$$||\boldsymbol{x}||_{\infty} = \max_{i} |x_{i}|$$

Special vectors and matrices

• Unit vector:

$$||x||_2 = 1$$

Symmetric Matrix:

$$oldsymbol{A} = oldsymbol{A}^{ op}$$

Orthogonal matrix:

$$oldsymbol{A}^ op oldsymbol{A} = oldsymbol{A} oldsymbol{A}^ op = oldsymbol{I}$$
 $oldsymbol{A}^{-1} = oldsymbol{A}^ op$

Matrix eigendecomposition

Eigenvector and eigenvalue of a square matrix A

$$Av = \lambda v$$

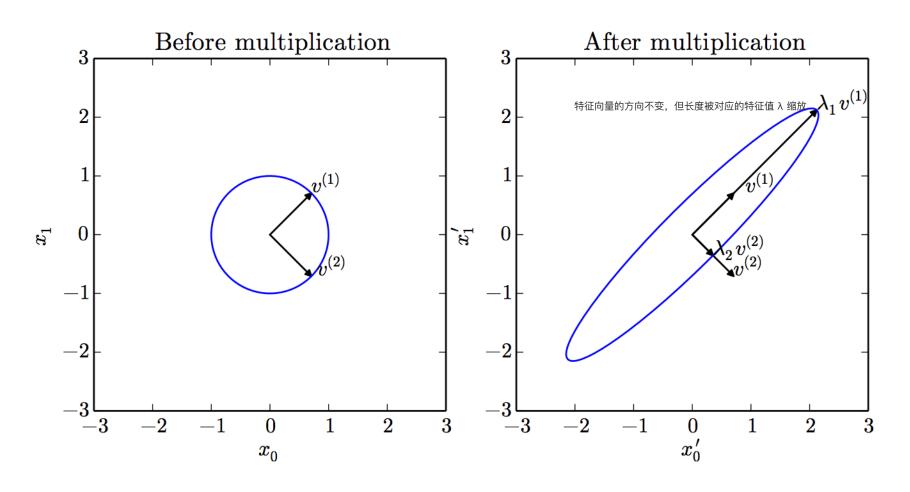
Eigendecomposition of a diagonalisable matrix

$$\mathbf{A} = \mathbf{V} \operatorname{diag}(\boldsymbol{\lambda}) \mathbf{V}^{-1}$$

Every real symmetric matrix has a real, orthogonal eigendecomposition

$$oldsymbol{A} = oldsymbol{Q} oldsymbol{\Lambda} oldsymbol{Q}^{ op}$$

Eigenvalues interpretation



What if the matrix A is not square?

$$oldsymbol{A} = oldsymbol{U}oldsymbol{D}oldsymbol{V}^{ op}$$

What if the matrix A is not square?

$$A = UDV^{\top}$$

 $m \times m$ orthogonal matrix (left-singular vectors - eigenvectors of $\mathbf{A}\mathbf{A}^{\mathsf{T}}$)

More general; matrix need not be square

What if the matrix A is not square?

$$A = UDV$$

 $n \times n$ orthogonal matrix (right-singular vectors - eigenvectors of A^TA)

More general; matrix need not be square

What if the matrix A is not square?

$$A = UDV^{\top}$$

 $m \times n$ diagonal matrix (singular values - square roots of eigenvalues of A^TA)

More general; matrix need not be square

What if the matrix A is not square?

$$oldsymbol{A} = oldsymbol{U}oldsymbol{D}oldsymbol{V}^{ op}$$

SVD 的一个重要应用是计算 Moore-Penrose 伪逆

- More general; matrix need not be square
- Allows to compute Moore-Penrose pseudoinverse

$$oldsymbol{A}^+ = oldsymbol{V} oldsymbol{D}^+ oldsymbol{U}^ op$$

What if the matrix A is not square?

$$oldsymbol{A} = oldsymbol{U} oldsymbol{D} oldsymbol{V}^ op$$

- More general; matrix need not be square
- Allows to compute Moore-Penrose pseudoinverse

