Regression

Terminology

- Data consists of **pairs** $(\mathbf{x}_n, y_n)$, where y_n is the n'th output and x_n is a vector of D inputs. The number of pairs N is the data-size and D is the dimensionality.
- Two goals of regression: **prediction** and **interpretation**
- The regression function: $y_n \approx f_w(\mathbf{x}_n)\ \forall n$
- Regression finds correlation not a causal relationship.
- **Input variables** a.k.a. covariates, independent variables, explanatory variables, exogenous variables, predictors, regressors.
- **Output variables** a.k.a. target, label, response, outcome, dependent variable, endogenous variables, measured variable, regressands.

Linear Regression

- Assumes linear relationship between inputs and output.
- $y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1} + ... + w_D x_{nD}$ $:= \tilde{\mathbf{x}}_n^T \tilde{\mathbf{w}}$ contain the additional offset term (a.k.a. bias).
- Given data we learn the weights $\mathbf{w}$ (a.k.a. estimate or fit the model)
- Overparameterisation $D > N$ eg. univariate linear regression with a single data point $y_1 \approx w_0 + w_1 x_{11}$. This makes the task under-determined (no unique solution).

Loss Functions $\mathcal{L}$

- A loss function (a.k.a. energy, cost, training objective) quantifies how well the model does (how costly its mistakes are).
- $y \in \mathbb{R} \Rightarrow$ desirable for cost to be symmetric around 0 since $\pm$ errors should be penalized equally.
- Cost function should penalize "large" mistakes and "very large" mistakes similarly to be robust to outliars.
- Mean Squared Error:

$\mathsf{MSE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}[y_n - f_{\mathrm{w}}(\mathbf{x}_n)]^2$
not robust to outliars.

- Mean Absolute Error:

$\mathsf{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}|y_n - f_{\mathrm{w}}(\mathbf{x}_n)|$

- Convexity: a function is convex iff a line segment between two points on the function's graph always lies above the function.
- Convexity: a function $h(\mathbf{u}), \mathbf{u} \in \mathbb{R}^D$ is convex if $\forall\ \mathbf{u}, \mathbf{v} \in \mathbb{R}^D, 0 \le \lambda \le 1$:

$h(\lambda\mathbf{u} + (1-\lambda)\mathbf{v}) \le \lambda h(\mathbf{u}) + (1-\lambda)h(\mathbf{v})$

Stirctly convex if $\le \Rightarrow <$

- Convexity, a desired computational property: A strictly convex function has a unique global minimum $\mathbf{w}^*$. For convex functions, every local minimum is a global minimum.
- Sums of convex functions are also convex $\Rightarrow$ MSE combined with a linear model is convex in $\mathbf{w}$.
- Proof of convexity for MAE:

$\mathsf{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}_n(\mathbf{w}), \mathcal{L}_n(\mathbf{w}) = |y_n - f_{\mathrm{w}}(\mathbf{x}_n)|$
$\mathcal{L}_n(\lambda w_1 + (1-\lambda)w_2) \le \lambda\mathcal{L}_n(w_1) + (1-\lambda)\mathcal{L}_n(w_2)$
$|y_n - x_n^T(\lambda w_1 + (1-\lambda)w_2)| \le \lambda|y_n - x_n^T w_1| + (1-\lambda)|y_n - x_n^T w_2|$
$(1-\lambda) \ge 0 \Rightarrow (1-\lambda)|y_n - x_n^T w_2| = |(1-\lambda)y_n - (1-\lambda)x_n^T w_2|$
$a = \lambda y_n - \lambda x_n^T w_1, b = (1-\lambda)y_n - (1-\lambda)x_n^T w_2$
$a + b = y_n - x_n^T(\lambda w_1 + (1-\lambda)w_2)$
$|a+b| \le |a| + |b| \Rightarrow \mathcal{L}_n(\mathbf{w})$ convex $\Rightarrow \mathsf{MAE}(\mathbf{w})$ convex

- Huber loss:

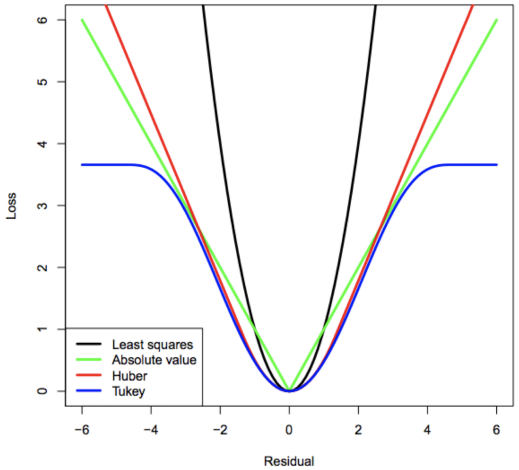
$$\mathcal{H}uber(e) := \begin{cases} \frac{1}{2}e^2 & ,\text{if } |e| \le \delta \\ \delta|e| - \frac{1}{2}\delta^2 & ,\text{if } |e| > \delta \end{cases} \quad \text{convex,}$$

differentiable, and robust to outliers but setting δ is not easy.

- Tukey's bisquare loss:

$$\frac{\partial\mathcal{L}}{\partial e} := \begin{cases} e\{1 - e^2/\delta^2\}^2 & ,\text{if } |e| \le \delta \\ 0 & ,\text{if } |e| > \delta \end{cases} \quad \text{non-convex,}$$

but robust to outliers.



Optimisation

- Given $\mathcal{L}(\mathbf{w})$ we want $\mathbf{w}^* \in \mathbb{R}^D$ which minimises the cost: $\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}) \rightarrow$ formulated as an optimisation problem
- Local minimum $\mathbf{w}^* \Rightarrow \exists\epsilon > 0$ s.t. $\mathcal{L}(\mathbf{w}^*) \le \mathcal{L}(\mathbf{w})\ \forall\mathbf{w}$ with $\|\mathbf{w} - \mathbf{w}^*\| < \epsilon$
- Global minimum $\mathbf{w}^*$, $\mathcal{L}(\mathbf{w}^*) \le \mathcal{L}(\mathbf{w})\ \forall\mathbf{w} \in \mathbb{R}^D$

Smooth Optimization

- A gradient is the slope of the tangent to the function. It points to the direction of largest increase of the function.

$\nabla\mathcal{L}(\mathbf{w}) := \left[\frac{\partial\mathcal{L}(\mathbf{w})}{\partial w_1}, \ldots, \frac{\partial\mathcal{L}(\mathbf{w})}{\partial w_D}\right]^\top \in \mathbb{R}^D$

Gradient Descent

- To minimize the function, we iteratively take a step in the opposite direction of the gradient

$$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma\nabla\mathcal{L}\left(\mathbf{w}^{(t)}\right)$$

where $\gamma > 0$ is the step-size (or learning rate). Then repeat with the next t.

- Example: Gradient descent for 1parameter model to minimize MSE:

$f_w(x) = w_0 \Rightarrow \mathcal{L}(w) = \frac{1}{2N}\sum_{n=1}^{N}(y_n - w_0)^2 = \nabla\mathcal{L} = \frac{\partial}{\partial w_0}\mathcal{L} = \frac{1}{2N}\sum -2(y_n - w_0) = (-\frac{1}{N}\sum y_n) + w_0 = w_0 - \bar{y}$
$(min_w L(w) = w_0 - \bar{y} = 0 \Rightarrow w_0 = \bar{y})$
$w_0^{(t+1)} := (1-\gamma)w_0^{(t)} + \gamma\bar{y}$
where $\bar{y} := \sum_n y_n/N$. When is this sequence guaranteed to converge? When $\gamma > 2$ you start having an exploding GD.

Gradient Descent for Linear MSE

We define the error vector $\mathbf{e}$: $\mathrm{e} = \mathbf{y} - \mathbf{X}\mathbf{w}$ and MSE as follows:
$\mathcal{L}(\mathbf{w}) := \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2 = \frac{1}{2N}\mathbf{e}^\top\mathbf{e}$
then the gradient is given by
$\nabla\mathcal{L}(\mathbf{w}) = -\frac{1}{N}\mathbf{X}^\top\mathbf{e}$
Computational cost: $\Theta(N \times D)$

Stochastic Gradient Descent

$\mathcal{L}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}_n(\mathbf{w})$
$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma\nabla\mathcal{L}_n\left(\mathbf{w}^{(t)}\right)$

- Compuational cost: $\Theta(D)$
- Cheap and unbiased estimate of the gradient!

$E[\nabla\mathcal{L}_n(w)] = \frac{1}{n}\sum_{n=1}^{N}\nabla\mathcal{L}_n(w) = \nabla\left(\frac{1}{N}\sum\cdots\right) = \nabla\mathcal{L}(n)$ which is the true gradient direction.

Mini-batch SGD

$\mathbf{g} := \frac{1}{|B|}\sum_{n\in B}\nabla\mathcal{L}_n\left(\mathbf{w}^{(t)}\right)$
$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma\mathbf{g}.$

- Randomly chosen a subset $B \subseteq [N]$ of the training examples. For each of these selected examples n, we compute the respective gradient $\nabla\mathcal{L}_n$, at the same current point $\mathbf{w}^{(t)}$.
- The computation of $\mathbf{g}$ can be parallelized easily. This is how current deep-learning applications utilize GPUs (by running over $|B|$ threads in parallel).
- $B := [N]$, we obtain $\mathbf{g} = \nabla\mathcal{L}$.

Non-Smooth Optimization

- An alternative characterization of convexity, for differentiable functions is given by

$\mathcal{L}(\mathbf{u}) \ge \mathcal{L}(\mathbf{w}) + \nabla\mathcal{L}(\mathbf{w})^\top(\mathbf{u} - \mathbf{w})\quad \forall\mathbf{u}, \mathbf{w}$

meaning that the function must always lie above its linearization.

Subgradients

- A vector $\mathbf{g} \in \mathbb{R}^D$ such that

$\mathcal{L}(\mathbf{u}) \ge \mathcal{L}(\mathbf{w}) + \mathbf{g}^\top(\mathbf{u} - \mathbf{w})\quad \forall\mathbf{u}$

is called a subgradient to the function $\mathcal{L}$ at $\mathbf{w}$.

- This definition makes sense for objectives $\mathcal{L}$ which are not necessarily differentiable (and not even necessarily convex).
- If $\mathcal{L}$ is convex and differentiable at $\mathbf{w}$, then the only subgradient at $\mathbf{w}$ is $\mathbf{g} = \nabla\mathcal{L}(\mathbf{w})$.

Subgradient Descent

$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma\mathbf{g}$
for $\mathbf{g}$ a subgradient to $\mathcal{L}$ at the current iterate $\mathbf{w}^{(t)}$.

Example: Optimizing Linear MAE

1) Compute a subgradient of the absolute value function $h : \mathbb{R} \rightarrow \mathbb{R}, h(e) := |e|$.

$$g = \begin{cases} -1 & \text{if } e < 0 \\ [-1, 1] & \text{if } e = 0 \\ 1 & \text{if } e > 0 \end{cases}$$

2) Recall the definition of the mean absolute error:
$\mathcal{L}(\mathbf{w}) = \mathrm{MAE}(\mathbf{w}) := \frac{1}{N}\sum_{n=1}^{N}|y_n - f_{\mathbf{w}}(\mathbf{x}_n)|$
For linear regression, its (sub)gradient is easy to compute using the chain rule. Compute it!
The subgradient is given by:
$\partial\mathcal{L}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}g(e_n)\nabla f_{\mathbf{w}}(\mathbf{x}_n) = \frac{1}{N}\sum_{n=1}^{N}g(e_n)\mathbf{x}_n$
since $f_{\mathbf{w}}(\mathbf{x}_n) = \mathbf{w}^T\mathbf{x}_n$, then $\nabla f_{\mathbf{w}}(\mathbf{x}_n) = \mathbf{x}_n$ where $e_n = y_n - f_{\mathbf{w}}(\mathbf{x}_n)$.
See Exercise Sheet 2.

Stochastic Subgradient Descent

- still abbreviated SGD commonly.
- Same, $\mathbf{g}$ being a subgradient to the randomly selected $\mathcal{L}_n$ at the current iterate $\mathbf{w}^{(t)}$.
- SGD update for linear MAE:

$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} + \gamma g(e_n)\mathbf{x}_n$

Variants of SGD

SGD with Momentum

pick a stochastic gradient $\mathbf{g}$
$\mathbf{m}^{(t+1)} := \beta_1\mathbf{m}^{(t)} + (1-\beta_1)\,\mathbf{g}$ (momentum term)
$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma\mathbf{m}^{(t+1)}$

- momentum from previous gradients (acceleration)

Adam

- pick a stochastic gradient $\mathbf{g}$

$\mathbf{m}^{(t+1)} := \beta_1\mathbf{m}^{(t)} + (1-\beta_1)\,\mathbf{g}$
$\mathbf{v}_i^{(t+1)} := \beta_2\mathbf{v}_i^{(t)} + (1-\beta_2)\,(\mathbf{g}_i)^2 \quad \forall i$ (Momentum t
$\mathbf{w}_i^{(t+1)} := \mathbf{w}_i^{(t)} - \frac{\gamma}{\sqrt{\mathbf{v}_i^{(t+1)}}}\mathbf{m}_i^{(t+1)} \quad \forall i$

- faster forgetting of older weights
- is a momentum variant of Adagrad
- coordinate-wise adjusted learning rate

-strong performance in practice, e.g. for self-attention networks

SignSGD

pick a stochastic gradient $\mathbf{g}$

$\mathbf{w}_i^{(t+1)} := \mathbf{w}_i^{(t)} - \gamma \operatorname{sign}(\mathbf{g}_i)$

- only use the sign (one bit) of each gradient entry $\rightarrow$ communication efficient for distributed training
- convergence issues

Constrained Optimization

- Sometimes, optimization problems come posed with additional constraints:

$\min_{\mathbf{w}} \mathcal{L}(\mathbf{w})$, subject to $\mathbf{w} \in \mathcal{C}$.

- The set $\mathcal{C} \subset \mathbb{R}^D$ is called the constraint set.

Convex Sets

A set $\mathcal{C}$ is convex iff the line segment between any two points of $\mathcal{C}$ lies in $\mathcal{C}$, i.e., if for any $\mathbf{u}, \mathbf{v} \in \mathcal{C}$ and any θ with $0 \leq \theta \leq 1$, we have

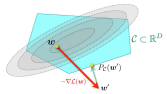
$\theta\mathbf{u} + (1-\theta)\mathbf{v} \in \mathcal{C}$

- Intersubsections of convex sets are convex - Projections onto convex sets are unique.(and often efficient to compute)
- Formal definition:

$P_{\mathcal{C}}(\mathbf{w}') := \arg\min_{\mathbf{v} \in \mathcal{C}} \|\mathbf{v} - \mathbf{w}'\|$.

Projected Gradient Descent

- Idea: add a projection onto $\mathcal{C}$ after every step:



$P_{\mathcal{C}}(\mathbf{w}') := \arg\min_{\mathbf{v} \in \mathcal{C}} \|\mathbf{v} - \mathbf{w}'\|$.

$\mathbf{w}^{(t+1)} := P_{\mathcal{C}}\left[\mathbf{w}^{(t)} - \gamma \nabla \mathcal{L}\left(\mathbf{w}^{(t)}\right)\right]$

- Projected SGD. Same SGD step, followed by the projection step. Same convergence properties.

Constrained $\rightarrow$ Unconstrained Problems

$\min_{w \in C} \mathcal{L}(w) \sim \min_w \mathcal{L}(w) + P(w)$

- Alternatives to projected gradient methods
- Use penalty functions instead of directly solving $\min_{\mathbf{w} \in \mathcal{C}} \mathcal{L}(\mathbf{w})$.
- "brick wall" (indicator function)

$$P(w) = I_{\mathcal{C}}(\mathbf{w}) := \begin{cases} 0 & \mathbf{w} \in \mathcal{C} \\ \infty & \mathbf{w} \notin \mathcal{C} \end{cases}$$

Can't run GD because non-continuous objective.

- Penalize error. Example:

$\mathcal{C} = \{\mathbf{w} \in \mathbb{R}^D \mid A\mathbf{w} = \mathbf{b}\} \Rightarrow P(w) = \lambda \|A\mathbf{w} - \mathbf{b}\|^2$

- ℓ_1 norm encourages sparsity which reduces memory: $P(w) = \lambda \|\mathbf{w}\|_1$
- Linearized Penalty Functions (see Lagrange Multipliers)

Implementation Issues

1) Stopping criteria: $\nabla \mathcal{L}(\mathbf{w}) \approx 0$

2) Optimality:

1st order optimiality condition: if $\mathcal{L}$ is convex and $\nabla \mathcal{L}(w^*) = 0 \Rightarrow$ global optimality

2nd order: $\mathcal{L}$ potentially non-convex, if $\nabla \mathcal{L}(w^*) = 0$ & $\nabla^2 \mathcal{L}(w^*) \geq 0 \Rightarrow w$ local minimum.

$\nabla^2 \mathcal{L}(\mathbf{w}) := \frac{\partial^2 \mathcal{L}}{\partial \mathbf{w} \partial \mathbf{w}^\top}(\mathbf{w})$ is expensive.

3) Step-size selection: $\gamma >>$ might diverge. $\gamma <<$ slow convergence. Convergence to local minimum guaranteed only when $\gamma < \gamma_{\min}$, $\gamma_{\min}$ depends on the problem.

4) Line-search methods: For some $\mathcal{L}$, set step-size automatically.

5) Feature normalization: GD is sensitive to ill-conditioning $\rightarrow$ Normalize your input features i.e. pre-condition the optimization problem.

Non-Convex Optimization

- Real-world problems are not convex!
- All we have learnt on algorithm design and performance of convex algorithms still helps us in the nonconvex world.

SGD Theory

- For convergence, $\gamma^{(t)} \rightarrow 0$ "appropriately". Robbins-Monroe condition suggests to take $\gamma^{(t)}$ s.t.:

$\sum_{t=1}^{\infty} \gamma^{(t)} = \infty, \quad \sum_{t=1}^{\infty} \left(\gamma^{(t)}\right)^2 < \infty$

Example: $\gamma^{(t)} := 1/(t+1)^r$ where $r \in (0.5, 1)$.

Least Squares

- Linear regression + MSE $\rightarrow$ compute the optimum of the cost function analytically by solving a linear system of D equations (normal equations)
- Derive the normal equations, proove convexity, optimality conditions for convex functions ($\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}$.)

Normal Equations

$\mathcal{L}(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2$

$= \frac{1}{2N} (\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w})$,

- Proof of convexity:

1) Simplest way: observe that $\mathcal{L}$ is naturally represented as the sum (with positive coefficients) of the simple terms $\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2$. Further, each of these simple terms is the composition of a linear function with a convex function (the square function). Therefore, each of these simple terms is convex and hence the sum is convex.

2) Directly verify the definition, that for any $\lambda \in [0,1]$ and $\mathbf{w}, \mathbf{w}'$

$\mathcal{L}(\lambda\mathbf{w} + (1-\lambda)\mathbf{w}') - (\lambda \mathcal{L}(\mathbf{w}) + (1-\lambda)\mathcal{L}(\mathbf{w}')) \leq 0.$

$\text{LHS} = -\frac{1}{2N}\lambda(1-\lambda)\left\|\mathbf{X}(\mathbf{w} - \mathbf{w}')\right\|_2^2 < 0,$

3) We can compute the second derivative (the Hessian) and show that it is positive semidefinite (all its eigenvalues are non-negative).

$$\begin{aligned}
\mathbf{H}(\mathbf{w}) &= \frac{1}{2N} \nabla^2 \left((\mathbf{y} - \mathbf{X}\mathbf{w})^\top (\mathbf{y} - \mathbf{X}\mathbf{w})\right) \\
&= \frac{1}{2N} \nabla \left(-2(\mathbf{y} - \mathbf{X}\mathbf{w})\mathbf{X}^\top\right) \\
&= \frac{-2}{2N} \nabla (\mathbf{X}^\top (\mathbf{y} - \mathbf{X}\mathbf{w})) \\
&= \frac{-1}{N} \mathbf{X}^\top \nabla (\mathbf{y} - \mathbf{X}\mathbf{w}) \\
&= \frac{-1}{N} \mathbf{X}^\top (\nabla \mathbf{y} - \nabla (\mathbf{X}\mathbf{w})) \\
&= \frac{-1}{N} \mathbf{X}^\top (\mathbf{0} - \mathbf{X}) \\
&= \frac{1}{N} \mathbf{X}^\top \mathbf{X}
\end{aligned}$$

Singular value decomposition (SVD): $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$

U and V are orthogonal matrices, and S is a diagonal matrix with the singular values σ_i on the diagonal.

$\mathbf{H}(\mathbf{w}) = \frac{1}{N}\mathbf{X}^\top\mathbf{X} = \frac{1}{N}\mathbf{V}\mathbf{S}^2\mathbf{V}^\top$

where $\mathbf{S}^2$ is a diagonal matrix with the squares of the singular values.

Let $\mathbf{v}$ be a non-zero vector,

$$\begin{aligned}
\mathbf{v}^\top \mathbf{H}(\mathbf{w}) \mathbf{v} &= \frac{1}{N} \mathbf{v}^\top \mathbf{V}\mathbf{S}^2\mathbf{V}^\top \mathbf{v} \\
&= \frac{1}{N} (\mathbf{V}^\top \mathbf{v})^\top \mathbf{S}^2 (\mathbf{V}^\top \mathbf{v}) \\
&= \frac{1}{N} \|\mathbf{S}(\mathbf{V}^\top \mathbf{v})\|^2 \geq 0
\end{aligned}$$

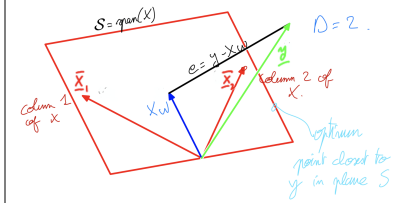
$\mathbf{S}$ diagonal matrix with non-negative entries, $\mathbf{V}^\top\mathbf{v}$ vector.

- Now find its minimum

$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N}\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$

$\Rightarrow \mathbf{X}^\top \underbrace{(\mathbf{y} - \mathbf{X}\mathbf{w})}_{\text{error}} = \mathbf{0}$

Geometric Interpretation



Closed form

- $\mathbf{X}^\top\mathbf{X} \in \mathbb{R}^{D \times D}$ is called the Gram matrix.
- If invertible, we can get a closed-form expression for the minimum:

$\mathbf{w}^\star = \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{y}$

Invertibility and Uniqueness

- $\mathbf{X}^\top\mathbf{X} \in \mathbb{R}^{D \times D}$ invertible iff $\operatorname{rank}(\mathbf{X}) = D$.
- Proof: assume $\operatorname{rank}(\mathbf{X}) < D$. Then there exists a non-zero vector $\mathbf{u}$ so that $\mathbf{X}\mathbf{u} = \mathbf{0}$. It follows that $\mathbf{X}^\top\mathbf{X}\mathbf{u} = \mathbf{0}$, and so $\operatorname{rank}\left(\mathbf{X}^\top\mathbf{X}\right) < D$. Therefore, $\mathbf{X}^\top\mathbf{X}$ is not invertible.

Conversely, assume that $\mathbf{X}^\top\mathbf{X}$ is not invertible. Hence, there exists a non-zero vector $\mathbf{v}$ so that $\mathbf{X}^\top\mathbf{X}\mathbf{v} = \mathbf{0}$. It follows that

$$\mathbf{0} = \mathbf{v}^\top\mathbf{X}^\top\mathbf{X}\mathbf{v} = (\mathbf{X}\mathbf{v})^\top(\mathbf{X}\mathbf{v}) = \|\mathbf{X}\mathbf{v}\|^2$$

This implies that $\mathbf{X}\mathbf{v} = \mathbf{0}$, i.e., $\operatorname{rank}(\mathbf{X}) < D$.

Rank Deficiency and Ill-Conditioning

- In practice, $\mathbf{X}$ is often rank deficient.
- If $D > N$, we always have $\operatorname{rank}(\mathbf{X}) < D$ (since row rank = col. rank)
- If $D \leq N$, but some of the columns $\mathbf{x}_i$are (nearly) collinear, then the matrix is illconditioned, leading to numerical issues when solving the linear system.
- Using a linear system solver, one can solve this problem.

Closed-form solution for MAE

Can you derive closed-form solution for 1-parameter model when using MAE cost function?

Maximum Likelihood

Gaussian distribution and independence

- A Gaussian random variable in $\mathbb{R}$ with mean μ and variance σ^2 has a density of

$p\left(y \mid \mu, \sigma^2\right) = \mathcal{N}\left(y \mid \mu, \sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\mu)^2}{2\sigma^2}\right]$.

- The density of a Gaussian random vector with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$ (which must be a positive semi-definite matrix) is

$\mathcal{N}(\mathbf{y} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$

$= \frac{1}{\sqrt{(2\pi)^D \det(\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2}(\mathbf{y} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{y} - \boldsymbol{\mu})\right]$.

- Two random variables X and Y are called independent when $p(x, y) = p(x)p(y)$.

A probabilistic model for least-squares

- Data generation: $y_n = \mathbf{x}_n^\top\mathbf{w} + \epsilon_n$ where the ϵ_n (the noise) is a zero mean Gaussian random variable.
- Given N samples, the likelihood of the data vector $\mathbf{y} = (y_1, \cdots, y_N)$ given the input $\mathbf{X}$ and the model $\mathbf{w}$ is equal to

$p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \prod_{n=1}^N p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \prod_{n=1}^N \mathcal{N}\left(y_n \mid \mathbf{x}_n^\top\mathbf{w}, \sigma^2\right)$.

- The probabilistic view point is that we should maximize this likelihood over the choice of model w. I.e., the "best" model is the one that maximizes this likelihood.

Defining cost with log-likelihood

$\mathcal{L}_{\text{LL}}(\mathbf{w}) := \log p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2}\sum_{n=1}^N \left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2 + \text{cnst}.$

Maximum-likelihood estimator (MLE)

$\arg\min_{\mathbf{w}} \mathcal{L}_{\text{MSE}}(\mathbf{w}) = \arg\max_{\mathbf{w}} \mathcal{L}_{\text{LL}}(\mathbf{w})$.

- MLE $\rightarrow$ finding the model under which the observed data is most likely to have been generated from (probabilistically).

Properties of MLE

- MLE is a sample approximation to the expected log-likelihood:

$$\mathcal{L}_{\text{LL}}(\mathbf{w}) \approx \mathbb{E}_{p(y,\mathbf{x})}[\log p(y \mid \mathbf{x}, \mathbf{w})]$$

- MLE is consistent, i.e., it will give us the correct model assuming that we have a sufficient amount of data. (can be proven under some weak conditions)

$\mathbf{w}_{\text{MLE}} \longrightarrow^{p} \mathbf{w}_{\text{true}}$ in probability

- The MLE is asymptotically normal, i.e.,

$(\mathbf{w}_{\text{MLE}} - \mathbf{w}_{\text{true}}) \longrightarrow^{d}$

$\frac{1}{\sqrt{N}}\mathcal{N}\left(\mathbf{w}_{\text{MLE}} \mid \mathbf{0}, \mathbf{F}^{-1}(\mathbf{w}_{\text{true}})\right)$

where $\mathbf{F}(\mathbf{w}) = -\mathbb{E}_{p(\mathbf{y})}\left[\frac{\partial^2 \mathcal{L}}{\partial \mathbf{w} \partial \mathbf{w}^\top}\right]$ is the Fisher information.

- MLE is efficient, i.e. it achieves the Cramer-Rao lower bound. Covariance $(\mathbf{w}_{\text{MLE}}) = \mathbf{F}^{-1}(\mathbf{w}_{\text{true}})$

Laplace distribution

$p(y_n \mid \mathbf{x}_n, \mathbf{w}) = \frac{1}{2b} e^{-\frac{1}{b}|y_n - \mathbf{x}_n^\top \mathbf{w}|}$

Regularization

$\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}) + \Omega(\mathbf{w})$

L_2-Regularization: Ridge Regression

- Standard Euclidean norm (L_2- norm):

$\Omega(\mathbf{w}) = \lambda\|\mathbf{w}\|_2^2$ where $\|\mathbf{w}\|_2^2 = \sum_i w_i^2$.

- When $\mathcal{L}$ is MSE, this is called ridge regression:

$\min_{\mathbf{w}} \frac{1}{2N}\sum_{n=1}^{N}\left[y_n - \mathbf{x}_n^\top \mathbf{w}\right]^2 + \lambda\|\mathbf{w}\|_2^2$

- Least squares is a special case of this: set $\lambda := 0$.

Explicit solution for w:

$\nabla = \nabla\mathcal{L} + \nabla\Omega = -\frac{1}{N}X^T(y - Xw) + \lambda 2w = 0 \Rightarrow$

$\mathbf{w}^\star_{\text{ridge}} = \left(\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I}\right)^{-1}\mathbf{X}^\top\mathbf{y}$

(here for simpler notation $\frac{\lambda'}{2N} = \lambda$)

Ridge Regression Fights Ill-Conditioning

- Lifting the eigenvalues : The eigenvalues of $\left(\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I}\right)$ are all at least λ' and so the inverse always exists.

- Proof: Write the Eigenvalue decomposition of $\mathbf{X}^\top\mathbf{X}$ as $\mathbf{USU}^\top$. We then have

$\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I} = \mathbf{USU}^\top + \lambda'\mathbf{UIU}^\top = \mathbf{U}\left[\mathbf{S} + \lambda'\mathbf{I}\right]\mathbf{U}^\top$

- Alternative proof: Recall that for a symmetric matrix $\mathbf{A}$ we can also compute eigenvalues by looking at the so-called Rayleigh ratio,

$R(\mathbf{A}, \mathbf{v}) = \frac{\mathbf{v}^\top\mathbf{A}\mathbf{v}}{\mathbf{v}^\top\mathbf{v}}$

Note that if $\mathbf{v}$ is an eigenvector with eigenvalue λ then the Rayleigh coefficient indeed gives us λ. We can find the smallest and largest eigenvalue by minimizing and maximizing this coefficient. But note that if we apply this to the symmetric matrix $\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I}$ then for any vector $\mathbf{v}$ we have

$\frac{\mathbf{v}^\top(\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I})\mathbf{v}}{\mathbf{v}^\top\mathbf{v}} \geq \frac{\lambda'\mathbf{v}^\top\mathbf{v}}{\mathbf{v}^\top\mathbf{v}} = \lambda'$

L_1-Regularization: The Lasso

- L_1-norm in combination with the MSE cost function, this is known as the Lasso:

$\min_{\mathbf{w}} \frac{1}{2N}\sum_{n=1}^{N}\left[y_n - \mathbf{x}_n^\top\mathbf{w}\right]^2 + \lambda\|\mathbf{w}\|_1$

where $\|\mathbf{w}\|_1 := \sum_i |w_i|$

- For L_1-regularization the optimum solution is likely going to be sparse (only has few non-zero components) compared to the case where we use L_2-regularization. Sparsity is desirable, since it leads to a "simple" model.

Geometric Interpretation

- Assume that $\mathbf{X}^\top\mathbf{X}$ is invertible. We claim that in this case the set $\left\{\mathbf{w} : \|\mathbf{y} - \mathbf{Xw}\|^2 = \alpha\right\}$ is an ellipsoid and this ellipsoid simply scales around its origin as we change α.

- First look at $\alpha = \|\mathbf{Xw}\|^2 = \mathbf{w}^\top\mathbf{X}^\top\mathbf{Xw}$. This is a quadratic form. Let $\mathbf{A} = \mathbf{X}^\top\mathbf{X}$. Note that $\mathbf{A}$ is a symmetric matrix and by assumption it has full rank. If $\mathbf{A}$ is a diagonal matrix with strictly positive elements a_i along the diagonal then this describes the equation $\sum_i a_i\mathbf{w}_i^2 = \alpha$ which is indeed the equation for an ellipsoid. In the general case, $\mathbf{A}$ can be written as (using the SVD) $\mathbf{A} = \mathbf{UBU}^T$, where $\mathbf{B}$ is a diagonal matrix with strictly positive entries. This then corresponds to an ellipsoid with rotated axes. If we now look at $\alpha = \|\mathbf{y} - \mathbf{Xw}\|^2$, where $\mathbf{y}$ is in the column space of $\mathbf{X}$ then we can write it as $\alpha = \|\mathbf{X}(\mathbf{w}_0 - \mathbf{w})\|^2$ for a suitable chosen $\mathbf{w}_0$ and so this corresponds to a shifted ellipsoid. Finally, for the general case, write $\mathbf{y}$ as $\mathbf{y} = \mathbf{y}_\parallel + \mathbf{y}_\perp$, where $\mathbf{y}_\parallel$is the component of $\mathbf{y}$ that lies in the subspace spanned by the columns of $\mathbf{X}$ and $\mathbf{y}_\perp$ is the component that is orthogonal. In this case

$$\begin{aligned}\alpha &= \|\mathbf{y} - \mathbf{Xw}\|^2 \\ &= \|\mathbf{y}_\parallel + \mathbf{y}_\perp - \mathbf{Xw}\|^2 \\ &= \|\mathbf{y}_\perp\|^2 + \|\mathbf{y}_\parallel - \mathbf{Xw}\|^2 \\ &= \|\mathbf{y}_\perp\|^2 + \|\mathbf{X}(\mathbf{w}_0 - \mathbf{w})\|^2 .\end{aligned}$$

Hence this is then equivalent to the equation $\|\mathbf{X}(\mathbf{w}_0 - \mathbf{w})\|^2 = \alpha - \|\mathbf{y}_\perp\|^2$, proving the claim. From this we also see that if $\mathbf{X}^\top\mathbf{X}$ is not full rank then what we get is not an ellipsoid but a cylinder with an ellipsoidal cross-subsection.

Ridge Regression as MAP estimator

- Least squares as MLE:

$$\begin{aligned}\mathbf{w}_{\text{lse}} &\overset{(a)}{=} \arg\min_{\mathbf{w}} -\log p(\mathbf{y}, \mathbf{X} \mid \mathbf{w}) \\ &\overset{(b)}{=} \arg\min_{\mathbf{w}} -\log p(\mathbf{X} \mid \mathbf{w})p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) \\ &\overset{(c)}{=} \arg\min_{\mathbf{w}} -\log p(\mathbf{X})p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) \\ &\overset{(d)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) \\ &\overset{(e)}{=} \arg\min_{\mathbf{w}} \quad -\log\left[\prod_{n=1}^{N} p(y_n \mid \mathbf{x}_n, \mathbf{w})\right] \\ &\overset{(f)}{=} \arg\min_{\mathbf{w}} -\log\left[\prod_{n=1}^{N}\mathcal{N}\left(y_n \mid \mathbf{x}_n^\top\mathbf{w}, \sigma^2\right)\right] \\ &= \arg\min_{\mathbf{w}} -\log\left[\prod_{n=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2\sigma^2}\left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2}\right] \\ &= \arg\min_{\mathbf{w}} -N\log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) \\ &\quad + \sum_{n=1}^{N}\frac{1}{2\sigma^2}\left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2 \\ &= \arg\min_{\mathbf{w}} \frac{1}{2\sigma^2}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2\end{aligned}$$

- Ridge as MAP:

$$\begin{aligned}\mathbf{w}_{\text{ridge}} &= \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{w} \mid \mathbf{X}, \mathbf{y}) \\ &\overset{(a)}{=} \arg\min_{\mathbf{w}} -\log\frac{p(\mathbf{y}, \mathbf{X} \mid \mathbf{w})p(\mathbf{w})}{p(\mathbf{y}, \mathbf{X})} \\ &\overset{(b)}{=} \arg\min_{\mathbf{w}} -\log p(\mathbf{y}, \mathbf{X} \mid \mathbf{w})p(\mathbf{w}) \\ &\overset{(c)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{y} \mid \mathbf{X}, \mathbf{w})p(\mathbf{w}) \\ &= \arg\min_{\mathbf{w}} -\log\left[p(\mathbf{w})\prod_{n=1}^{N} p(y_n \mid \mathbf{x}_n, \mathbf{w})\right] \\ &= \arg\min_{\mathbf{w}} -\log\mathcal{N}\left(\mathbf{w} \mid 0, \frac{1}{\lambda}\mathbf{I}\right) \\ &\quad \times \prod_{n=1}^{N}\mathcal{N}\left(y_n \mid \mathbf{x}_n^\top\mathbf{w}, \sigma^2\right) \\ &= \arg\min_{\mathbf{w}} -\log\frac{1}{\left(2\pi\frac{1}{\lambda}\right)^{D/2}}e^{-\frac{\lambda}{2}\|\mathbf{w}\|^2} \\ &\quad \times \prod_{n=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2\sigma^2}\left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2} \\ &= \arg\min_{\mathbf{w}} \sum_{n=1}^{N}\frac{1}{2\sigma^2}\left(y_n - \mathbf{x}_n^\top\mathbf{w}\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2\end{aligned}$$

- Ridge regression has a very similar interpretation.