$$oldsymbol{A}^+ = oldsymbol{V} oldsymbol{D}^+ oldsymbol{U}^ op$$

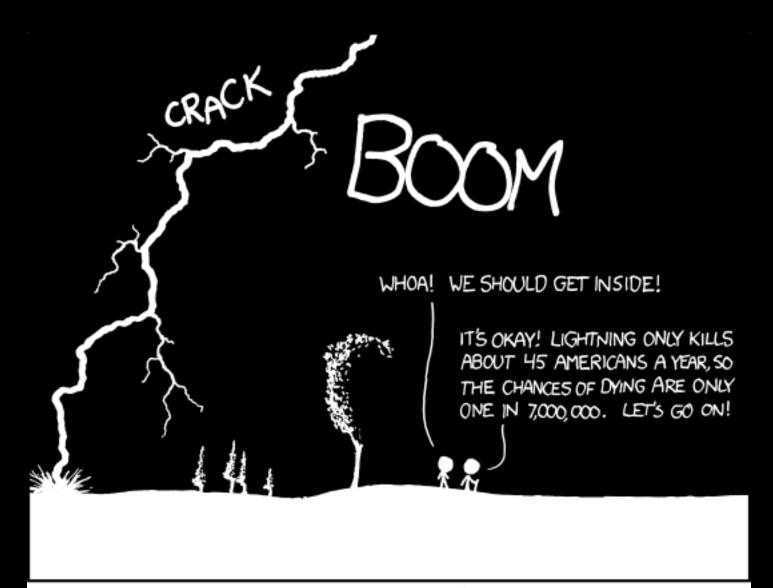
Reciprocal of nonzero elements of **D** and then transpose

What if the matrix A is not square?

$$oldsymbol{A} = oldsymbol{U}oldsymbol{D}oldsymbol{V}^{ op}$$

- More general; matrix need not be square
- Allows to compute Moore-Penrose pseudoinverse
- If ${f A}$ has more rows than cols ${m x}={m A}^+{m y}^-$ gives solution with min $||{m A}{m x}-{m y}||_2$.

Probability & information theory



THE ANNUAL DEATH RATE AMONG PEOPLE WHO KNOW THAT STATISTIC IS ONE IN SIX.

Probability mass function

- The domain of P must be the set of all possible states of x.
- $\forall x \in x, 0 \le P(x) \le 1$. An impossible event has probability 0 and no state can be less probable than that. Likewise, an event that is guaranteed to happen has probability 1, and no state can have a greater chance of occurring.
- $\sum_{x \in \mathbf{x}} P(x) = 1$. We refer to this property as being **normalized**. Without this property, we could obtain probabilities greater than one by computing the probability of one of many events occurring.

$$P(\mathbf{x} = x_i) = \frac{1}{k}$$

Example: uniform distribution

Probability density function

- The domain of p must be the set of all possible states of x.
- $\forall x \in \mathbf{x}, p(x) \geq 0$. Note that we do not require $p(x) \leq 1$.
- $\bullet \int p(x)dx = 1.$

$$u(x;a,b) = \frac{1}{b-a}$$
.

Example: uniform distribution

A few important rules...

Marginal probabilities (discrete and continuous)

$$\forall x \in \mathbf{x}, P(\mathbf{x} = x) = \sum_{y} P(\mathbf{x} = x, \mathbf{y} = y)$$
 $p(x) = \int p(x, y) dy$

Conditional probability

$$P(y = y \mid x = x) = \frac{P(y = y, x = x)}{P(x = x)}$$

Chain rule

$$P(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}) = P(\mathbf{x}^{(1)}) \prod_{i=2}^{n} P(\mathbf{x}^{(i)} \mid \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(i-1)})$$

A few important rules...

Independence

$$\forall x \in x, y \in y, \ p(x = x, y = y) = p(x = x)p(y = y)$$

Conditional independence

$$\forall x \in x, y \in y, z \in z, \ p(x = x, y = y \mid z = z) = p(x = x \mid z = z)p(y = y \mid z = z)$$

Bayes' Rule

$$P(\mathbf{x} \mid \mathbf{y}) = \frac{P(\mathbf{x})P(\mathbf{y} \mid \mathbf{x})}{P(\mathbf{y})}$$

MODIFIED BAYES' THEOREM:

$$P(H|X) = P(H) \times \left(1 + P(C) \times \left(\frac{P(X|H)}{P(X)} - 1\right)\right)$$

H: HYPOTHESIS

X: OBSERVATION

P(H): PRIOR PROBABILITY THAT H IS TRUE

P(x): PRIOR PROBABILITY OF OBSERVING X

P(C): PROBABILITY THAT YOU'RE USING BAYESIAN STATISTICS CORRECTLY

Bayes' Rule

$$P(\mathbf{x} \mid \mathbf{y}) = \frac{P(\mathbf{x})P(\mathbf{y} \mid \mathbf{x})}{P(\mathbf{y})}$$

MODIFIED BAYES' THEOREM:

$$P(H|X) = P(H) \times \left(1 + P(C) \times \left(\frac{P(X|H)}{P(X)} - 1\right)\right)$$

H: HYPOTHESIS

X: OBSERVATION

P(H): PRIOR PROBABILITY THAT H IS TRUE

P(x): PRIOR PROBABILITY OF OBSERVING X

P(C): PROBABILITY THAT YOU'RE USING

NB: I hope there's no need to point this out but this is just a joke...

Expectation

of a discrete random variable

$$\mathbb{E}_{\mathbf{x} \sim P}[f(x)] = \sum P(x)f(x)$$

of a continuous random variable

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

Linearity of expectations

$$\mathbb{E}_{\mathbf{x}}[\alpha f(x) + \beta g(x)] = \alpha \mathbb{E}_{\mathbf{x}}[f(x)] + \beta \mathbb{E}_{\mathbf{x}}[g(x)]$$

Variance and covariance

Variance

$$Var(f(x)) = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])^2 \right]$$

Covariance

$$Cov(f(x), g(y)) = \mathbb{E}\left[\left(f(x) - \mathbb{E}\left[f(x)\right]\right)\left(g(y) - \mathbb{E}\left[g(y)\right]\right)\right]$$

Covariance matrix given a random vector x

$$Cov(\mathbf{x})_{i,j} = Cov(\mathbf{x}_i, \mathbf{x}_j)$$

Bernoulli distribution

$$P(\mathbf{x} = 1) = \phi$$

$$P(\mathbf{x} = 0) = 1 - \phi$$

$$P(\mathbf{x} = x) = \phi^{x} (1 - \phi)^{1 - x}$$

$$\mathbb{E}_{\mathbf{x}}[\mathbf{x}] = \phi$$

$$\operatorname{Var}_{\mathbf{x}}(\mathbf{x}) = \phi(1 - \phi)$$

Gaussian distribution

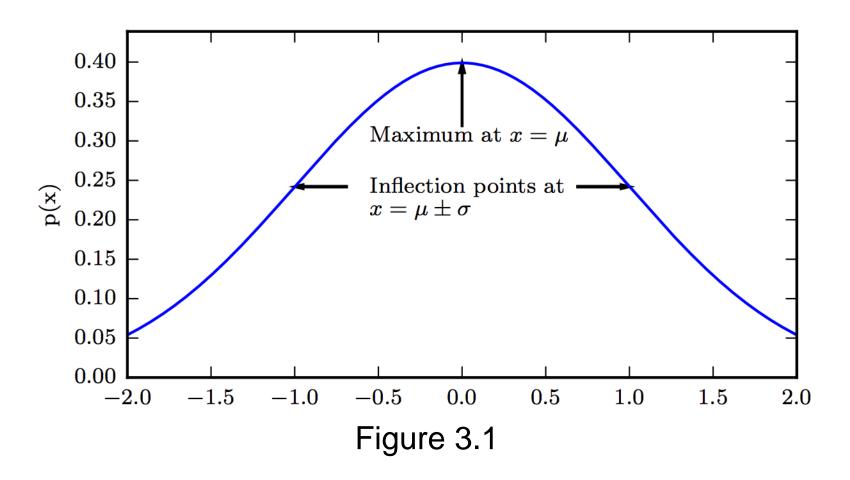
Parametrised by variance

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

Parametrised by precision

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

Gaussian distribution



Multivariate Gaussian

Parametrised by variance

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sqrt{\frac{1}{(2\pi)^n \text{det}(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu})\right)$$

Parametrised by precision

$$\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\beta}^{-1}) = \sqrt{\frac{\det(\boldsymbol{\beta})}{(2\pi)^n}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^{\top} \boldsymbol{\beta}(\boldsymbol{x} - \boldsymbol{\mu})\right)$$

More distributions

Exponential

$$p(x;\lambda) = \lambda \mathbf{1}_{x \ge 0} \exp(-\lambda x)$$

Laplacian

Laplace
$$(x; \mu, \gamma) = \frac{1}{2\gamma} \exp\left(-\frac{|x - \mu|}{\gamma}\right)$$

Dirac

$$p(x) = \delta(x - \mu)$$

More distributions

Exponential

$$p(x; \lambda) = \lambda \mathbf{1}_{x \ge 0} \exp(-\lambda x)$$

Laplacian Assign probability zero to all negative values of x

Laplace
$$(x; \mu, \gamma) = \frac{1}{2\gamma} \exp\left(-\frac{|x - \mu|}{\gamma}\right)$$