- We start with the posterior $p(\mathbf{w} \mid \mathbf{X}, \mathbf{y})$ and chose that parameter $\mathbf{w}$ that maximizes this posterior. Hence this is called the maximum-a-posteriori (MAP) estimate.

- As before, we take the log and add a minus sign and minimize instead.

- In order to compute the posterior we use Bayes law and we assume that the components of the weight vector are iid Gaussians with mean zero and variance $\frac{1}{\lambda}$.

In step (a) we used Bayes' law. In step (b) and (c) we eliminated quantities that do not depend on $\mathbf{w}$.

Model Selection

Probabilistic Setup

- Unknown distribution $\mathscr{D}$ with range $\mathscr{X} \times \mathscr{Y}$

- We see a dataset S of independent samples from $\mathscr{D}$: $S = \{(x_n, y_n)\}_{n=1}^{N} \sim \mathscr{D}$ i.i.d.

Learning Algorithm: $\mathscr{A}(S) = f_S$

Generalization Error

- How accurate is f at predicting?

- We compute the expected error over all samples drawn from distribution $\mathscr{D}$:

$L_{\mathscr{D}}(f) = \mathbb{E}_{(x,y)\sim\mathscr{D}}[\ell(y, f(x))]$

where $\ell(\cdot, \cdot)$ is the loss function

The quantity $L_{\mathscr{D}}(f)$ has many names:

True	Risk
Expected	Error
Generalization	Loss

- Problem: $mathscrD$ is unknown!

Empirical Error

- approximate the true error by averaging the loss function over the dataset

$L_S(f) = \frac{1}{|S|}\sum_{(x_n,y_n)\in S}\ell(y_n, f(x_n))$

Also called: empirical risk/error/loss

- The samples are random thus $L_S(f)$ is a random variable It is an unbiased estimator of the true error

- Law of large number: $L_S(f) \underset{|S|\to\infty}{\rightarrow} L_{\mathscr{D}}(f)$ but fluctuations!

- Generalization gap: $|L_{\mathscr{D}}(f) - L_S(f)|$

Training error

- what we are minimizing

- the prediction function f_S is itself a function of the data S

- trained on the same data it is applied to, the empirical error is called the training error:

$L_S(f_S) = \frac{1}{|S|}\sum_{(x_n,y_n)\in S}\ell(y_n, f_S(x_n))$

- might not be representative of the error we see on "fresh" samples

- $L_S(f_S)$ might not be close to $L_{\mathscr{D}}(f_S)$ i.e. overfitting

Generalization gap

- How far is the test from the true error?

- Claim: given a model f and a test set $S_{\text{test}} \sim \mathscr{D}$ i.i.d. (not used to learn f) and a loss $\ell(\cdot,\cdot) \in [a,b]$:

$$\mathbb{P}\left[\underbrace{|L_{\mathscr{D}}(f) - L_{S_{\text{test}}}(f)|}_{\text{Generalization Gap}} \geq \sqrt{\frac{(b-a)^2\ln(2/\delta)}{2|S_{\text{test}}|}}\right] \leq \delta$$

- The error decreases as $\mathcal{O}\left(1/\sqrt{|S_{\text{test}}|}\right)$ with the number of test points High probability bound: δ is only in the ln

$\rightarrow$ The more data points we have, the more confident we are that the empirical loss we measure is close to the true loss

- Given a dataset S

1. Split: $S = S_{\text{train}} \cup S_{\text{test}}$
2. Train: $\mathscr{A}(S_{\text{train}}) = f_{S_{\text{train}}}$
3. Validate: $\mathbb{P}\left(L_{\mathscr{D}}(f_{S_{\text{train}}}) \geq L_{S_{\text{test}}}(f_{S_{\text{train}}}) + \sqrt{\frac{(a-b)^2\ln(2/\delta)}{2|S_{\text{test}}|}}\right) \leq \delta$

$\Rightarrow$ We can obtain a probabilistic upper bound on the expected risk

The proof relies only on concentration inequalities

- $(x_n, y_n) \in S_{\text{test}}$ are chosen independently, the associated losses $\Theta_n = \ell(y_n, f(x_n)) \in [a,b]$ given a fixed model f, are also i.i.d. random variables

- Empirical loss:
$\frac{1}{N}\sum_{n=1}^N \Theta_n = \frac{1}{N}\sum_{n=1}^N \ell(y_n, f(x_n)) = L_{S_{\text{test}}}(f)$
- True loss: $\mathbb{E}[\Theta_n] = \mathbb{E}[\ell(y_n, f(x_n))] = L_{\mathscr{D}}(f)$

- What is the chance that the empirical loss $L_{S_{\text{test}}}(f)$ deviates from the true loss by more than a given constant? $\rightarrow$ concentration inequalities

Hoeffding inequality: a simple concentration bound

- Claim: Let $\Theta_1, \ldots, \Theta_N$ be a sequence of i.i.d. random variables with mean $\mathbb{E}[\Theta]$ and range $[a,b]$. Then, for any $\varepsilon > 0$

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{n=1}^N \Theta_n - \mathbb{E}[\Theta]\right| \geq \varepsilon\right] \leq 2e^{-2N\varepsilon^2/(b-a)^2}$$

- Concentration bound: the empirical mean is concentrated around its mean

A. Use it with $\Theta_n = \ell(y_n, f(x_n))$

B. Equating $\delta = 2e^{-2|S_{\text{test}}|\varepsilon^2/(b-a)^2}$ we get
$\varepsilon = \sqrt{\frac{(b-a)^2\ln(2/\delta)}{2|S_{\text{test}}|}}$

- Does model selection work? $L_{S_{\text{test}}}(f_{S_{\text{train}},\lambda_k}) \approx L_{\mathscr{D}}(f_{S_{\text{train}},\lambda_k})$?

How far is each of the K test errors $L_{S_{\text{test}}}(f_k)$ from the true $L_{\mathscr{D}}(f_k)$?

- Claim: we can bound the maximum deviation for all K candidates, by

$$\mathbb{P}\left[\max_k |L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k)| \geq \sqrt{\frac{(b-a)^2\ln(2K/\delta)}{2|S_{\text{test}}|}}\right] \leq \delta$$

- The error decreases as $\mathcal{O}\left(1/\sqrt{|S_{\text{test}}|}\right)$ with the number test points
- When testing K hyper-parameters, the error only goes up by $\sqrt{\ln(K)}$

$\Rightarrow$ So we can test many different models without incurring a large penalty

- It can be extended to infinitely many models

Proof: A simple union bound

- Special case $K = 1$

$\mathbb{P}[\max_k |L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k)| \geq \varepsilon]$
$= \mathbb{P}[\cup_k \{|L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k)| \geq \varepsilon\}]$
$\leq \sum_k \mathbb{P}[|L_{\mathscr{D}}(f_k) - L_{S_{\text{test}}}(f_k)| \geq \varepsilon]$
$\leq 2Ke^{-2N\varepsilon^2/(b-a)^2}$

- Equating $\delta = 2Ke^{-2N\varepsilon^2/(b-a)^2}$, we get $\varepsilon = \sqrt{\frac{(b-a)^2\ln(2K/\delta)}{2N}}$ as stated

- If we choose the "best" function according to the empirical risk then its true risk is not too far away from the true risk of the optimal choice

- Let $k^* = \text{argmin}_k L_{\mathscr{D}}(f_k)$ (smallest true risk) and $\hat{k} = \text{argmin}_k L_{S_{\text{test}}}(f_k)$ (smallest empirical risk) then:

$$\mathbb{P}\left[L_{\mathscr{D}}(f_{\hat{k}}) \geq L_{\mathscr{D}}(f_{k^*}) + 2\sqrt{\frac{(b-a)^2\ln(2K/\delta)}{2|S_{\text{test}}|}}\right] \leq \delta$$

Hoeffding's inequality Proof

- We equivalently assume that $\mathbb{E}[\Theta] = 0$ and that $\Theta_n \in [a,b]$
- We will only show that
$\mathbb{P}\left\{\frac{1}{N}\sum_{n=1}^N \Theta_n \geq \varepsilon\right\} \leq e^{-2N\varepsilon^2/(b-a)^2}$

This, together with the equivalent bound
$\mathbb{P}\left\{\frac{1}{N}\sum_{n=1}^N \Theta_n \leq -\varepsilon\right\} \leq e^{-2N\varepsilon^2/(b-a)^2}$
will prove the claim:

For any $s \geq 0$, $\mathbb{P}\left\{\frac{1}{N}\sum_{n=1}^N \Theta_n \geq \varepsilon\right\} = \mathbb{P}\left\{s\frac{1}{N}\sum_{n=1}^N \Theta_n \geq s\varepsilon\right\}$
$= \mathbb{P}\left\{e^{s\frac{1}{N}\sum_{n=1}^N \Theta_n} \geq e^{s\varepsilon}\right\}$
$\leq \mathbb{E}\left[e^{s\frac{1}{N}\sum_{n=1}^N \Theta_n}\right] e^{-s\varepsilon}$ (Markov inequality)
$= \prod_{n=1}^N \mathbb{E}\left[e^{\frac{s\Theta_n}{N}}\right] e^{-s\varepsilon}$ (the r.v Θ_n are indep.)
$= \mathbb{E}\left[e^{\frac{s\Theta}{N}}\right]^N e^{-s\varepsilon}$ (the r.v Θ_n are i.d.)
$\leq e^{s^2(b-a)^2/(8N)} e^{-s\varepsilon}$ (Hoeffding lemma)

What do we do now? We have for any $s \geq 0$
$\mathbb{P}\left\{\frac{1}{N}\sum_{n=1}^N \Theta_n \geq \varepsilon\right\} \leq e^{s^2(b-a)^2/(8N)} e^{-s\varepsilon}$

In particular for the minimum value obtained for $s = \frac{4N\varepsilon}{(b-a)^2}$
$\mathbb{P}\left\{\frac{1}{N}\sum_{n=1}^N \Theta_n \geq \varepsilon\right\} \leq e^{-2N\varepsilon^2/(b-a)^2}$

Hoeffding lemma

For any random variable X, with $\mathbb{E}[X] = 0$ and $X \in [a,b]$ we have
$\mathbb{E}\left[e^{sX}\right] \leq e^{\frac{1}{8}s^2(b-a)^2}$ for any $s \geq 0$

Proof outline:

Consider the convex function $s \mapsto e^{sx}$. In the range $[a,b]$ it is upper bounded by the chord
$e^{sx} \leq \frac{x-a}{b-a}e^{sb} + \frac{b-x}{b-a}e^{sa}$

Taking the expectation and recalling that $\mathbb{E}[X] = 0$, we get
$\mathbb{E}\left[e^{sX}\right] \leq \frac{b}{b-a}e^{sa} - \frac{a}{b-a}e^{sb} \leq e^{s^2(b-a)^2/8}$

Bias Variance Decomposition

- Simple models have large bias but low variance
- Complex models have low bias but high variance
- We need to balance bias & variance correctly
- Data model: output perturbed by some noise
$y = f(x) + \varepsilon$
$\varepsilon \sim \mathscr{D}_\varepsilon \approx$ i.i.d. independent of x $\mathbb{E}[\varepsilon] = 0$
- We consider the square loss and will provide a decomposition of the true error

Error Decomposition

- We are interested in how the expected error of f_S: $\mathbb{E}_{(x,y)\sim D}\left[(y - f_S(x))^2\right]$
- The decomposition will hold true at every single point x. Therefore, to simplify, we consider the expected error of f_S for a fixed element x_0 :
$L(f_S) = \mathbb{E}_{\varepsilon\sim\mathscr{D}_\varepsilon}\left[(f(x_0) + \varepsilon - f_S(x_0))^2\right]$
- This is a random variable. The randomness comes for the train set S
- We run the experiment many times, and we are interested in the average and the variance of the predictions $(f_{S_1}, \cdots, f_{S_k})$ over these multiple runs

A decomposition in three terms

We are interested in the expectation of the true risk over the training set S
$\mathbb{E}_{S\sim\mathscr{D}}[L(f_S)]$
$= \mathbb{E}_{S\sim\mathscr{D}}[\mathbb{E}_{\varepsilon\sim D_\varepsilon}[(f(x_0) + \varepsilon - f_S(x_0))^2]]$
$= \mathbb{E}_{S\sim\mathscr{D},\varepsilon\sim\mathscr{D}_\varepsilon}[(f(x_0) + \varepsilon - f_S(x_0))^2]$
$= \mathbb{E}_{\varepsilon\sim\mathscr{D}_\varepsilon}\left[\varepsilon^2\right]$
$+ 2\mathbb{E}_{S\sim\mathscr{D},\varepsilon\sim\mathscr{D}_\varepsilon}\left[\varepsilon\left(f(x_0) - f_S(x_0)\right)\right]$
$+ \mathbb{E}_{S\sim\mathscr{D}}\left[\left(f(x_0) - f_S(x_0)\right)^2\right]$

Using that $\mathbb{E}_{\varepsilon\sim\mathscr{D}}[\varepsilon] = 0$ and $\varepsilon \perp\!\!\!\perp S$:
- $\mathbb{E}_{\varepsilon\sim\mathscr{D}_\varepsilon}\left[\varepsilon^2\right] = \text{Var}_{\varepsilon\sim\mathscr{D}_\varepsilon}[\varepsilon]$
- $\mathbb{E}_{S\sim\mathscr{D},\varepsilon\sim\mathscr{D}_\varepsilon}\left[\varepsilon\left(f(x_0) - f_S(x_0)\right)\right] = \mathbb{E}_{\varepsilon\sim\mathscr{D}\varepsilon}[\varepsilon] \times \mathbb{E}_{S\sim\mathscr{D}}\left[f(x_0) - f_S(x_0)\right] = 0$

$\Rightarrow$
$\mathbb{E}_{S\sim\mathscr{D},\varepsilon\sim\mathscr{D}_\varepsilon}\left[(f(x_0) + \varepsilon - f_S(x_0))^2\right] =$
$\text{Var}_{\varepsilon\sim D_\varepsilon}[\varepsilon] + \mathbb{E}_{S\sim\mathscr{D}}\left[(f(x_0) - f_S(x_0))^2\right]$

Trick: we add and subtract the constant term $\mathbb{E}_{S'\sim D}[f_{S'}(x_0)]$, where S' is a second training set independent from S

$$\begin{aligned}\mathbb{E}_{S\sim\mathscr{D}}\left[(f(x_0) - f_S(x_0))^2\right] &= \mathbb{E}_{S\sim\mathscr{D}}\left[(f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] + \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] - f_S(x_0))^2\right] \\ &= \mathbb{E}_{S\sim\mathscr{D}}\left[(f(x_0) - \mathbb{E}_{S'\sim D}[f_{S'}(x_0)])^2 + (\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] - f_S(x_0))^2\right. \\ &\quad \left. + 2\left(f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]\right)\left(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] - f_S(x_0)\right)\right]\end{aligned}$$

Cross-term:
$$\begin{aligned}&\mathbb{E}_{S\sim\mathscr{D}}[(f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]) \cdot (\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] - f_S(x_0))] \\ &= (f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]) \cdot \mathbb{E}_{S\sim\mathscr{D}}[(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] - f_S(x_0))] \\ &= (f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]) \cdot (\mathbb{E}_{S'\sim D}[f_{S'}(x_0)] - \mathbb{E}_{S\sim\mathscr{D}}[f_S(x_0)]) = 0.\end{aligned}$$

$\Rightarrow \mathbb{E}_{S\sim\mathscr{D}}\left[(f(x_0) - f_S(x_0))^2\right]$
$= (f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2$
$+ \mathbb{E}_{S\sim\mathscr{D}}\left[(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)] - f_S(x_0))^2\right]$

Bias-Variance Decomposition

- We obtain the following decomposition into three positive terms:

$\mathbb{E}_{S\sim\mathscr{D},\varepsilon\sim\mathscr{D}_\varepsilon}\left[(f(x_0) + \varepsilon - f_S(x_0))^2\right]$
$= \text{Var}_{\varepsilon\sim\mathscr{D}_\varepsilon}[\varepsilon] \leftarrow$ Noise variance
$+ (f(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2 \leftarrow$ Bias
$+ \mathbb{E}_{S\sim\mathscr{D}}\left[(f_S(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2\right] \leftarrow$ Var.

- each of which always provides a lower bound of the true error

- $\Rightarrow$ To minimize the true error, we must choose a method that achieves low bias and low variance simultaneously

Noise: $\text{Var}_{\varepsilon\sim\mathscr{D}_\varepsilon}[\varepsilon]$

- a strict lower bound on the achievable error
- It is not possible to go below the noise level
- Even if we know the true model f, we still suffer from the noise: $L(f) = \mathbb{E}\left[\varepsilon^2\right]$
- It is not possible to predict the noise from the data since they are independent

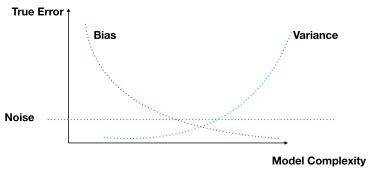
Bias: $(f(x_0) - \mathbb{E}_{S\sim\mathscr{D}}[f_S(x_0)])^2$

- Squared of the difference between the actual value $f(x_0)$ and the expected prediction
- It measures how far off in general the models' predictions are from the correct value
- If model complexity is low, bias is typically high
- If model complexity is high, bias is typically low

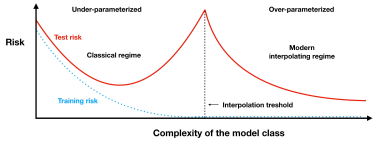
Variance: $\mathbb{E}_{S\sim\mathscr{D}}\left[\left(f_S(x_0) - \mathbb{E}_{S\sim D}[f_S(x_0)]\right)^2\right]$

- Variance of the prediction function
- It measures the variability of predictions at a given point across different training set realizations
- If we consider complex models, small variations in the training set can lead to significant changes in the predictions

Bias Variance tradeoff



Double descent curve



Classification

- Linear Decision boundaries: Assume we restrict ourselves to linear decision boundaries (hyperplane):

$\Rightarrow$ Prediction: $f(x) = \text{sign}\left(x^\top w\right)$

- Assume the data are linearly separable, i.e., a separating hyperplane exists

Margin

- Key concept: The margin is the distance from the hyperplane to the closest point

$\Rightarrow$ Take the one with the largest margin!