Dirac

$$p(x) = \delta(x - \mu)$$

Mixture distributions

$$P(\mathbf{x}) = \sum_{i} P(\mathbf{c} = i) P(\mathbf{x} \mid \mathbf{c} = i)$$

Gaussian mixture with three components

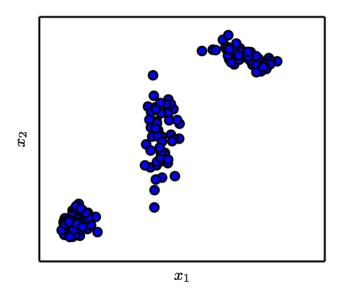


Figure 3.2

Logistic sigmoid

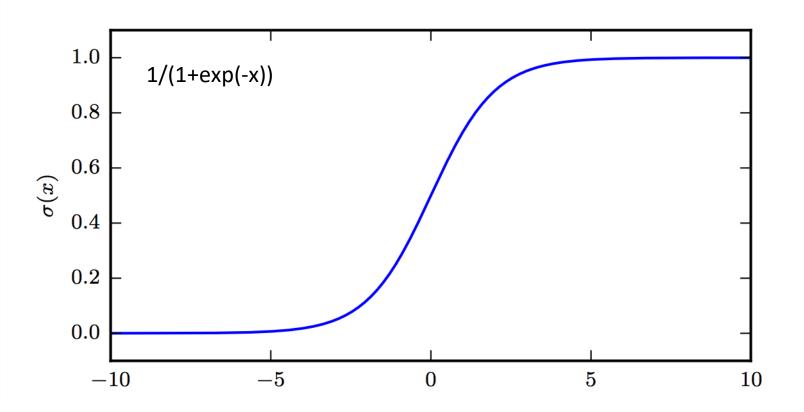


Figure 3.3: The logistic sigmoid function.

Commonly used to parametrise Bernoulli distributions

Softplus function

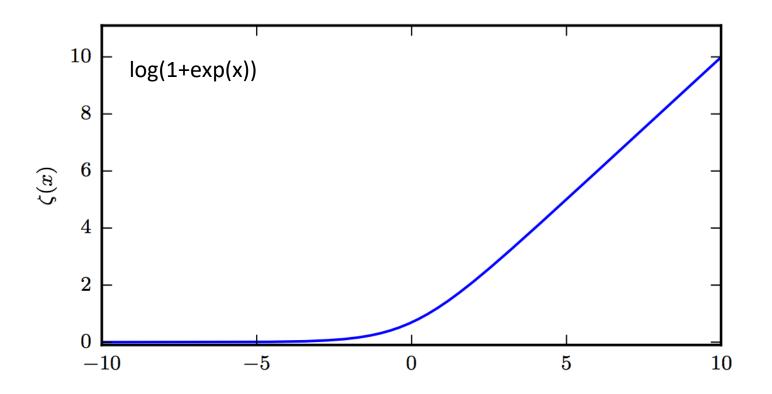


Figure 3.4: The softplus function.

Commonly used to parametrise normal distribution (beta)

Information theory

Information

$$I(x) = -\log P(x)$$

Entropy

$$H(\mathbf{x}) = \mathbb{E}_{\mathbf{x} \sim P}[I(x)] = -\mathbb{E}_{\mathbf{x} \sim P}[\log P(x)]$$

KL divergence

$$D_{\mathrm{KL}}(P||Q) = \mathbb{E}_{\mathbf{x} \sim P} \left[\log \frac{P(x)}{Q(x)} \right] = \mathbb{E}_{\mathbf{x} \sim P} \left[\log P(x) - \log Q(x) \right]$$

Entropy of a Bernoulli variable

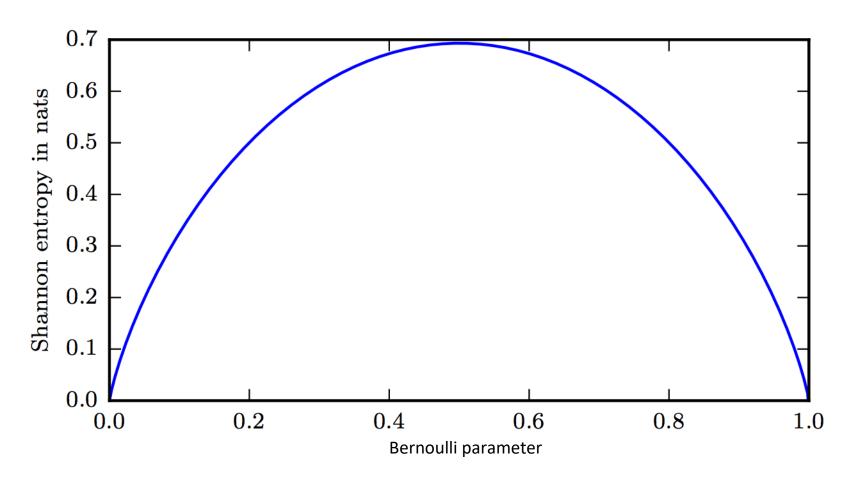
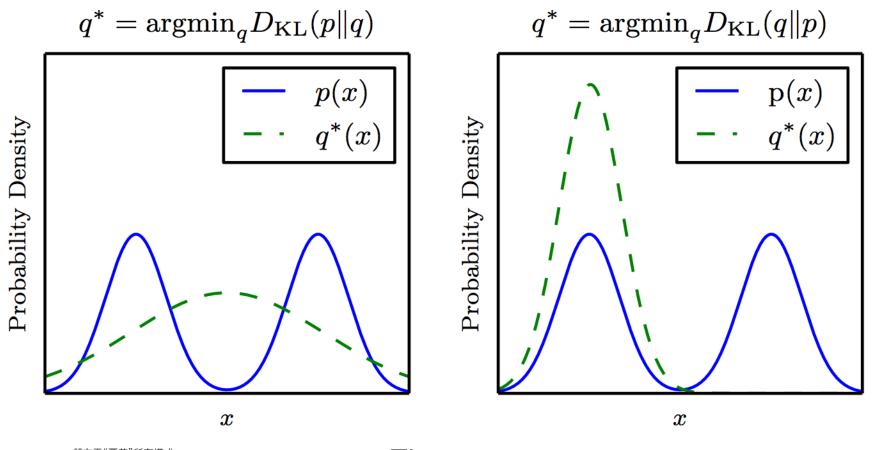