- Max-margin separating hyperplane: Choose the hyperplane which maximizes the margin Why: If we slightly change the training set, the number of misclassifications will stay low

$\Rightarrow$ It will lead us to support vector machine (SVM) and logistic regression

Formalizing Binary Classification

- Setting: $(X, Y) \sim \mathscr{D}$ with ranges $\mathscr{X}, \mathscr{Y} = \{-1, 1\}$
- Loss function: (0-1 Loss) $\ell(y, y') = 1_{y \neq y'} = \begin{cases} 1 & \text{if } y \neq y' \\ 0 & \text{if } y = y' \end{cases}$
- True risk for the classification:

$L_{\mathscr{D}}(f) = \mathbb{E}_{\mathscr{D}}\left[1_{Y \neq f(X)}\right] = \mathbb{P}_{\mathscr{D}}[Y \neq f(X)]$ (resp. classification error = probability of making an error)

- Goal: minimize $L_{\mathscr{D}}(f)$

Bayes classifier

- Def: The classifier $f_* = \arg\min L_{\mathscr{D}}(f)$ is called the Bayes classifier f
- Claim: $f_*(x) = \arg\max_{y \in \{-1,1\}} \mathbb{P}(Y = y \mid X = x)$
- Note: Bayes classifier is an unattainable gold standard, as we never know the underlying data distribution $\mathscr{D}$ in practice

Proof of the Bayes classifier

- Claim 1: $\forall x \in \mathscr{X}, f_*(x) \in \arg\min_{y \in \mathscr{Y}} \mathbb{P}(Y \neq y \mid X = x) \Longrightarrow f_* \in \arg\min_{f: \mathscr{X} \to \mathscr{Y}} L_{\mathscr{D}}(f)$

$L_{\mathscr{D}}(f) = \mathbb{E}_{X,Y}\left[1_{Y \neq f(X)}\right] = \mathbb{E}_X\left[\mathbb{E}_{Y|X}\left[1_{Y \neq f(X)} \mid X\right]\right]$
$= \mathbb{E}_X[\mathbb{P}(Y \neq f(X) \mid X)]$
$\geq \mathbb{E}_X[\min_{y \in \mathscr{Y}} \mathbb{P}(Y \neq y \mid X)]$
$= \mathbb{E}_X[\mathbb{P}(Y \neq f_*(X) \mid X)] = \mathbb{E}_{X,Y}\left[1_{Y \neq f_*(X)}\right] = L_{\mathscr{D}}(f_*)$

- Claim 2: $f_*(x) = \arg\min_{y \in \mathscr{Y}} \mathbb{P}(Y \neq y \mid X = x)$

$f_*(x) = \arg\max_{y \in \mathscr{Y}} \mathbb{P}(Y = y \mid X = x) = \arg\min_{y \in \mathscr{Y}} \mathbb{P}(Y \neq y \mid X = x)$

Two classes of classification algorithms

- Non-parametric: approximate the conditional distribution $\mathbb{P}(Y = y \mid X = x)$ via local averaging $\Rightarrow$ KNN
- Parametric: approximate true distribution $\mathscr{D}$ via training data $\Rightarrow$ Minimize the empirical risk on training data (ERM)

Classification by empirical risk minimization

- How: minimize the empirical risk instead of the true risk:

$\min_{f: X \to Y} L_{\text{train}}(f) := \frac{1}{N}\sum_{n=1}^N 1_{f(x_n) \neq y_n} = \frac{1}{N}\sum_{n=1}^N 1_{y_n f(x_n) \leq 0}$

- Problem: L_{train} is not convex:

The set of classifiers is not convex because $\mathcal{Y}$ is discrete

The indicator function 1 is not convex because it is not continuous

Convex relaxation of the classification risk

- Instead of learning $f: \mathscr{X} \to \mathscr{Y}$, learn $g: \mathscr{X} \to \mathbb{R}$ in a convex subset of continuous functions $\mathscr{G}$, and predict with $f(x) = \text{sign}(g(x))$. The problem becomes

$\min_{g \in \mathscr{G}} \frac{1}{N}\sum_{n=1}^N 1_{y_n g(x_n) \leq 0}$

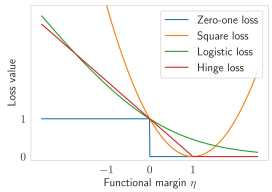
- Replace the indicator function by a convex $\phi: \mathbb{R} \to \mathbb{R}$ and minimize

$\min_{g \in \mathscr{G}} \frac{1}{N}\sum_{n=1}^N \phi(y_n g(x_n))$

ϕ is a function of the functional margin $y_n g(x_n)$

$\Rightarrow$ This is a convex problem!

Remark: possible to bound the zero-one risk $L(f)$ by the ϕ risk



Losses for Classification

- Logistic loss $\rightarrow$ logistic regression
- Hinge loss $\rightarrow$ max margin classification

Good regressor $\Rightarrow$ good classifier

- Consider $\mathscr{Y} = \{0, 1\}$, for all regression functions $\eta: \mathscr{X} \to \mathbb{R}$ we can define a classifier as $\mathscr{X} \to \{0, 1\}$

$f_\eta: x \mapsto 1_{\eta(x) \geq 1/2}$

- Claim:

$L_{\mathscr{D}}^{\text{classif}}(f_\eta) - L_{\mathscr{D}}^{\text{classif}}(f^*) \leq 2\sqrt{L_{\mathscr{D}}^{\ell_2}(\eta) - L_{\mathscr{D}}^{\ell_2}(\eta^*)}$

Where $L_{\mathscr{D}}^{\text{classif}}(f_\eta) = \mathbb{E}_{\mathscr{D}}\left[1_{f(X) \neq Y}\right], L_{\mathscr{D}}^{\ell_2}(f) = \mathbb{E}_{\mathscr{D}}\left[(Y - f(X))^2\right]$ and $\eta_* = \arg\min_\eta L_{\mathscr{D}}^{\ell_2}(\eta)$

$\Rightarrow$ If η is good for regression then f_η is good for classification too (converse is not true)

Logistic Regression

- Binary classification : We observe some data $S = \{x_n, y_n\}_{n=1}^N \in \mathscr{X} \times \{0, 1\}$

Motivation for logistic regression

Instead of directly modeling the output Y, we can model the probability that Y belongs to a specific class. Map the prediction from $(-\infty, +\infty)$ to $[0, 1]$

The logistic function

$\sigma(\eta) := \frac{e^\eta}{1+e^\eta}$

- Properties of the logistic function:

$1 - \sigma(\eta) = \frac{1+e^\eta - e^\eta}{1+e^\eta} = (1+e^\eta)^{-1}$ $\sigma'(\eta) = \frac{e^\eta(1+e^\eta) - e^\eta e^\eta}{(1+e^\eta)^2} = \frac{e^\eta}{(1+e^\eta)^2} = \sigma(\eta)(1-\sigma(\eta))$

Logistic Regression

$p(1 \mid x) := \mathbb{P}(Y = 1 \mid X = x) = \sigma\left(x^\top w + w_0\right)$

$p(0 \mid x) := \mathbb{P}(Y = 0 \mid X = x) = 1 - \sigma\left(x^\top w + w_0\right)$

Logistic regression models the probability that Y belongs to a particular class using the logistic function σ

Label prediction: quantize the probability:

If $p(1 \mid x) \geq 1/2$, you predict the class 1

If $p(1 \mid x) < 1/2$, you predict the class 0

- Interpretation:

Very large $\left|x^\top w + w_0\right|$ corresponds to $p(1 \mid x)$ very close to 0 or 1 (high confidence)

Small $\left|x^\top w + w_0\right|$ corresponds to $p(1 \mid x)$ very close to .5 (low confidence)

Comparison of logistic and linear regression for data with extreme values

- More robust to unbalanced data and extremes.

Geometric Interpretation

- The vector w is orthogonal to the "surface of transition"
- The transition between the two levels happens at the hyperplane $w^\perp = \{v, v^\top w = 0\}$
- Scaling w makes the transition faster or slower
- Changing w_0 shifts the decision region along the w vector
- The transition happens at the hyperplane $\{v, v^\top w + w_0 = 0\}$
- Bias term: should consider a shift w_0 as there is no reason for the transition hyperplane to pass through the origin: $p(1 \mid x) = \sigma\left(w^\top x + w_0\right)$ For simplicity, add the constant 1 to the feature vector $x = \begin{pmatrix} x \\ 1 \end{pmatrix}$ It is crucial for allowing to shift the decision region

MLE for logistic regression

- Assumption: The inputs $\mathbf{X}$ do not depend on the parameter w we choose:

$\mathscr{L}(w) = p(\mathbf{y}, \mathbf{X} \mid w) = p(\mathbf{X} \mid w)p(\mathbf{y} \mid \mathbf{X}, w)$
$\underset{\mathbf{X} \perp\!\!\!\perp w}{=} p(\mathbf{X})p(\mathbf{y} \mid \mathbf{X}, w)$

$p(\mathbf{y} \mid \mathbf{X}, w) = \Pi_{n=1}^N p(y_n \mid x_n, w)$
$= \Pi_{n:y_n=1} p(y_n = 1 \mid x_n, w) \times \Pi_{n:y_n=0} p(y_n = 0 \mid x_n, w)$
$= \Pi_{n=1}^N \sigma\left(x_n^\top w\right)^{y_n}\left[1 - \sigma\left(x_n^\top w\right)\right]^{1-y_n}$

The likelihood is proportional to:

$\mathscr{L}(w) \propto \prod_{n=1}^N \sigma\left(x_n^\top w\right)^{y_n}\left[1 - \sigma\left(x_n^\top w\right)\right]^{1-y_n}$

Minimum of the NLL

$-\log(p(\mathbf{y} \mid \mathbf{X}, w))$

$= -\log\left(\prod_{n=1}^N \sigma\left(x_n^\top w\right)^{y_n}\left[1 - \sigma\left(x_n^\top w\right)\right]^{1-y_n}\right)$

$= -\sum_{n=1}^N y_n \log\sigma\left(x_n^\top w\right) + (1 - y_n)\log\left(1 - \sigma\left(x_n^\top w\right)\right)$

$= \sum_{n=1}^N y_n \log\left(\frac{1 - \sigma\left(x_n^\top w\right)}{\sigma\left(x_n^\top w\right)}\right) - \log\left(1 - \sigma\left(x_n^\top w\right)\right)$

$= \sum_{n=1}^N -y_n x_n^\top w + \log\left(1 + e^{x_n^\top w}\right)$

$\longleftarrow 1 - \sigma(\eta) = \frac{1}{1+e^\eta} \Longrightarrow \frac{1-\sigma(\eta)}{\sigma(\eta)} = e^{-\eta}$

We obtain the following cost function we will minimize to learn the parameter $w_* = \arg\min L(w)$

$:= \frac{1}{N}\sum_{n=1}^N -y_n x_n^\top w + \log\left(1 + e^{x_n^\top w}\right)$

- If we are considering $y \in \{-1, 1\}$, we will have a different function

A side note on logistic loss

- In logistic regression, the negative log likelihood is equivalent to ERM for the logistic loss (a surrogate for $0-1$ loss, as discussed yesterday)
- Logistic loss for $y \in \{0, 1\}$:

$\ell(y, g(x)) = -yg(x) + \log(1 + \exp(g(x)))$

- Logistic loss for $y \in \{-1, 1\}$:

$\ell(y, g(x)) = \log(1 + \exp(-yg(x)))$

- Note: the logistic loss can be applied in modern machine learning as well: $g(x)$ can represent the output of a neural network

Gradient of the negative log likelihood

$$\nabla L(w) = \nabla \left[\frac{1}{N} \sum_{n=1}^{N} \log \left(1 + e^{x_n^\top w} \right) - y_n x_n^\top w \right] =$$

$$\frac{1}{N} \sum_{n=1}^{N} \frac{e^{x_n^\top w} x_n}{1 + e^{x_n^\top w}} - y_n x_n = \frac{1}{N} \sum_{n=1}^{N} \left(\sigma \left(x_n^\top w \right) - y_n \right) x_n$$

$$\nabla L(w) = \frac{1}{N} \mathbf{X}^\top (\sigma(\mathbf{X}w) - \mathbf{y})$$

- Same gradient as in LS but with σ - No closed form solution to $\nabla L(w) = 0$ - Good news: the cost function L is convex

Convexity of the loss function L

$L(w) = \frac{1}{N} \sum_{n=1}^{N} -y_n x_n^\top w + \log \left(1 + e^{x_n^\top w} \right)$ is convex in the weight vector w

- Proof: L is obtained through simple convexity preserving operations:

1) Positive combinations of convex functions is convex

2) Composition of a convex and a linear functions is convex

3) A linear function is both convex and concave

4) $\eta \mapsto \log(1 + e^\eta)$ is convex

- Proof of 4: $h(\eta) := \log(1 + e^\eta)$ is cvx

$h'(\eta) = \frac{e^\eta}{1+e^\eta} = \sigma(\eta)$

$h''(\eta) = \sigma'(\eta) = \frac{e^\eta}{(1+e^\eta)^2} \geq 0$

- 2) + 4) $\Rightarrow \log \left(1 + e^{x_n^\top w} \right)$ is convex

- 3) $\Rightarrow -y_n x_n^\top w$ is convex

- 1) $\Rightarrow L(w)$ is convex

Second proof: Hessian of L is psd

- The Hessian $\nabla^2 L$ is the matrix whose entries are the second derivatives $\frac{\partial^2}{\partial w_i \partial w_j} L(w)$

$$\nabla^2 L(w) = \nabla [\nabla L(w)]^\top$$

$$= \nabla \left[\frac{1}{N} \sum_{n=1}^{N} x_n \left(\sigma \left(x_n^\top w \right) - y_n \right) \right]^\top$$

$$= \frac{1}{N} \sum_{n=1}^{N} \nabla \sigma \left(x_n^\top w \right) x_n^\top$$

$$= \frac{1}{N} \sum_{n=1}^{N} \sigma \left(x_n^\top w \right) \left(1 - \sigma \left(x_n^\top w \right) \right) x_n x_n^\top$$

It can be written under the matrix form:

$\nabla^2 L(w) = \frac{1}{N} \mathbf{X}^\top S \mathbf{X}$

where $S = \text{diag} \left[\sigma \left(x_n^\top w \right) \left(1 - \sigma \left(x_n^\top w \right) \right) \right] \succcurlyeq 0$

$\Rightarrow$ L is convex since $\nabla^2 L(w) \geqslant 0$

How to minimize the convex function L?

GD:

$$\begin{cases} w_0 \in \mathbb{R}^d \\ w_{t+1} = w_t - \frac{\gamma_t}{N} \sum_{n=1}^{N} \left(\sigma \left(x_n^\top w_t \right) - y_n \right) x_n \end{cases}$$

- can be slow ($\Theta(N \times T)$)

SGD:

$$\begin{cases} w_0 \in \mathbb{R}^d \\ w_{t+1} = w_t - \gamma_t \left(\sigma \left(x_{n_t}^\top w_t \right) - y_{n_t} \right) x_{n_t} \end{cases}$$

where $\mathbb{P}[n_t = n] = 1/N$

- is faster but converges slower

Newton's method uses second order information

- Newton's method minimizes the quadratic approximation:

$L(w) \sim L(w_t) + \nabla L(w_t)^\top (w - w_t) + \frac{1}{2} (w - w_t)^\top \nabla^2 L(w_t) (w - w_t) := \phi_t(w)$

$\tilde{w} = \arg\min \phi_t(w) \Rightarrow$

$\nabla L(w_t) + \nabla^2 L(w_t) (\tilde{w} - w_t) = 0$

- Newton's method:

$w_{t+1} = w_t - \gamma_t \nabla^2 L(w_t)^{-1} \nabla L(w_t)$

- The step-size is needed to ensure convergence (damped Newton's method)

- The convergence is typically faster than with gradient descent but the computational complexity is higher (computing Hessian and solving a linear system)

Problem when the data are linearly separable

- Weights go to infinity.

$\inf_w L(w) = 0 = \lim_{\alpha \to \infty} L(\alpha \cdot \bar{w})$

- The inf value is not attained for a finite w

- If we use an optimization algorithm, the weights will go to ∞

- Solution: add a ℓ_2-regularization

- Ridge logistic regression:

$\frac{1}{N} \sum_{n=1}^{N} -y_n x_n^\top w + \log \left(1 + e^{x_n^\top w} \right) + \frac{\lambda}{2} \|w\|_2^2$

- Optimization perspective: stabilize the optimization process

- Statistical perspective: avoid overfitting

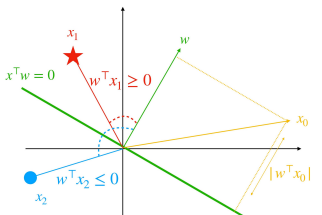
Support Vector Machines

- Vapnik's invention: A training algorithm for optimal margin classifiers

Linear Classifier

- Define a hyperplane as $\{x : w^\top x = 0\}$ where $\|w\| = 1$

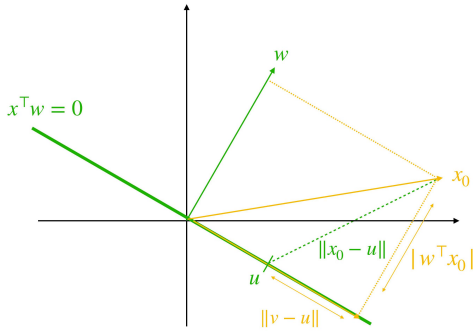
- Prediction: $f(x) = \text{sign} \left(x^\top w \right)$



- Claim: The distance between a point x_0 and the hyperplane defined by w is $|w^\top x_0|$

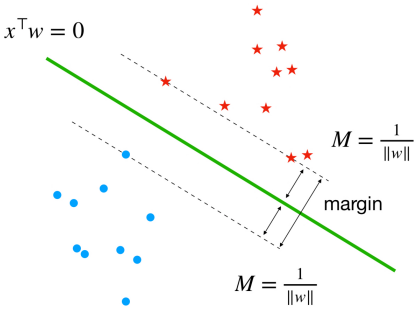
- Proof: The distance between x_0 and the hyperplane is given by $\min_{u : w^\top u = 0} \|x_0 - u\|$

Let $v = x_0 - w^\top x_0 w$ then by the Pythagorean theorem for any u s.t. $w^\top u = 0$



$\|x_0 - u\|^2 = \left(w^\top x_0 \right)^2 + \|v - u\|^2 \geq \left(w^\top x_0 \right)^2$

Hard-SVM rule: max-margin separating hyperplane



- First assume the dataset $(x_n, y_n)_{n=1}^N$ is linearly separable

- Margin of a hyperplane: $\min_{n \leq N} |w^\top x_n|$

- Max-margin separating hyperplane:

$\max_{w, \|w\|=1} \min_{n \leq N} |w^\top x_n|$ s.t. $\forall n, y_n x_n^\top w \geq 0$

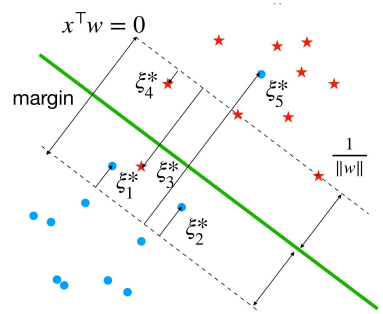
- Equivalent to:

$\max_{M \in \mathbb{R}, w, \|w\|=1} M$ s.t. $\forall n, y_n x_n^\top w \geq M$

- Also equivalent to:

$\min_w \frac{1}{2} \|w\|^2$ such that $\forall n, y_n x_n^\top w \geq 1$

Soft SVM



- A relaxation of the Hard-SVM rule that can be applied even if the training set is not linearly separable

- Idea: Maximize the margin while allowing some constraints to be violated

- Introduce positive slack variables $\xi_1, \cdots, \xi_N$ and replace the constraints with $y_n x_n^\top w \geq 1 - \xi_n$

- Soft SVM:

$$\min_{w, \xi} \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^{N} \xi_n$$

s.t. $\forall n, y_n x_n^\top w \geq 1 - \xi_n$ and $\xi_n \geq 0$

- Equivalent to:

$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^{N} \left[1 - y_n x_n^\top w \right]_+$

(A hinge loss)

$\xi_i^* = \frac{\xi_i}{\|w\|}$

- Proof: Fix w and consider the minimization over ξ :

1) If $y_n x_n^\top w \geq 1$, then $\xi_n = 0$

2) If $y_n x_n^\top w < 1, \xi_n = 1 - y_n x_n^\top w$

Therefore $\xi_n = \left[1 - y_n x_n^\top w \right]_+$

Classification by risk minimization

- $(X, Y) \sim \mathscr{D}$ with ranges $\mathscr{X}$ and $\mathscr{Y} = \{-1, 1\}$

- Goal: Find a classifier $f : \mathscr{X} \to \mathscr{Y}$ that minimizes the true risk $L(f) = \mathbb{E}_{\mathscr{D}} \left(1_{Y \neq f(X)} \right)$

- How: Through Empirical Risk Minimization (ERM):

$\min_w L_{\text{train}}(w) = \frac{1}{N} \sum_{n=1}^{N} \phi \left(y_n w^\top x_n \right)$

ϕ represents the loss function of the functional margin $y_n x_n^\top w$

ϕ also serves as a convex surrogate for the $0 - 1$ loss

Losses for Classification

Examples of margin-based losses $\left(\eta = y x^\top w \right)$:

- Quadratic loss: $\text{MSE}(\eta) = (1 - \eta)^2$ Penalizes any deviation from 1

- Logistic loss: $\text{Logistic}(\eta) = \frac{\log(1 + \exp(-\eta))}{\log(2)}$ Asymmetric cost - a penalty is always incurred.

- Hinge loss: $\text{Hinge}(\eta) = [1-\eta]_+$ A penalty is applied if the prediction is incorrect or lacks confidence
- Common features: these losses are convex and provide an upper bound for the zero-one loss
- Behavioral differences:

Summary

- ERM for the hinge loss with ridge regularization: $\min_w \frac{\lambda}{2}\|w\|^2 + \frac{1}{N}\sum_{n=1}^N \left[1-y_n x_n^\top w\right]_+$
- Interpretation for separable data with small λ :
1) Choose the direction of w such that $w^\perp$ acts as a separating hyperplane
2) Adjust the scale of w to ensure that no point lies with the margin
3) Select the hyperplane with the largest margin

Optimization

$\min_w \frac{1}{N}\sum_{n=1}^N \left[1-y_n x_n^\top w\right]_+ + \frac{\lambda}{2}\|w\|^2$
- How to get w ?
- Convex (but non-smooth) objective which can be minimized with: 1) Subgradient method, 2) Stochastic Subgradient method

Convex duality

- Assume you can define an auxiliary function $G(w,\alpha)$ such that
$\min_w L(w) = \min_w \max_\alpha G(w,\alpha)$
- Primal problem: $\min_w \max_\alpha G(w,\alpha)$
- Dual problem: $\max_\alpha \min_w G(w,\alpha)$
$\Rightarrow$ Sometimes, the dual problem is easier to solve than the primal problem.

How do we find a suitable $G(w,\alpha)$?

$[z]_+ = \max(0,z) = \max_{\alpha\in[0,1]} \alpha z$
- $\left[1-y_n x_n^\top w\right]_+ = \max_{\alpha_n\in[0,1]} \alpha_n \left(1-y_n x_n^\top w\right)$
- The SVM problem is equivalent to: $\min_w L(w) =$

$$\min_w \max_{\alpha\in[0,1]^n} \underbrace{\frac{1}{N}\sum_{n=1}^N \alpha_n\left(1-y_n x_n^\top w\right) + \frac{\lambda}{2}\|w\|_2^2}_{G(w,\alpha)}$$

- The function G is convex in w and concave in α

Can min and max be interchanged?

$\max_\alpha \min_w G(w,\alpha) \le \min_w \max_\alpha G(w,\alpha)$
- Equality if G is convex in w, concave in α and the domains of w and α are convex and compact:
$\max_\alpha \min_w G(w,\alpha) = \min_w \max_\alpha G(w,\alpha)$
- Proof:
$\min_w G(\alpha,w) \le G(\alpha,w')\,\forall w'$
$\max_\alpha \min_w G(\alpha,w) \le \max_\alpha G(\alpha,w')\,\forall w'$
$\max_\alpha \min_w G(\alpha,w) \le \min_{w'} \max_\alpha G(\alpha,w')$

Application to SVM

- For SVM, the condition is met, allowing us to interchange min and max: $\min_w L(w) =$
$\max_{\alpha\in[0,1]^n} \min_w \frac{1}{N}\sum_{n=1}^N \alpha_n\left(1-y_n x_n^\top w\right) + \frac{\lambda}{2}\|w\|_2^2$
- Minimizer computation:
$\mathbf{Y} = \text{diag}(\mathbf{y})$
$\nabla_w G(w,\alpha) = -\frac{1}{N}\sum_{n=1}^N \alpha_n y_n x_n + \lambda w = 0 \Longrightarrow$
$w(\alpha) = \frac{1}{\lambda N}\sum_{n=1}^N \alpha_n y_n x_n = \frac{1}{\lambda N}\mathbf{X}^\top\mathbf{Y}\alpha$
- Dual optimization problem:

$$\begin{aligned}\min_w L(w) &= \max_{\alpha\in[0,1]^n} \frac{1}{N}\sum_{n=1}^N \alpha_n\left(1-\frac{1}{\lambda N}y_n x_n^\top \mathbf{X}^\top\mathbf{Y}\alpha\right) + \frac{1}{2\lambda N^2}\left\|\mathbf{X}^\top\mathbf{Y}\alpha\right\|_2^2 \\ &= \max_{\alpha\in[0,1]^n} \frac{1^\top\alpha}{N} - \frac{1}{\lambda N^2}\alpha^\top\mathbf{Y}\mathbf{X}\mathbf{X}^\top\mathbf{Y}\alpha + \frac{1}{2\lambda N^2}\left\|\mathbf{X}^\top\mathbf{Y}\alpha\right\|_2^2 \\ &= \max_{\alpha\in[0,1]^n} \frac{1^\top\alpha}{N} - \frac{1}{2\lambda N^2}\alpha^\top \underbrace{\mathbf{Y}\mathbf{X}\mathbf{X}^\top\mathbf{Y}}_{\text{PSD matrix}}\alpha\end{aligned}$$

Advantages?

$$\max_{\alpha\in[0,1]^n} \alpha^\top 1 - \frac{1}{2\lambda N}\alpha^\top \underbrace{\mathbf{Y}\mathbf{X}\mathbf{X}^\top\mathbf{Y}}_{\text{PSD matrix}}\alpha$$

1. Differentiable Concave Problem: Efficient solutions can be achieved using
- Quadratic programming solvers
- Coordinate ascent
2. Kernel Matrix Dependency: The cost function only depends on the data via the kernel matrix $K = \mathbf{X}\mathbf{X}^\top \in \mathbb{R}^{N\times N}$ - no dependency on d
3. Dual Formulation Insight: α is typically sparse and non-zero exclusively for the training examples that are crucial in determining the decision boundary

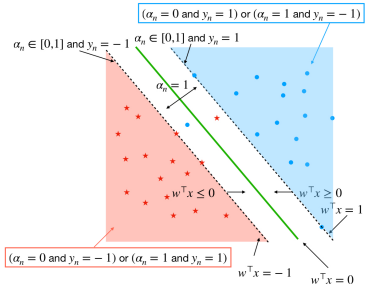
Interpretation of the dual formulation

- $\forall (x_n,y_n)\,\exists\alpha_n$ given by:

$$\max_{\alpha_n\in[0,1]} \alpha_n\left(1-y_n x_n^\top w\right)$$

- If x_n is on the correct side and outside the margin, $1-y_n x_n^\top w < 0$, then $\alpha_n = 0$
- If x_n is on the correct side and on the margin, $1-y_n x_n^\top w = 0$, then $\alpha_n \in [0,1]$
- If x_n is strictly inside the margin or or the incorrect side, $1-y_n x_n^\top w > 0$, then $\alpha_n = 1$

$\rightarrow$ The points for which $\alpha_n > 0$ are referred to as support vectors



- The SVM hyperplane is supported by the support vectors $w = \frac{1}{\lambda N}\sum_{n=1}^N \alpha_n y_n x_n$
$\Rightarrow w$ does not depend on the observation (x_n,y_n) if $\alpha_n = 0$

Recap

- Hard SVM - finds max-margin separating hyperplane $\min_w \frac{1}{2}\|w\|^2$ such that $\forall n, y_n x_n^\top w \ge 1$
- Soft SVM - relax the constraint for non-separable data
$\min_w \frac{\lambda}{2}\|w\|^2 + \frac{1}{N}\sum_{n=1}^N \left[1-y_n x_n^\top w\right]_+$
- Hinge loss can be optimized with (stochastic) sub-gradient method
- Duality: min max problem is equivalent to max min (convex-concave objective)
- Efficient solutions with quadratic programming and coordinate ascent
- The cost depends on the data via the kernel matrix (no dependency on d)

---

k-Nearest Neighbors

Remarks:
- Different metrics can be employed
- High computational complexity for large N (but efficient data structure may exist)

k-NN regression ($y \in \mathbb{R}$)

$f_{S_{\text{train}},k}(x) = \frac{1}{k}\sum_{n:x_n\in nbh_{S_{\text{train}},k}(x)} y_n$

k-NN classification ($y \in \{0,1\}$)

$f_{S_{\text{train}},k}(x) = \text{majority}\left\{y_n : x_n \in \text{nbh}_{S_{\text{train}},}(x)\right\}$
- Remarks:
- Choose an odd value for k to prevent ties
- Generalization: smoothing kernels; weighted linear combination of elements
- Why does it make sense?
- Relevant in the presence of spatial correlation
- Implicitly models intricate decision boundaries in low-dimensional spaces

Bias-variance tradeoff in k-NN

For small k:
- Low bias - complex decision boundary
- High variance - overfitting

For large k:
(When $k = N$, prediction is constant)
- High bias
- Low variance

- 1-NN classification has max train acc

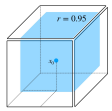
Summary: k-Nearest Neighbor

Pros:
- No optimization or training
- Easy to implement
- Works well in low dimensions, allowing for very complex decision boundaries

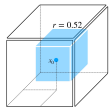
Cons:
- Slow at query time
- Not suitable for high-dimensional data
- Choosing the right local distance is crucial

Curse of dimensionality

- Claim 1: As the dimensionality grows, fixed-size training sets cover a diminishing fraction of the input space



- Assume the data $x \sim \mathcal{U}\left([0,1]^d\right)$
- Blue box around the center x_0 of size r
$\mathbb{P}(x \in \square) = r^d := \alpha$
- If $\alpha = 0.01$, to have: $d = 10$, we need $r = 0.63$; $d = 100$, we need $r = 0.95$
$d = 100 \rightarrow$ need to explore almost the whole box
- Claim 2: In high-dimension, data-points are far from each other.
- Consider N i.i.d. points uniform in the $[0,1]^d$
$\mathbb{P}\left(\exists x_i \in \square\right) \ge 1/2 \Longrightarrow r \ge \left(1-\frac{1}{2^{1/N}}\right)^{1/d}$
- Proof: $\mathbb{P}(x \notin \square) = 1-r^d$
$\mathbb{P}\left(x_i \notin \square\,, \forall i \le N\right) = \left(1-r^d\right)^N$
$\mathbb{P}\left(\exists x_i \in \square\right) = 1-\left(1-r^d\right)^N$
- For $d = 10, N = 500$, $r \ge 0.52$



Generalization bound for 1-NN (I)

- Setup: $(X,Y) \sim \mathscr{D}$ over $\mathscr{X}\times\mathscr{Y} = [0,1]^d \times \{0,1\}$
- Goal: Bound the classification error:
$L(f) = \mathbb{P}_{(X,Y)\sim D}(Y \ne f(X))$
- Baseline:
- Bayes classifier: minimizes L over all classifiers $f_*(x) = 1_{\eta(x)\ge 1/2}$ where $\eta(x) = \mathbb{P}(Y=1 \mid X=x)$

Proof 1:

$$\begin{aligned}\eta(x) \ge 1/2 &\Longleftrightarrow \mathbb{P}(Y=1|X=x) \ge 1/2 \\ &\Longleftrightarrow \mathbb{P}(Y=1 \mid X=x) \ge \mathbb{P}(Y=0 \mid X=x) \\ &\Longleftrightarrow 1 \in \arg\max_{y\in\{0,1\}} \mathbb{P}(Y=y|X=x) \\ &\Rightarrow 1_{\eta(x)\ge 1/2} = \arg\max_{y\in\{0,1\}} \mathbb{P}(Y=y|X=x) = f_*(x)\end{aligned}$$

- Bayes risk: represents the minimum probability of misclassification
$L(f_*) = \mathbb{P}\left(f_*(X) \ne Y\right)$
$= \mathbb{E}_{X\sim D_X}\left[\min\{\eta(X), 1-\eta(X)\}\right]$

Proof 2:

$$\begin{aligned}&L(f_*) = \mathbb{E}_{(X,Y)\sim\mathscr{D}}[1_{f_*(X)\ne Y}] \\ &= \mathbb{E}_{X\sim\mathscr{D}_X}[\mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{f_*(X)\ne Y} \mid X]1_{\eta(X)\ge 1/2} + \mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{f_*(X)\ne Y} \mid X]1_{\eta(X)<1/2}] \\ &= \mathbb{E}_{X\sim\mathscr{D}_X}[\mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{1\ne Y} \mid X]1_{\eta(X)\ge 1/2} + \mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{0\ne Y} \mid X]1_{\eta(X)<1/2}] \\ &= \mathbb{E}_{X\sim D_X}[\mathbb{P}(Y=0 \mid X)1_{\eta(X)\ge 1/2} + \mathbb{P}(Y=1 \mid X)1_{\eta(X)<1/2}] \\ &= \mathbb{E}_{X\sim\mathscr{D}_X}[\min\{\eta(X), 1-\eta(X)\}]\end{aligned}$$

Generalization bound for 1-NN (II)

- Assumption: $\exists c \ge 0, \forall x, x' \in \mathscr{X}$:
$|\eta(x) - \eta(x')| \le c\|x-x'\|_2$
$\Rightarrow$ Nearby points are likely to share the same label
- Claim: $\mathbb{E}_{S_{\text{train}}}\left[L\left(f_{S_{\text{train}}}\right)\right]$

$$\le 2L(f_*) + c\mathbb{E}_{S_{\text{train}},X\sim\mathscr{D}_X}\left[\underbrace{\|X - \text{nbh}_{S_{\text{train}},1}(X)\|}_{\text{geometric term}}\right]$$

$\leq 2L(f_*) + 4c\sqrt{d}N^{-\frac{1}{d+1}}$

- Interpretation:

• For constant d and $N \to \infty$: $\mathbb{E}_{S_{\text{train}}}[L(f_{S_{\text{train}}})] \leq 2L(f_*)$

• To achieve a constant error, we need $N \propto d^{(d+1)/2}$ - curse of dimensionality

• Despite common belief: Interpolation method can generalize well

Proof (I)

- We want to bound:

$\mathbb{E}_{S_{\text{train}}}[L(f_{S_{\text{train}}})]$
$= \mathbb{E}_{S_{\text{train}}}[\mathbb{P}_{(X,Y)\sim\mathscr{D}}[f_{S_{\text{train}}}(X) \neq Y]]$

- We first sample N unlabeled examples $S_{\text{train},X} = (X_1, \cdots X_N) \sim \mathscr{D}_X$, an unlabeled example $X \sim \mathscr{D}_X$ and define $X' = \text{nbh}_{S_{\text{train}},1}(X)$

- Finally we sample $Y \sim \eta(X)$ and $Y' \sim \eta(X')$

$\mathbb{E}_{S_{\text{train}}}[L(f_{S_{\text{train}}})]$

$= \mathbb{E}_{S_{\text{train},X}, X\sim D_X, Y\sim\eta(X), Y'\sim\eta(X')}\left[1_{Y\neq f_{S_{\text{train}}}(X)}\right]$

$= \mathbb{E}_{S_{\text{train},X}, X\sim\mathscr{D}_X, Y\sim\eta(X), Y'\sim\eta(X')}[1_{Y\neq Y'}]$

$= \mathbb{E}_{S_{\text{train},X}, X\sim\mathscr{D}_X}[\mathbb{P}_{Y\sim\eta(X), Y'\sim\eta(X')}(Y \neq Y')]$

Proof (II)

- Consider two points $x, x' \in [0,1]^d$.