Figure 3.5

The KL divergence is asymmetric

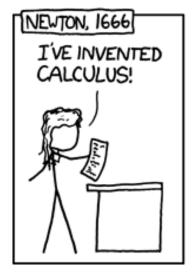
不对称性

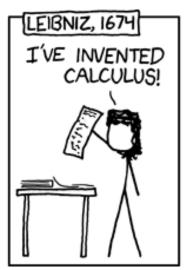


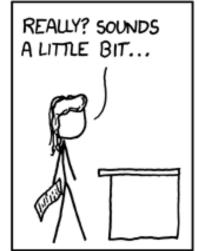
倾向于"覆盖"所有模式

Figure 3.6 倾向于"选择"一个模式

Optimisation and numerical computation











First order derivatives

First order derivatives

$$\frac{dy}{dx}$$

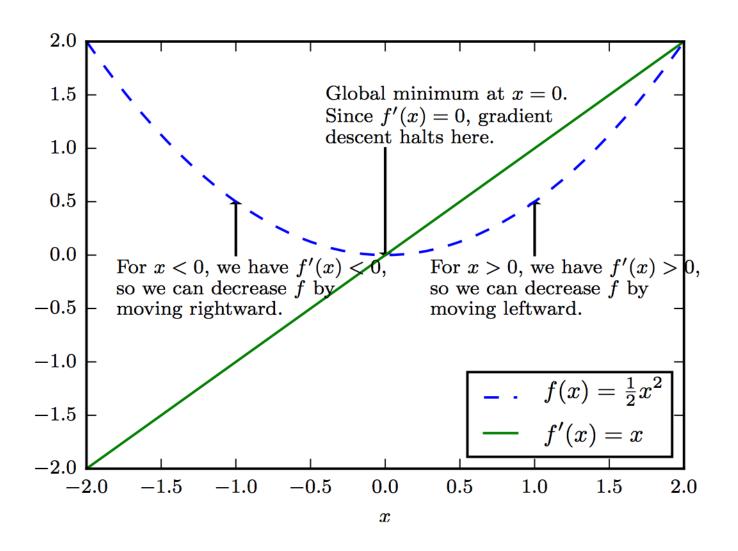
Partial derivatives and gradient

$$\frac{\partial}{\partial x_i} f(\boldsymbol{x}) \qquad \nabla_{\boldsymbol{x}} f(\boldsymbol{x})$$

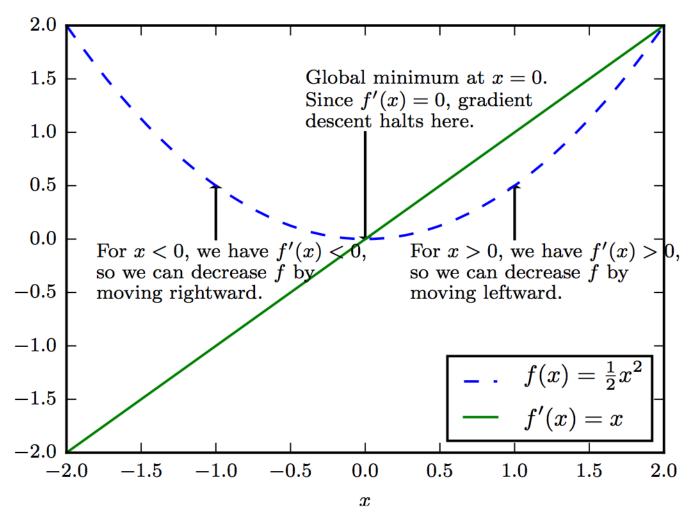
Jacobian matrix

$$J_{i,j} = rac{\partial}{\partial x_j} f(m{x})_i$$

Gradient descent

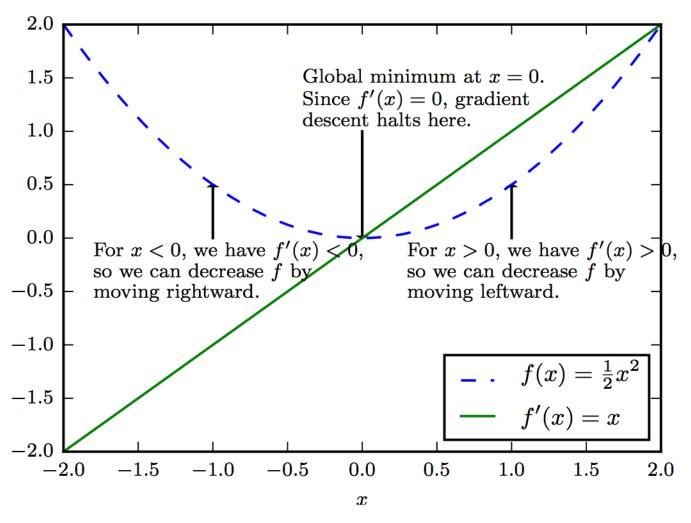


Gradient descent

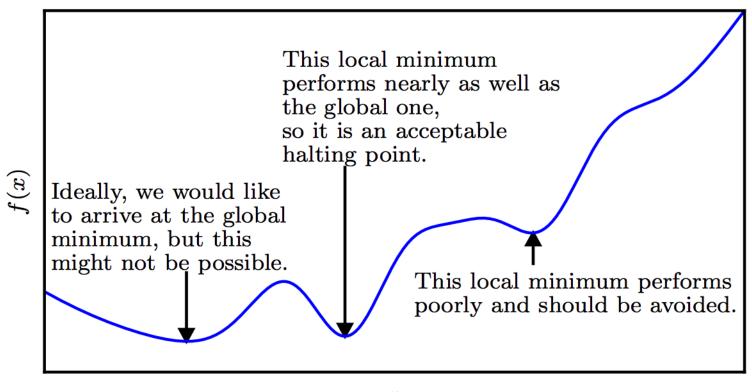


If **x** is multi-dimensional we follow the gradient, i.e., vector of partial derivatives 53

Gradient descent



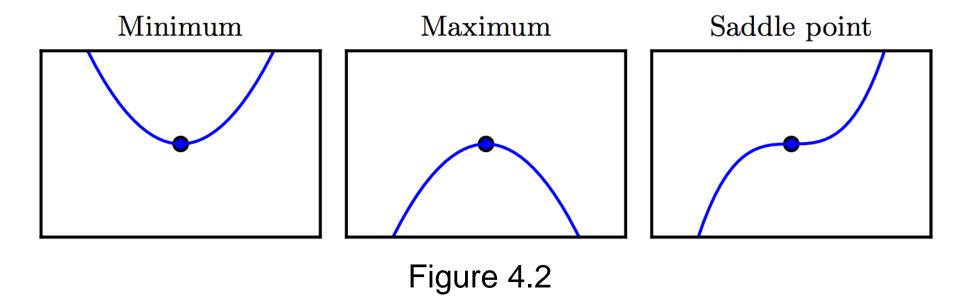
Approximate optimisation



 \boldsymbol{x}

Figure 4.3

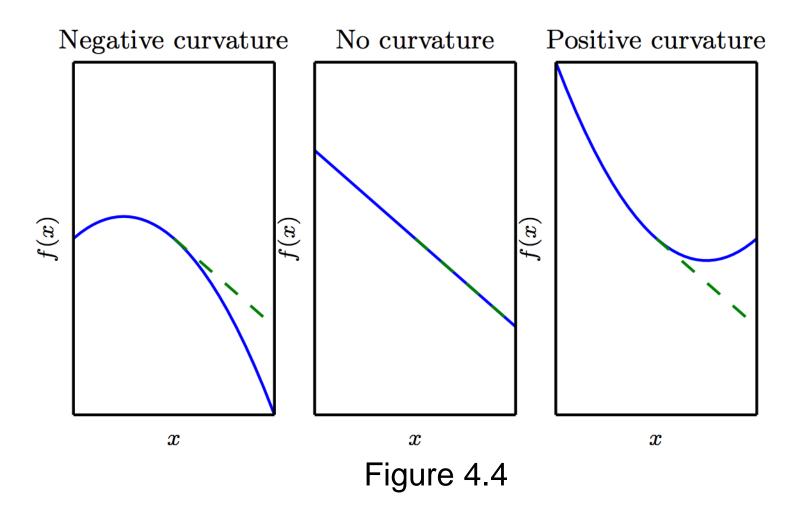
Critical points



Optimising in deep learning

- Pure math way of life:
 - Find literally the smallest value of f(x)
 - Or maybe: find some critical point of f(x) where the value is locally smallest
- Deep learning way of life:
 - Decrease the value of f(x) a lot