- Sample their labels $Y \sim \eta(x)$ and $Y' \sim \eta(x')$

- Claim:

$\mathbb{P}(Y' \neq Y) \leq 2\min\{\eta(x), 1-\eta(x)\} + c\|x - x'\|$

- Simple case: $x = x'$

$$\begin{aligned}\mathbb{P}(Y' \neq Y) &= \mathbb{E}[1_{Y'\neq Y} 1_{Y'=1} + 1_{Y'\neq Y} 1_{Y'=0}] \\ &= \mathbb{P}(Y'=1)\mathbb{P}(Y=0) + \mathbb{P}(Y'=1)\mathbb{P}(Y=0) \\ &= 2\eta(x)(1-\eta(x)) \\ &\leq 2\min\{\eta(x), 1-\eta(x)\}\end{aligned}$$

- Case 1: $\mathbf{Y=0}$ $(1-\eta(x))$ $Y'=1$ $\eta(x)$

- Case 2: $\mathbf{Y=1}$ $\eta(x)$ $Y'=0$ $(1-\eta(x))$

Proof (III)

• General case:

$$\begin{aligned}\mathbb{P}(Y \neq Y') =& \eta(x)(1-\eta(x')) + \eta(x')(1-\eta(x)) \\ =& \eta(x)(1-\eta(x)) + \eta(x)(\eta(x) - \eta(x')) \\ &+ \eta(x)(1-\eta(x)) + (\eta(x') - \eta(x))(1-\eta(x)) \\ =& 2\eta(x)(1-\eta(x)) + (2\eta(x)-1)(\eta(x) - \eta(x')) \\ \leq& 2\eta(x)(1-\eta(x)) + |(2\eta(x)-1)||\eta(x) - \eta(x')| \\ \leq& 2\eta(x)(1-\eta(x)) + |\eta(x) - \eta(x')| \\ \leq& 2\eta(x)(1-\eta(x)) + c\|x - x'\| \\ \leq& 2\min\{\eta(x), 1-\eta(x)\} + c\|x - x'\|\end{aligned}$$

Proof (IV)

$$\begin{aligned}\mathbb{E}_{S_{\text{train}}}[L(f_{S_{\text{train}}})] &= \mathbb{E}_{S_{\text{train},X}, X\sim\mathscr{D}_X, Y\sim\eta(X), Y'\sim\eta(X')}\left[1_{Y\neq f_{\text{train}}(X)}\right] \\ &= \mathbb{E}_{S_{\text{train},X}, X\sim\mathscr{D}_X, Y\sim\eta(X), Y'\sim\eta(X')}[1_{Y\neq Y'}] \\ &= \mathbb{E}_{S_{\text{train},X}, X\sim D_X}[\mathbb{P}_{Y\sim\eta(X), Y'\sim\eta(X)}(Y \neq Y')] \\ &\leq \mathbb{E}_{S_{\text{train},X}, X\sim\mathscr{D}_X}[2\min\{\eta(X), 1-\eta(X)\} + c\|X - X'\|] \\ &\leq 2L(f_*) + c\mathbb{E}_{S_{\text{train},X}\sim\mathscr{D}_X}[\|X - \text{nbh}_{S_{\text{train}},1}(X)\|]\end{aligned}$$

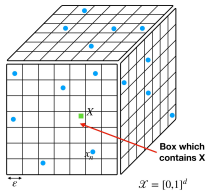
Bound on the geometric term (I)

- Consider a fresh sample $X \sim \mathscr{D}$ and denote by $p_k = \mathbb{P}(X \in \text{Box}_k)$

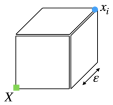
- Consider the box which contains X. Two options:

• The box contains an element of S_{train} X has a neighbor in S_{train} at distance at most $\sqrt{d}\varepsilon$

It happens with probability $1-(1-p_k)^N$



Proof: Consider the worst case:



$\|X - x_i\| = \sqrt{\sum_{i=1}^d \varepsilon^2} = \sqrt{d}\varepsilon$

• There is no element of S_{train} . The nearest neighbor of X can be at worst at a distance $\sqrt{d}$ It happens with probability $(1-p_k)^N$

Bound on the geometric term (II)

$\mathbb{E}[\|X - \text{nbh}(X)\|]$
$\leq \sum_k p_k \left[(1-p_k)^N \sqrt{d} + \left(1-(1-p_k)^N\right)\sqrt{d}\varepsilon\right]$

- Claim: The bound is derived by optimizing over p_k and ε

- Intuition:

• If p_k is large: it is likely that we pick that box but it is also likely that we find a training point in that box

• If p_k is small, we are generally safe, as by its definition, this scenario occurs infrequently

Nearest Neighbors is a local averaging method

- Local averaging methods aim to approximate the Bayes predictor directly - without the need for optimization

- This is achieved by approximating the conditional distribution $p(y \mid x)$ by some $\hat{p}(y \mid x)$ These "plug-in" estimators are:

• $f(x) \in \arg\max \hat{\mathbb{P}}(Y = y \mid x)$ for classification with the $0-1$ loss $y \in \mathcal{Y}$

• $f(x) = \hat{\mathbb{E}}[Y \mid x] = \int y\hat{p}(y \mid x)dy$ for regression with the square loss

- In the case of nearest neighbors:

$\hat{p}(y \mid x) = \sum_{n=1}^N \hat{w}_n(x) 1_{y=y_n}$

where $\hat{w}(x) = 1/k$ for the k nearest neighbors (0 otherwise)

Recap

• Curse of dimensionality: as $d \nearrow \infty$, it is harder to define local neighborhoods

• For $N \to \infty, 1-\text{NN}$ is competitive with Bayes classifier

• N needs to scale exponentially in d to achieve the same error

---

Kernel Regression

- Objective for ridge regression:

$\min_w \frac{1}{2N}\sum_{n=1}^N (y_n - w^\top x_n)^2 + \frac{\lambda}{2}\|w\|^2$

- Solution:

$\mathcal{W}_* = \frac{1}{N}(\underbrace{\frac{1}{N}\mathbf{X}^\top\mathbf{X} + \lambda I_d}_{d\times d})^{-1}\mathbf{X}^\top\mathbf{y}$

- Alternative solution:

$\mathcal{W}_* = \frac{1}{N}\mathbf{X}^\top(\underbrace{\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda I_N}_{N\times N})^{-1}\mathbf{y}$

- Proof: Let $P \in \mathbb{R}^{m\times n}$ and $Q \in \mathbb{R}^{n\times m}$

$P(QP + I_n) = PQP + P = (PQ + I_m)P$

Assuming that both $QP + I_n$ and $PQ + I_m$ are invertible

$(PQ + I_m)^{-1}P = P(QP + I_n)^{-1}$

We deduce the result with $P = \mathbf{X}^\top$ and $Q = \frac{1}{\lambda N}\mathbf{X}$

Usefulness of the alternative form

$\mathcal{W}_* = \underbrace{\frac{1}{N}\mathbf{X}^\top}_{d\times N}(\underbrace{\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda I_N}_{N\times N})^{-1}\mathbf{y}$

1. Computational complexity:

• For the original formulation

$\frac{1}{N}\left(\frac{1}{N}\mathbf{X}^\top\mathbf{X} + \lambda I_d\right)^{-1}\mathbf{X}^\top\mathbf{y} \to O(d^3 + Nd^2)$

• For the new formulation

$\frac{1}{N}\mathbf{X}^\top\left(\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda I_N\right)^{-1}\mathbf{y} \to O(N^3 + dN^2)$

$\Rightarrow$ Depending on d, N one formulation may be more efficient than the other

2. Structural difference:

$w_* = \mathbf{X}^\top\alpha_*$ where $\alpha_* = \frac{1}{N}\left(\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda I_N\right)^{-1}\mathbf{y}$

$\Rightarrow w_* \in \text{span}\{x_1, \cdots, x_N\}$

These two insights are fundamental to understanding the kernel trick

Representer Theorem

- Claim: For any loss function ℓ, there exists $\alpha_* \in \mathbb{R}^N$ such that $w_* := \mathbf{X}^\top\alpha_* \in \arg\min_w \frac{1}{N}\sum_{n=1}^N \ell(x_n^\top w, y_n) + \frac{\lambda}{2}\|w\|^2$

- Meaning: There exists an optimal solution within $\text{span}\{x_1, \cdots, x_N\}$

- Consequence: This is more general than LS, enabling the kernel trick to various problems, including Kernel SVM, Kernel LS, and Kernel PCA

Proof of the representer theorem

- Let w_* be an optimal solution of $\min_w \frac{1}{N}\sum_{n=1}^N \ell(x_n^\top w, y_n) + \frac{\lambda}{2}\|w\|^2$

- We can always rewrite w_* as $w_* = \sum_{n=1}^N \alpha_n x_n + u$ where $u^\top x_n = 0$ for all n

- Let's define $w = w_* - u$

• $\|w_*\|^2 = \|w\|^2 + \|u\|^2 \Rightarrow \|w\|^2 \leq \|w_*\|^2$

• $\forall n, w^\top x_n = (w_* - u)^\top x_n = w_*^\top x_n \Rightarrow \ell(x_n^\top w, y_n) = \ell(x_n^\top w_*, y_n)$

Therefore

$\frac{1}{N}\sum_{n=1}^N \ell(x_n^\top w, y_n) + \frac{\lambda}{2}\|w\|^2$
$\leq \frac{1}{N}\sum_{n=1}^N \ell(x_n^\top w_*, y_n) + \frac{\lambda}{2}\|w_*\|^2$

And w is an optimal solution for this problem.

Kernelized ridge regression

- Classic formulation in w :

$w_* = \arg\min_w \frac{1}{2N}\|\mathbf{y} - \mathbf{X}w\|^2 + \frac{\lambda}{2}\|w\|^2$

- Alternative formulation in α :

$\alpha_* = \arg\min_\alpha \frac{1}{2}\alpha^\top\left(\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda I_N\right)\alpha - \frac{1}{N}\alpha^\top\mathbf{y}$

- Claim: These two formulations are equivalent

- Proof: Set the gradient to 0 , to obtain $\alpha_* = \frac{1}{N}\left(\frac{1}{N}\mathbf{X}\mathbf{X}^\top + \lambda I_N\right)^{-1}\mathbf{y}$, and $w_* = \mathbf{X}^\top\alpha_*$

- Key takeaways:

• Computational complexity - depending on d, N

• The dual formulation only uses $\mathbf{X}$ through the kernel matrix $\mathbf{K} = \mathbf{X}\mathbf{X}^\top$

Kernel matrix

$$\mathbf{K} = \mathbf{X}\mathbf{X}^\top = \begin{pmatrix} x_1^\top x_1 & x_1^\top x_2 & \cdots & x_1^\top x_N \\ x_2^\top x_1 & x_2^\top x_2 & \cdots & x_2^\top x_N \\ \vdots & \vdots & \ddots & \vdots \\ x_N^\top x_1 & x_N^\top x_2 & \cdots & x_N^\top x_N \end{pmatrix} = \left(x_i^\top x_j\right)_{i,j} \in \mathbb{R}^{N\times N}$$

- Depends on the dimensions only through the scalar product.

- If we have a scalar product independent of the dimensions it can be fast.

Kernel matrix with feature spaces

- When a feature map $\phi : \mathbb{R}^d \to \mathbb{R}^{\tilde{d}}$ is used, $(x_n)_{n=1}^N \hookrightarrow (\phi(x_n))_{n=1}^N$

$\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\top \in \mathbb{R}^{N\times N}$

- Problem: when $d \lll \tilde{d}$ computing $\phi(x)^\top\phi(x')$ costs $O(\tilde{d})$ - too expensive

Kernel trick

- Kernel function: $\kappa(x, x')$ such that $\kappa(x, x') = \phi(x)^\top\phi(x')$

It is equivalent to

• Directly compute $\kappa(x, x')$

• First map the features to $\phi(x)$, then compute $\phi(x)^\top\phi(x')$

- Purpose: enable computation of linear classifiers in high-dimensional space without performing computations in this high-dimensional space directly.

Predicting with kernels

- Problem: The prediction is $y = \phi(x)^\top w_*$ but computing $\phi(x)$ can be expensive

- Question: How can we make predictions using only the kernel function, without the need to compute $\phi(x)$?

- Answer: $\phi(x)^\top w_* = \phi(x)^\top\phi(\mathbf{X})^\top\alpha_* = \sum_{n=1}^N \kappa(x, x_n)\alpha_{*n}$ We can do a prediction only using the kernel function

- Important remark:

$y = \underbrace{\phi(x)^\top w_*}_{\text{Linear prediction in the feature space}} = \overbrace{f_{W_*}(x)}^{\text{Non linear prediction in the } \mathcal{X} \text{ space}}$

1. Linear Kernel

$\kappa(x,x') = x^\top x' \rightarrow$ Feature map is $\phi(x) = x$

2. Quadratic kernel

$\kappa(x,x') = (xx')^2$ for $x, x' \in \mathbb{R} \Rightarrow$ Feature map is $\phi(x) = x^2$

3. Polynomial kernel

Let $x, x' \in \mathbb{R}^3$

$\kappa(x,x') = (x_1x_1' + x_2x_2' + x_3x_3')^2$

- Feature map:

$\phi(x) = [x_1^2, x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3] \in \mathbb{R}^6$

- Proof:

$\kappa(x,x') = \phi(x)^\top \phi(x')$

$\kappa(x,x') = (x_1x_1' + x_2x_2' + x_3x_3')^2$

$= (x_1x_1')^2 + (x_2x_2')^2 + (x_3x_3')^2 + 2x_1x_2x_1'x_2' + 2x_1x_3x_1'x_3' + 2x_2x_3x_2'x_3'$

$= \left(x_1^2, x_2^2, x_3^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \sqrt{2}x_2x_3\right)^\top \left(x_1'^2, x_2'^2, x_3'^2, \sqrt{2}x_1'x_2', \sqrt{2}x_1'x_3', \sqrt{2}x_2'x_3'\right)$

We obtain ϕ by identification

4. Radial basis function (RBF) kernel

- Let $x, x' \in \mathbb{R}^d$ $\kappa(x,x') = e^{-(x-x')^\top (x-x')}$

Taylor:

- For $x, x' \in \mathbb{R}$ $\kappa(x,x') = e^{-(x-x')^2}$
- Feature map: $\phi(x) = e^{-x^2}\left(\cdots, \frac{2^{k/2}x^k}{\sqrt{k!}}\cdots\right)$
- Proof: $\kappa(x,x') = e^{-x^2-x^2+2xx'} = e^{-x^2}e^{-x'^2}\sum_{k=0}^{\infty}\frac{2^k x^k x'^k}{k!}$ (Taylor: $e^x = \sum_{k=0}^{\infty}\frac{x^k}{k!}$)

$\phi(x) = e^{-x^2}\left(\cdots, \frac{2^{k/2}x^k}{\sqrt{k!}}\cdots\right) \Longrightarrow \phi(x)^\top\phi(x') = \kappa(x,x')$

- Interest: it cannot be represented as an inner product in a finite-dimensional space

Building new kernels from existing kernels

- Let κ_1, κ_2 be two kernel functions and ϕ_1, ϕ_2 the corresponding feature maps

Claim 1: Positive linear combinations of kernel are kernels:

$\kappa(x,x') = \alpha\kappa_1(x,x') + \beta\kappa_2(x,x')$ for $\alpha, \beta \geq 0$

Proof 1:

$\kappa(x,x') = \alpha\kappa_1(x,x') + \beta\kappa_2(x,x')$

$= \alpha\phi_1(x)^\top\phi_1(x') + \beta\phi_2(x)^\top\phi_2(x')$

$= \phi(x)^\top\phi(x')$

where $\phi(x) = \begin{pmatrix}\sqrt{\alpha}\phi_1(x)\\ \sqrt{\beta}\phi_2(x)\end{pmatrix} \in \mathbb{R}^{d_1+d_2}$

Claim 2: Products of kernels are kernels:

$\kappa(x,x') = \kappa_1(x,x')\kappa_2(x,x')$

Proof 2:

$\kappa(x,x') = \kappa_1(x,x')\kappa_2(x,x')$

$= \phi_1(x)^\top\phi_1(x')\phi_2(x)^\top\phi_2(x')$

Let $\phi(x)^\top = (\phi_1(x)_1\phi_2(x)_1, \cdots, \phi_1(x)_1\phi_2(x)_{d_2}, \cdots, \phi_1(x)_{d_1}\phi_2(x)_1, \cdots, \phi_1(x)_{d_1}\phi_2(x)_{d_2}) \in \mathbb{R}^{d_1d_2}$

then

$\phi(x)^\top\phi(x') = \sum_{i,j}(\phi_1(x))_i(\phi_2(x))_j(\phi_1(x'))_i(\phi_2(x'))_j$

$= \sum_i(\phi_1(x))_i(\phi_1(x'))_i\sum_j(\phi_2(x))_j(\phi_2(x'))_j$

$= \phi_1(x)^\top\phi_1(x')\phi_2(x)^\top\phi_2(x') = \kappa(x,x')$

Mercer's condition

- Given a kernel function κ, we can ensure the existence of a feature map ϕ such that $\kappa(x,x') = \phi(x)^\top\phi(x')$ if and only if the following Mercer's conditions are fulfilled:
- The kernel function is symmetric: $\forall x, x', \kappa(x,x') = \kappa(x',x)$
- The kernel matrix is psd for all possible input sets: $\forall N \geq 0, \forall (x_n)_{n=1}^N, \quad \mathbf{K} = (\kappa(x_i,x_j))_{i,j=1}^N \geqslant 0$

Proof of Mercer theorem

- If κ represents an inner product then it is symmetric and the kernel matrix is psd: $v^\top Kv = \sum_{i,j}v_iv_j\phi(x_i)^\top\phi(x_j) = \left\|\sum_i v_i\phi(x_i)\right\|^2$
- Define $\phi(x) = \kappa(\cdot, x)$. Define a vector space of functions by considering all linear combinations $\left\{\sum_i \alpha_i\kappa(\cdot,x_i)\right\}$. Define an inner product on this vector space by $\left\langle\sum_i\alpha_i\kappa(\cdot,x_i), \sum_j\beta_j\kappa(\cdot,x_j')\right\rangle = \sum_{i,j}\alpha_i\beta_j\kappa(x_i,x_j')$

This is a valid inner product (symmetric, bilinear and positive definite, with equality holding only if $\phi(x)$ is the zero function)

Consequently $\langle\phi(x),\phi(x')\rangle = \langle\kappa(\cdot,x),\kappa(\cdot,x')\rangle = \kappa(x,x')$

Deep Learning

From Linear Models to NNs

- Linear prediction (with augmented features): $y = f_{\text{Lin}}(x) = \phi(x)^\top w$
- Prediction with a neural network (NN): $y = f_{\mathbf{NN}}(x) = f(x)^\top w$

Why Neural Networks?