Curvature



Second order derivatives

Second order derivatives

$$\frac{d^2}{dx^2}f$$

Hessian

$$\boldsymbol{H}(f)(\boldsymbol{x})_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(\boldsymbol{x})$$

Second order derivatives

Second order derivatives

$$\frac{d^2}{dx^2}f$$

Hessian

$$\boldsymbol{H}(f)(\boldsymbol{x})_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(\boldsymbol{x})$$

In deep learning usually **H** is a symmetric real-valued matrix, thus it can be decomposed in a set of eigenvalues and orthogonal eigenvectors

$$f(oldsymbol{x}) pprox f(oldsymbol{x}^{(0)}) + (oldsymbol{x} - oldsymbol{x}^{(0)})^{ op} oldsymbol{g} + rac{1}{2} (oldsymbol{x} - oldsymbol{x}^{(0)})^{ op} oldsymbol{H} (oldsymbol{x} - oldsymbol{x}^{(0)})$$
 $f(oldsymbol{x}^{(0)} - \epsilon oldsymbol{g}) pprox f(oldsymbol{x}^{(0)}) - \epsilon oldsymbol{g}^{ op} oldsymbol{g} + rac{1}{2} \epsilon^2 oldsymbol{g}^{ op} oldsymbol{H} oldsymbol{g}$

$$f(x) \approx f(x^{(0)}) + (x - x^{(0)})^{\top} g + \frac{1}{2} (x - x^{(0)})^{\top} H(x - x^{(0)})$$

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) pprox f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^{ op} \boldsymbol{g} + rac{1}{2} \epsilon^2 \boldsymbol{g}^{ op} \boldsymbol{H} \boldsymbol{g}$$

Second order Taylor series approximation of f(x) around x(0)

$$f(x) \approx f(x^{(0)}) + (x - x^{(0)})^{\top} g + \frac{1}{2} (x - x^{(0)})^{\top} H(x - x^{(0)})$$

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) pprox f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^{ op} \boldsymbol{g} + rac{1}{2} \epsilon^2 \boldsymbol{g}^{ op} \boldsymbol{H} \boldsymbol{g}$$

Value of the function after gradient descent step

$$f(\boldsymbol{x}) pprox f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{g} + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{H} (\boldsymbol{x} - \boldsymbol{x}^{(0)})$$

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) pprox f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^{\top} \boldsymbol{g} + \frac{1}{2} \epsilon^2 \boldsymbol{g}^{\top} \boldsymbol{H} \boldsymbol{g}$$

Value of the function before the step

$$f(\boldsymbol{x}) pprox f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{g} + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{H} (\boldsymbol{x} - \boldsymbol{x}^{(0)})$$

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) pprox f(\boldsymbol{x}^{(0)}) + \epsilon \boldsymbol{g}^{\top} \boldsymbol{g} + \frac{1}{2} \epsilon^2 \boldsymbol{g}^{\top} \boldsymbol{H} \boldsymbol{g}.$$

这正是 梯度下降 的核心: 顺着负梯度方向走, 函数值会下降 (因为g^T g>0)

梯度方向的下降 带来的改进

Improvement due to slope of function

$$f(\boldsymbol{x}) pprox f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{g} + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{H} (\boldsymbol{x} - \boldsymbol{x}^{(0)})$$

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) pprox f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^{\top} \boldsymbol{g} + \frac{1}{2} \epsilon^{2} \boldsymbol{g}^{\top} \boldsymbol{H} \boldsymbol{g}$$

Correction due to curvature

二阶修正项, 反映了函数的 曲率 (curvature) 对下降的影响

限制因素 (correction), 提醒我们不要走太大步

$$f(\boldsymbol{x}) pprox f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{g} + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{x}^{(0)})^{\top} \boldsymbol{H} (\boldsymbol{x} - \boldsymbol{x}^{(0)})$$

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) pprox f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^{\top} \boldsymbol{g} + \frac{1}{2} \epsilon^{2} \boldsymbol{g}^{\top} \boldsymbol{H} \boldsymbol{g}$$

If this is positive, we can look for the optimal step size that minimises the Taylor-series approximation

$$f(oldsymbol{x}) pprox f(oldsymbol{x}^{(0)}) + (oldsymbol{x} - oldsymbol{x}^{(0)})^ op oldsymbol{g} + rac{1}{2}(oldsymbol{x} - oldsymbol{x}^{(0)})^ op oldsymbol{H}(oldsymbol{x} - oldsymbol{x}^{(0)})$$
 $f(oldsymbol{x}^{(0)} - \epsilon oldsymbol{g}) pprox f(oldsymbol{x}^{(0)}) - \epsilon oldsymbol{g}^ op oldsymbol{g} + rac{1}{2}\epsilon^2 oldsymbol{g}^ op oldsymbol{H}oldsymbol{g}$
 $\epsilon^* = rac{oldsymbol{g}^ op oldsymbol{g}}{oldsymbol{g}^ op oldsymbol{H}oldsymbol{g}}$

$$f(oldsymbol{x}) pprox f(oldsymbol{x}^{(0)}) + (oldsymbol{x} - oldsymbol{x}^{(0)})^{ op} oldsymbol{g} + rac{1}{2} (oldsymbol{x} - oldsymbol{x}^{(0)})^{ op} oldsymbol{H} (oldsymbol{x} - oldsymbol{x}^{(0)})$$
 $f(oldsymbol{x}^{(0)} - \epsilon oldsymbol{g}) pprox f(oldsymbol{x}^{(0)}) - \epsilon oldsymbol{g}^{ op} oldsymbol{g} + rac{1}{2} \epsilon^2 oldsymbol{g}^{ op} oldsymbol{H} oldsymbol{g}$
 $\epsilon^* = oldsymbol{g} oldsymbol{g}^{ op} oldsymbol{H} oldsymbol{g}$

Big gradients speed you up (larger numerator means larger step size)

$$f(m{x})pprox f(m{x}^{(0)}) + (m{x}-m{x}^{(0)})^{ op}m{g} + rac{1}{2}(m{x}-m{x}^{(0)})^{ op}m{H}(m{x}-m{x}^{(0)})$$
 $f(m{x}^{(0)}-\epsilonm{g})pprox f(m{x}^{(0)}) - \epsilonm{g}^{ op}m{g} + rac{1}{2}\epsilon^2m{g}^{ op}m{H}m{g}$ $\epsilon^* = m{g}^{ op}m{H}m{g}$ 代表函数的 曲率 (curvature) 在梯度方向上的大/

Big eigenvalues slow you down if you align with their eigenvectors (larger denominator means smaller step size)

"Real" issues

- Algorithms often specified in terms of real numbers
 - cannot be implemented with finite number of bits; does the algorithm still work?
- Do small changes in the input to a function cause large changes to an output?
 - Rounding/measurement errors, noise, can cause large changes
 - Iterative search for best input is difficult

Rounding and truncation errors

- In a digital computer, we use float32 or similar schemes to represent real numbers
- A real number x is rounded to x + delta for some small delta
- Overflow: large x replaced by inf
- Underflow: small x replaced by 0

Example

 Adding a very small number to a larger one may have no effect. This can cause large changes downstream:

```
>>> a = np.array([0., 1e-8]).astype('float3
>>> a.argmax()
1
>>> (a + 1).argmax()
0
```

Secondary effects

- Suppose we have code that computes x-y
- Suppose x overflows to inf
- Suppose y overflows to inf
- Then x y = inf inf = NaN

exp

- exp(x) overflows for large x
 - Doesn't need to be very large
 - float32: 89 overflows
 - Never use large x
- exp(x) underflows for very negative x
 - Possibly not a problem
 - Possibly catastrophic if exp(x) is a denominator, an argument to a logarithm, etc.

log and sqrt

- log(0) = inf
- log(<negative>) is imaginary, usually nan in software
- sqrt(0) is 0, but its derivative has a divide by zero
- Definitely avoid underflow or round-to-negative in the argument!

log exp

- log exp(x) is a common pattern
- Should be simplified to x
- Avoids:
 - Overflow in exp
 - Underflow in exp causing -inf in log

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Also see https://blog.feedly.com/tricks-of-the-trade-logsumexp/

Bug hunting strategies

- If you increase your learning rate and the loss *gets stuck*, you are probably rounding your gradient to zero somewhere: maybe computing cross-entropy using probabilities instead of logits
- For correctly implemented loss, too high of learning rate should usually cause <u>explosion</u>

Bug hunting strategies

- If you see explosion (NaNs, very large values) immediately suspect:
 - log
 - exp
 - sqrt
 - division
- Always suspect the code that changed most recently