- Classical machine learning:
- Relatively simple models on top of features handcrafted by domain experts
- Only works well when used with good handcrafted features
- Deep learning:
- Large neural networks that learn features directly from the data
- Can be viewed as a complicated feature extractor + linear prediction
- Requires large amounts of data and compute to train
- Quality often continues to improve substantially with more data and larger models

Recap: Logistic Regression

$f_{LR}(x) = p(1 \mid x) = \sigma\left(x^\top w + b\right)$

$= \sigma\left(\sum_{i=1}^d x_iw_i + b\right)$

where $\sigma(z) = (1+\exp(-z))^{-1}$ is the sigmoid

- Pattern-matching perspective:
- Task: classify between digit 1 and digit 0 using logistic regression
- We learn a single pattern w which we apply elementwise to each input x (very restrictive!)
- We classify the digit as 1 if $p(1 \mid x) \geq 0.5$ or, equivalently, if $\sum_{i=1}^d x_iw_i \geq -b$

Two-Layer Neural Networks

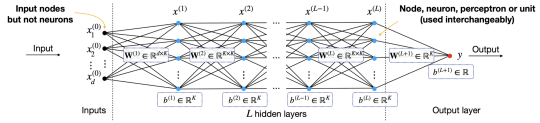
(aka two-layer perceptron)

- Stack logistic regression units $\phi(x)_j = \sigma\left(\sum_{i=1}^d x_iw_{i,j}^{(1)} + b_j\right)$ (aka hidden units or neurons) in a hidden layer
- Aggregate the hidden units using a linear function $\phi(x)^\top w^{(2)}$

Pattern-matching perspective:

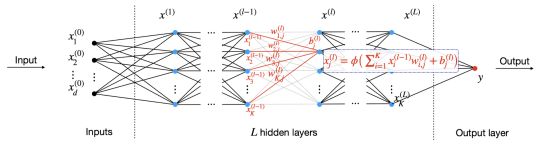
- Task: classify between digit 1 and digit 0 with a two-layer neural network
- Each hidden unit learns a different pattern (not necessarily interpretable!)
- We classify based on a linear combination of these patterns $\Rightarrow$ much more flexible

Multi-layer Neural Networks



- Learnable Parameters: Weight matrices $\mathbf{W}^{(l)}$ and bias vectors $b^{(l)}$ for $1 \leq l \leq L+1$
- Each column of $\mathbf{W}^{(l)}$ corresponds to the weights of one perceptron
- Outputs of hidden layer l given by vector: $x^{(l)} = f^{(l)}\left(x^{(l-1)}\right) := \phi\left(\left(\mathbf{W}^{(l)}\right)^\top x^{(l-1)} + b^{(l)}\right)$

Single Neuron View



$x_j^{(l)} = \phi\left(\sum_{i=1}^K x_i^{(l-1)}w_{i,j}^{(l)} + b_j^{(l)}\right)$

- Important: ϕ is non-linear otherwise we can only represent linear functions

NNs extract features from the input

- NN = feature extractor + output layer
- Feature extractor from $\mathbb{R}^d$ to $\mathbb{R}^K$:
- This function is defined by
- The biases $\left\{b^{(l)}\right\}_{l\in[L]}$ and weights $\left\{\mathbf{W}^{(l)}\right\}_{l\in[L]}$ so we learn

$\Rightarrow O\left(dK + K^2L\right) \approx O\left(K^2L\right)$ parameters

- The activation function ϕ we pick
- In practice: both L and K are large - overparametrized NNs

Neural Network: Inference and Training

- $h(x) = f(x)^\top w^{(L+1)} + b^{(L+1)}$
- Regression $h(x)$

$\ell(y, h(x)) = (h(x) - y)^2$

- Binary Classification with $y \in \{-1, 1\}$ $\text{sign}(h(x))$

$\ell(y, h(x)) = \log(1 + \exp(-yh(x)))$

- Multi-Class Classification with $y \in \{1, \ldots, K\}$ $\text{argmax}_{c\in\{1,\ldots,K\}} h(x)_c$

$\ell(y, h(x)) = -\log\frac{e^{h(x)_y}}{\sum_{i=1}^K e^{h(x)_i}}$

Popular activation functions

- Sigmoid: $\phi(x) = \sigma(x) = \frac{1}{1+e^{-x}}$
- ReLU : $\phi(x) = (x)_+ = \max\{0, x\}$
- GELU: $\phi(x) = x \cdot \Phi(x) \approx x \cdot \sigma(1.702x)$

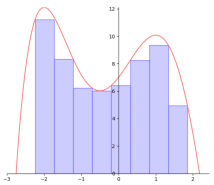
L_2 Approximation: Barron's result

- Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and define $\hat{f}(\omega) = \int_{\mathbb{R}^d} f(x)e^{-i\omega^\top x}dx$, its Fourier transform
- Assumption: $\int_{\mathbb{R}^d}|\omega||\hat{f}(\omega)|d\omega \leq C$ (smoothness assumption)
- Claim: $\forall n \geq 1$ and $r > 0$, $\exists$ f_n: $f_n(x) = \sum_{j=1}^n c_j\phi\left(x^\top w_j + b_j\right) + c_0$ such that $\int_{|x|\leq r}(f(x) - f_n(x))^2\,dx \leq \frac{(2Cr)^2}{n}$

$\Rightarrow$ All sufficiently smooth function can be approximated by a one-hidden-layer NN

- The more neurons allowed, the smaller the error.
- The smoother the function (the smaller C), the smaller the error
- The larger the domain (the larger r), the greater the error
- Approximation is in average (in ℓ_2-norm)
- Applicable for any "sigmoid-like" activation function
- The function f_n is a one-hidden-layer NN with n nodes $f_n = c^\top\phi\left(W^\top x + b\right) + c_0$

L_1 Approximation



- "A NN with sigmoid activation and at most two hidden layers can approximate well a smooth function in ℓ_1-norm"
- Approximation in ℓ_1-norm: $\int_{|x|\leq r} |f(x) - f_n(x)|\, dx \leq$ Something small
- $f : \mathbb{R} \to \mathbb{R}$ on a bounded domain, Riemann integrable - its integral can be approximated to any desired accuracy using "lower" and "upper" sums of the area of rectangles
- Approximation of the function by a sum of rectangle functions
- Approximation in ℓ_1-norm:

$$\begin{aligned}\int_{|x|\leq r} |f(x) - f_n(x)|\, dx &= \int_{|x|\leq r} (f(x) - f_n(x))\, dx \\ &= \int_{|x|\leq r} f(x)dx - \int_{|x|\leq r} f_n(x)dx \\ &= \int_{|x|\leq r} f(x) - \sum_i \text{Area(Rectangle }_i)\end{aligned}$$

Approximation of the rectangle

- A rectangle function is equal to the sum of two step functions
- Approximate a step function with a sigmoid $\tilde{\phi}(x) = \phi(w(x-b))$

By setting:

- b : where the transition happens
- w : makes the transition steeper

Derivative: $\tilde{\phi}'(b) = w/4$

$\Rightarrow$ The width of the transition is $O(4/w)$

$h(\phi(w(x-a)) - \phi(w(x-b)))$

Conclusion in the 1D case

1. Approximate the function in the Riemann sense by a sum of k rectangles
2. Represent each rectangle using two nodes in the hidden layer of a neural network
3. Compute the sum of all nodes in the hidden layer (considering appropriate weights and signs) to get the final output

$\Rightarrow$ NN with one hidden layer containing $2k$ nodes for a Riemann sum with k rectangles

- Remarks:
- The same intuition applies to any sigmoid-like function
- This is an intuitive explanation, not a quantitative one
- The weights w must be large

Larger dimension: $d = 2$

Same idea:

- Approximate the function by 2D rectangle functions
- Approximate a 2D rectangle function by sigmoids
- Two sigmoids can approximate an infinite rectangle function $(x_1, x_2) \mapsto \phi(w(x_1 - a_1)) - \phi(w(x_1 - b_1))$

The rectangle:

- ranges from a_1 to b_1 in the x_1 direction
- is unbounded in the x_2 direction

Two sigmoids can approximate an infinite rectangle function

$(x_1, x_2) \mapsto \phi(w(x_2 - a_2)) - \phi(w(x_2 - b_2))$

The rectangle:

- ranges from a_2 to b_2 in the x_2 direction
- is unbounded in the x_1 direction

Four sigmoids approximate a cross

$(x_1, x_2) \mapsto \phi(w(x_1 - a_1)) - \phi(w(x_1 - b_1)) + \phi(w(x_2 - a_2)) - \phi(w(x_2 - b_2))$

$\Rightarrow$ This approximation is close to our objective, with the exception of the two infinite "arms"

How can we eliminate the crossed arms?

Using the sigmoid to threshold unwanted infinite arms

Thresholding the function will eliminate the arms

It is equivalent to composing it with $1_{y\geq c}$ for $c \in (1, 2]$

$\Rightarrow$ Approximate $1_{y\geq c}$ using a sigmoid with a large weight w and an appropriate bias (e.g., $3w/2$)

Point-wise approximations

- Def: piecewise linear (PWL) function:

$q(x) = \sum_{i=1}^m (a_i x + b_i)\, 1_{r_{i-1}\leq x < r_i}$ with $a_i r_i + b_i = a_{i+1} r_i + b_{i+1}$

- ℓ_∞-approximation result (Shektman, 1982): Let f be a continuous function on $[c, d]$. $\forall\, \varepsilon > 0\ \exists\, q$ s.t. $\sup_{x\in[c,d]} |f(x) - q(x)| \leq \varepsilon$

Piecewise linear functions can be written as combination of RELU

- Claim 1: Any PWL q can be rewritten as

$q(x) = \tilde{a}_1 x + \tilde{b}_1 + \sum_{i=2}^m \tilde{a}_i \left(x - \tilde{b}_i\right)_+$

where $\tilde{a}_1 = a_1, \tilde{b}_1 = b_1, a_i = \sum_{j=1}^i \tilde{a}_i$ and $\tilde{b}_i = r_{i-1}$

- Claim 2: q can be implemented as a one-hidden-layer NN with RELU activation. Each term corresponds to one node:

- Bias $-\tilde{b}_i$
- Output weight $\tilde{a}_i$

The term $\tilde{a}_1 x + \tilde{b}_1$ also corresponds to one node:

- Bias $\tilde{b}_1$: bias of the output node
- Term $\tilde{a}_1 x = \tilde{a}_1(x)_+$since $x \in [0, 1]$

Proof of the equivalent formulation

$$q(x) = \sum_{i=1}^m (a_i x + b_i)\, 1_{r_{i-1}\leq x < r_i} \quad r(x) = \tilde{a}_1 x + \tilde{b}_1 + \sum_{i=2}^m \tilde{a}_i \left(x - \tilde{b}_i\right)_+$$

$$\tilde{a}_1 = a_1, \tilde{b}_1 = b_1 \text{ and } a_i = \sum_{j=1}^i \tilde{a}_j \text{ and } \tilde{b}_i = r_{i-1}$$

- For $x \in [0, r_1]$

$\left(\tilde{a}_1, \tilde{b}_1\right) = (a_1, b_1) \Longrightarrow q(x) = a_1 x + b_1 = \tilde{a}_1 x + \tilde{b}_1 = r(x)$ because $\tilde{b}_2 = r_1$

- For $x \in [r_1, r_2], r(x) = \tilde{a}_1 x + \tilde{b}_1 + (a_2 - a_1)(x - r_1)_+$

$= a_1 x + b_1 + (a_2 - a_1)(x - r_1) = a_2 x + b_1 - (a_2 - a_1) r_1$

$r'(x) = a_2$ and $r(r_1) = q(r_1)$ as shown above

$\Longrightarrow r(x) = q(x)$ for $x \in [r_1, r_2]$

Proof by induction

Let's assume that $r(x) = q(x)$ for $x \in [0, r_{i-1}]$

For $x \in [r_{i-1}, r_i]$

$$\begin{aligned} r(x) &= \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^m \tilde{a}_j \left(x - \tilde{b}_j\right)_+ \\ &= \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^i \tilde{a}_j \left(x - \tilde{b}_j\right) \\ &= \sum_{j=1}^i \tilde{a}_j x + \tilde{b}_1 - \sum_{j=2}^j \tilde{a}_j \tilde{b}_j \end{aligned}$$

Thus

- $r'(x) = \sum_{j=1}^i \tilde{a}_j = a_i$ good slope
- $r(r_{i-1}) = q(r_{i-1})$ good starting point

$\Longrightarrow r(x) = q(x)$ for $x \in [r_{i-1}, r_1]$

Why: two affine functions with the same starting point and the same slope are equal

Recap

- Neural networks consist of linear layers stacked together with non-linearities
- A neural network can be seen as a learned feature extractor + a linear predictor
- Neural networks typically require large amounts of data and compute to learn good features
- Neural networks have very high representational power (i.e., the universal approximation result) in contrast to simple models like linear regression

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Neural Network Training

Training of NNs with SGD

- SGD algorithm: Uniformly sample n, compute the gradient of $\mathscr{L}_n = \frac{1}{2}(y_n - f(x_n))^2$ to update:

$$\left(w_{i,j}^{(l)}\right)_{t+1} = \left(w_{i,j}^{(l)}\right)_t - \gamma \frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}}$$

$$\left(b_i^{(l)}\right)_{t+1} = \left(b_i^{(l)}\right)_t - \gamma \frac{\partial \mathscr{L}_n}{\partial b_i^{(l)}}$$

- In Practice: Step size schedule, mini-batch, momentum, Adam
- Problem: With $O\left(K^2 L\right)$ parameters, applying chain-rules independently is inefficient due to the compositional structure of f
- Solution: the Backpropagation algorithm computes gradients via the chain rule but reuses intermediate computations

Description of NN parameters

Weight matrices: $\mathbf{W}^{(l)}$ such that $\mathbf{W}_{i,j}^{(l)} = w_{i,j}^{(l)}$, of size

- $\mathbf{W}^{(1)} \in \mathbb{R}^{d\times K}$
- $\mathbf{W}^{(l)} \in \mathbb{R}^{K\times K}$ for $2 \leq l \leq L$
- $\mathbf{W}^{(L+1)} \in \mathbb{R}^K$

Bias vectors: $b^{(l)}$ such that the i-th component is $b_i^{(l)}$

- $b^{(l)} \in \mathbb{R}^K$ for $1 \leq l \leq L$
- $b^{(L+1)} \in \mathbb{R}$

Compact description of output

- $x^{(1)} = f^{(1)}\left(x^{(0)}\right) := \phi\left(\left(\mathbf{W}^{(1)}\right)^\top x^{(0)} + b^{(1)}\right)$
- $x^{(l)} = f^{(l)}\left(x^{(l-1)}\right) := \phi\left(\left(\mathbf{W}^{(l)}\right)^\top x^{(l-1)} + b^{(l)}\right)$
- $y = f^{(L+1)}\left(x^{(L)}\right) := \left(\mathbf{W}^{(L+1)}\right)^\top x^{(L)} + b^{(L+1)}$

The overall function $y = f\left(x^{(0)}\right)$ is just the composition of the layer functions:

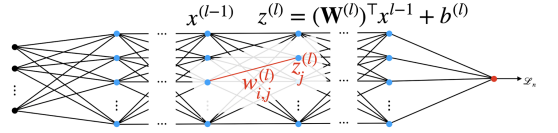
$f = f^{(L+1)} \circ f^{(L)} \circ \cdots \circ f^{(l)} \circ \cdots \circ f^{(2)} \circ f^{(1)}$

Cost function

$\mathscr{L} = \frac{1}{2N} \sum_{n=1}^N \left(y_n - f^{(L+1)} \circ \cdots \circ f^{(2)} \circ f^{(1)}(x_n)\right)^2$

Chain rule

$\mathscr{L}_n = \frac{1}{2}\left(y_n - f^{(L+1)} \circ \cdots \circ f^{(l+1)} \circ \phi\left(z^{(l)}\right)\right)^2$



$$\begin{aligned} \frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}} &= \sum_{k=1}^K \frac{\partial \mathscr{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} \\ &= \frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} \quad \text{since } \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = 0 \text{ for } k \neq j \\ &= \frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} \cdot x_i^{(l-1)} \quad \text{since } z_j^{(l)} = \sum_{k=1}^K w_{k,j}^{(l)} x_k^{(l-1)} + b_j^{(l)} \end{aligned}$$

We need to compute $\frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}}, z^{(l)}, x_i^{(l-1)}$ and reuse them for different $\frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}}$

Forward Pass

$x^{(0)} = x_n \in \mathbb{R}^d$

$z^{(l)} = \left(\mathbf{W}^{(l)}\right)^\top x^{(l-1)} + b^{(l)}\ ,\ x^{(l)} = \phi\left(z^{(l)}\right)$

Computational complexity $\Rightarrow O\left(K^2 L\right)$

Backward pass (I)

Define $\delta_j^{(l)} = \frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} = \sum_k \frac{\partial \mathscr{L}_n}{\partial z_k^{(l+1)}} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \sum_k \delta_k^{(l+1)} \frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}}$

Backward pass (II)

- Using $z_k^{(l+1)} = \sum_{i=1}^K w_{i,k}^{(l+1)} x_i^{(l)} + b_k^{(l+1)} = \sum_{i=1}^K w_{i,k}^{(l+1)} \phi\left(z_i^{(l)}\right) + b_k^{(l+1)}$

- We obtain $\frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \phi'\left(z_j^{(l)}\right) w_{j,k}^{(l+1)}$

- Thus $\delta_j^{(l)} = \sum_k \delta_k^{(l+1)} \phi'\left(z_j^{(l)}\right) w_{j,k}^{(l+1)}$

$\delta^{(l)} = \left(\mathbf{W}^{(l+1)} \delta^{(l+1)}\right) \odot \phi'\left(z^{(l)}\right)$

Backward pass (III)

Initialization (first derivative):

$\delta^{(L+1)} = \frac{\partial}{\partial z^{(L+1)}} \frac{1}{2}\left(y_n - z^{(L+1)}\right)^2 = z^{(L+1)} - y_n$

$\delta^{(l)} = \left(\mathbf{W}^{(l+1)} \delta^{(l+1)}\right) \odot \phi'\left(z^{(l)}\right)$

Computational complexity: $O\left(K^2 L\right)$

Derivatives computation

- Using $z_m^{(l)} = \sum_{k=1}^K w_{k,m}^{(l)} x_k^{(l-1)} + b_m^{(l)}$:

$\frac{\partial \mathscr{L}_n}{\partial b_j^{(l)}} = \sum_{k=1}^K \frac{\partial \mathscr{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial b_j^{(l)}} = \frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial b_j^{(l)}} = \delta_j^{(l)}$

$\frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}} = \sum_{k=1}^K \frac{\partial \mathscr{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = \frac{\partial \mathscr{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} = \delta_j^{(l)} \cdot x_i^{(l-1)}$

Backpropagation algorithm

Forward pass:

$x^{(0)} = x_n \in \mathbb{R}^d$

$z^{(l)} = \left(\mathbf{W}^{(l)}\right)^\top x^{(l-1)} + b^{(l)}$

$x^{(l)} = \phi\left(z^{(l)}\right)$

Backward pass:

$\delta^{(L+1)} = z^{(L+1)} - y_n$

$\delta^{(l)} = \left(\mathbf{W}^{(l+1)} \delta^{(l+1)}\right) \odot \phi'\left(z^{(l)}\right)$

Compute the derivatives:

$\frac{\partial \mathscr{L}_n}{\partial w_{i,j}^{(l)}} = \delta_j^{(l)} x_i^{(l-1)}$

$\frac{\partial \mathscr{L}_n}{\partial b_j^{(l)}} = \delta_j^{(l)}$

Parameter Initialization

- In deep networks, improper parameter initialization can lead to the vanishing or exploding gradients problem
- Problem: Extremely slow or unstable optimization
- Solution: Control the layerwise variance of neurons (aka He initialization)

Variance-Preserving Initialization

- for ReLU networks:

- $z^{(l)} \sim \mathcal{N}(0, \mathbf{I}_K)$: pre-activations at layer l (note: $\mathrm{Var}\left[z_i^{(l)}\right] = 1$)
- $w_i^{(l+1)} \sim \mathcal{N}(0, \sigma \mathbf{I}_K)$: the i-th weight vector at layer $l+1$
- $z_i^{(l+1)} = \mathrm{ReLU}\left(z^{(l)}\right)^\top w_i^{(l+1)}$: the i-th pre-activation at layer $l+1$
- We set $\sigma = \sqrt{2/K}$ so that $\mathrm{Var}\left[z_i^{(l+1)}\right] = 1$

Batch Normalization

- Batch $B = (x_1, \cdots, x_M)$ and denote by $z_n^{(l)}$ the layer's pre-activation input corresponding to the observation x_n

- Step 1: Normalize each layer's input using its mean and its variance over the batch:

$\bar{z}_n^{(l)} = \frac{z_n^{(l)} - \mu_B^{(l)}}{\sqrt{\left(\sigma_B^{(l)}\right)^2 + \varepsilon}}$ (Component-wise)

where $\mu_B^{(l)} = \frac{1}{M}\sum_{n=1}^M z_n^{(l)}$ and $\left(\sigma_B^{(l)}\right)^2 = \frac{1}{M}\sum_{n=1}^M \left(z_n^{(l)} - \mu_B^{(l)}\right)^2$, and $\varepsilon \in \mathbb{R}_{\geq 0}$ is a small value added for numerical stability

- Step 2: Introduce learnable parameters $\gamma^{(l)}, \beta^{(l)} \in \mathbb{R}^K$ to be able to reverse the normalization if needed: $\hat{z}_n^{(l)} = \gamma^{(l)} \odot \bar{z}_n^{(l)} + \beta^{(l)}$

- Scale-invariance: For $\varepsilon \approx 0$, the output is invariant to activation-wise affine scaling of $z_n^{(l)}$

$\mathrm{BN}\left(a \odot z_n^{(l)} + b\right) = \mathrm{BN}\left(z_n^{(l)}\right)$ for $a \in \mathbb{R}_{>0}^K$ and $b \in \mathbb{R}^K$ e.g. $\Rightarrow$ no need to include a bias before BatchNorm.

- Inference: The prediction for one sample should not depend on other samples

- Estimate $\hat{\mu}^{(l)} = \mathbf{E}\left[\mu_B^{(l)}\right]$ and $\hat{\sigma}^{(l)} = \mathbf{E}\left[\sigma_B^{(l)}\right]$ during training, use these for inference
- Exponential moving averages are commonly used in practice

- Implementation:

- Requires sufficiently large batches to get good estimates of $\mu_B^{(l)}, \sigma_B^{(l)}$
- BatchNorm is applied a bit differently for non-fully-connected nets

Batch Normalization - Results

- BatchNorm leads to much faster convergence
- BatchNorm allows to use much larger learning rates (up to 30×)

Layer Normalization

- Step 1: Normalize each layer's input using its mean and its variance over the features (instead of over the inputs): $\bar{z}_n^{(l)} = \frac{z_n^{(l)} - \mu_n^{(l)} \cdot 1_K}{\sqrt{\left(\sigma_n^{(l)}\right)^2 + \varepsilon}}$

where $\mu_n^{(l)} = \frac{1}{K}\sum_{k=1}^K z_n^{(l)}(k)$ and $\left(\sigma_n^{(l)}\right)^2 = \frac{1}{K}\sum_{k=1}^K \left(z_n^{(l)}(k) - \mu_n^{(l)}\right)^2$, and $\varepsilon \in \mathbb{R}_{\geq 0}$

- Step 2: Introduce learnable parameters $\gamma^{(l)}, \beta^{(l)} \in \mathbb{R}^K$: $\hat{z}_n^{(l)} = \gamma^{(l)} \odot \bar{z}_n^{(l)} + \beta^{(l)}$

- Normalize across features, independently for each observation
- Very common alternative, widely used for transformers and text data
- No batch dependency, use the same for training and inference

Normalization Benefits

- Stabilizes activation magnitudes / reduces initialization impact
- Additional regularization effect from noisy $\mu_B^{(l)}, \sigma_B^{(l)}$ in batch norm
- Stabilizes and speeds up training, allows larger learning rates
- Used in almost all modern deep learning architectures
- Often inserted after every convolutional layer, before non-linearity

Recap

- Neural networks are trained with gradient-based methods such as SGD
- To compute the gradients, we use backpropagation, which involves the chain rule to efficiently calculate the gradients based on the network's intermediate outputs $z^{(l)}$ and $\delta^{(l)}$
- Proper parameter initialization should avoid exploding and vanishing gradients by carefully controlling the layerwise variance
- Batch and Layer normalization dynamically stabilize the training process, allowing for faster convergence and the use of larger learning rates

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Convolutional Networks

CNN General Structure

- Convolutional networks consist of sparsely connected convolutional layers in place of fully-connected linear layers
- Pooling layers perform spatial downsampling (typically typically reducing the dimensions from $H \times W$ to $H/2 \times W/2$
- A fully-connected network at the end performs classification based on the extracted features
- Fully connected NNs have $O\left(K^2 L\right)$ parameters: training requires a lot of data
- Fully connected neural networks interpret an image as a flattened vector, disregarding the original spatial dependencies

Convolution

$x_{n,m}^{(1)} = \sum_{k,l} f_{k,l} \cdot x_{n-k,m-l}^{(0)}$

- We consider local filters: $f_{k,l} \neq 0$ for small values of $|k|$ and $|l|$

$\rightarrow x_{n,m}^{(1)}$ only depends on the value of $x^{(0)}$ close to (n, m)

$\rightarrow f$ represents the learnable weights

- We use the same filter at every position - weight sharing
- Translation equivariance - a shifted input results in a shifted output
- Convolution requires fewer parameters which are universal across different locations

Handling of borders

- Zero padding: Add zeros to each side of the input's boundaries $\Rightarrow$ same dimension as the input
- Valid padding: Perform the convolution only where the entire filter fits inside the original data $\Rightarrow$ smaller dimensions than the input

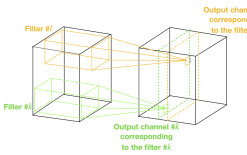
Filter for Multi-Channel Convolution

- For multi-channel inputs, the filter has the same number of channels as the input
- The filter channels and the bias are the learnable parameters of the filter

Multi-Channel Output from Multiple Filters

- It is common to use multiple filters. Each filter processes the input to produce a separate channel
- Applying different filters to an input generates multiple output channels.

Convolutional Layer



- A convolutional layer is composed of multiple filters
- Each output channel corresponds to its own independent filter
- Hyper-parameters of the convolutional layer: size, padding, stride

Pooling

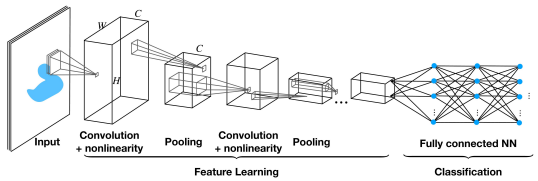
- often applied after the convolutional layer
- Max pooling: returns the maximum value of the portion of the convolved feature that is covered by the kernel

- Average pooling: returns the average value of the portion of the convolved feature that is covered by the kernel
- Pooling is a downsampling operation that reduces the spatial dimensions of the convolved feature
- Remark: Pooling layers do not have learnable parameters
- Hyperparameters are the size, type, and stride of the pooling operation

Non-linearity and CNNs

- Important: A non-linearity such as ReLU is included after each convolutional layer to make the model non-linear

CNNs: General Structure



- Depth: ↑ # channels, ↓ dimensions
- Receptive field (area of input that affects a given neuron) increases with depth:
• First layers extract low-level features, e.g., edges, colors (↓ receptive field + ↓ depth)
• Subsequent layers extract high-level features, e.g., objects (↑ receptive field + ↑ depth)
- ConvNet reduces the images to a form easier to process without losing essential features

Backpropagation with weight sharing

- Weight sharing is used in CNN: many edges use the same weights

Training:

1. Run backpropagation as if the weights were not shared (treat each weight as an independent variable)
2. Once the gradient is computed, sum the gradients of all edges that share the same weight

Let $f(x,y,z):\mathbb{R}^3\to\mathbb{R}$ and $g(x,y)=f(x,y,x)$

$$\left(\frac{\partial g}{\partial x}(x,y),\frac{\partial g}{\partial y}(x,y)\right)$$
$$\underset{\text{Chain rule}}{=}\left(\frac{\partial f}{\partial x}(x,y,x)+\frac{\partial f}{\partial z}(x,y,x),\frac{\partial f}{\partial y}(x,y,x)\right)$$

Learned Convolutional Filters

- Edge and color detectors typically emerge when trained on large datasets
- Individual Activations Can Be Interpretable
- Activations in later layers detect more complex patterns

Residual Networks

Skip Connections and Residuals

• Starting point: Adding more layers should lead to the same or lower training loss as they can learn the identity function
• ResNet paper indicates that this is not always the case
• Solution: add a skip connection around some layers $F(\mathbf{X})$
• Standard network: $\mathbf{Y}=F(\mathbf{X})$
• Residual network: $\mathbf{Y}=R(\mathbf{X})+\mathbf{X}$ where $R(\mathbf{X})$ is called a residual branch
• Technical detail: If size($\mathbf{Y}$) $\neq$ size($\mathbf{X}$), additional operations are needed on the skip connection to match the dimensions
• Skip connections address the observed convergence issue, making the training of very deep networks (with hundreds of layers) feasible
• Skip connections are used in almost all modern neural networks (including CNNs and transformers)

Popular architectures

VGG & ResNet

Data Augmentation

- Generate new data from the data
- Note dangers of excessive augmentation (e.g. rotation on MNIST)!
- Transformation $\tau:\mathbb{R}^d\to\mathbb{R}^d$ which preserves the labels (i.e., $y_x=y_{\tau(x)}$)

$$S=S_{\text{train}}\cup\{(\tau(x_i),y_i)\}_{i=1}^n$$

• We train on more data
• Encourages models to be invariant to τ
• It can be seen as regularization
• These transformations are task and dataset specific
- Pictures can also be cropped, resized, or perturbed by a small amount of noise

Weight Decay: l_2-regularization

- Regularize weights without regularizing bias terms: $\min\mathscr{L}+\frac{\lambda}{2}\sum_l\left\|\mathbf{W}^{(l)}\right\|_F^2$
- Favors small weights which can aid in generalization and optimization
- Optimization with gradient descent:

$$\left(w_{i,j}^{(l)}\right)_{t+1}=\left(w_{i,j}^{(l)}\right)_t-\eta\nabla\mathscr{L}-\eta\lambda\left(w_{i,j}^{(l)}\right)_t=\underbrace{(1-\eta\lambda)}_{\text{weight decay}}\left(w_{i,j}^{(l)}\right)_t-\eta\nabla\mathscr{L}$$

- Interaction with BatchNorm:
• $\text{BN}(\mathbf{WX})=\text{BN}(\alpha\mathbf{WX})$ for $\alpha\in\mathbb{R}_{>0}$ (assuming $\varepsilon\approx 0$)
• BN is scale invariant in $\mathbf{W}$, hence there is no direct regularization effect from WD
• However, the training dynamics differ

Dropout: randomly drop nodes

- Def: At each training step, retain with probability $p^{(l)}$ each node in layer (l) :
- We drop nodes independently for each element of a mini-batch
- Training phase: Run one step of SGD on the subnetwork and update the weights
- Testing phase:
• Use all nodes
• Scale each of them by the factor $p^{(l)}$ to ensure that the expected output (when considering the probability of dropping nodes during training) matches the actual output at test time
- Remark: Weight rescaling can be implemented during training time by scaling the weights by $1/p^{(l)}$ after each weight update - how it is implemented in practice
- Note: Variance is generally not preserved and as a result Dropout often works poorly with normalization

Dropout: results

• Setting: Fully-connected networks of different width and depth on MNIST
• Dropout results in lower test error
• However, dropout typically requires more iterations to converge due to increased stochastic noise

Recap

• Convolutional networks are composed of sparsely connected convolutional layers instead of fully-connected linear layers
• The same convolution is applied as a sliding window across all spatial locations
• Data augmentation usually results in a significant improvement in the model's generalization performance
• Weight decay and dropout can further enhance the performance, though typically to a lesser extent

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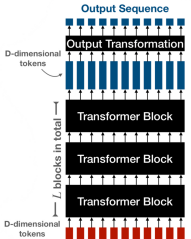
Transformers

- A transformer is a neural network that iteratively transforms a sequence to another sequence and mixes the information between the sequence elements via self-attention.

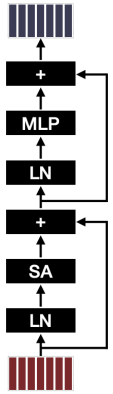
Architecture

- Self-Attention (SA): mixes information between tokens
- Multi-Layer Perceptron (MLP): mixes information within each token
- Skip connections are widely used



- Layer normalization (LN) is usually placed at the start of a residual branch

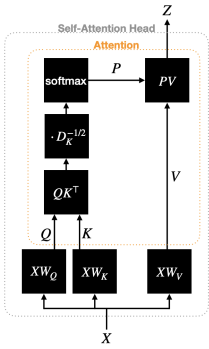
Text Token Embeddings



- Tokenization: split the input text into a sequence of input tokens (typically word fragments + some special symbols) according to some predefined tokenizer procedure:
- Convert each token ID $i\in\{1,\ldots,N_{vocab}\}$ into a real-valued vector $\mathbf{w}_i\in\mathbb{R}^D$
- This can be seen as a matrix multiplication $\mathbf{W}\cdot\mathbf{e}_i=\mathbf{W}_{:,i}=\mathbf{w}_i$ (with $\mathbf{W}\in\mathbb{R}^{\text{D}\times\text{N}_{\text{vocab}}}$)
- $\mathbf{W}$ is learned via backpropagation, along with all other transformer parameters (however, the tokenizer procedure is typically fixed in advance and not learned)
- The whole input sequence of T tokens leads to an input matrix $X\in\mathbb{R}^{T\times D}$

Attention

- Attention is a function that transforms a sequence of tokens to a new sequence of tokens using a learned input-dependent weighted average
- Input tokens : $V\in\mathbb{R}^{T_{in}\times D}$
- Output tokens : $Z\in\mathbb{R}^{T_{out}\times D}$
- Output tokens are simply a weighted average of the input tokens: $z_i=\sum_{j=1}^{T_i}p_{ij}v_j$ i.e. $Z=PV$
- Weighting coefficients $\mathcal{P}\in[0,1]^{T_{out}\times T_{in}}$ form valid probability distributions over the input tokens $\sum_{j=1}^{T_{in}}p_{ij}=1$
- Query tokens : $Q\in\mathbb{R}^{T_{out}\times D_K}$
- Key tokens : $K\in\mathbb{R}^{T_{in}\times D_K}$
- Determine weight $p_{i,j}$ based on how simmilar q_i and k_j are.
- Use inner product to obtain raw similarity scores.
- Normalize with softmax (scaled the temperature by $\sqrt{D_K}$) to obtain a probability distribution.



- $P=\text{softmax}\left(\frac{QK^\top}{\sqrt{D_K}}\right)$

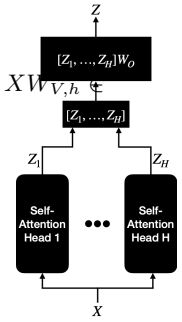
The softmax is applied on each row independently. Scaling ensures uniformity at initialization and faster convergence

Self-Attention

- V, K, Q are all derived from the same input token sequence $X \in \mathbb{R}^{T \times D}$
- Values : $V = XW_V \in \mathbb{R}^{T \times D}$, $W_V \in \mathbb{R}^{D \times D}$
- Keys : $K = XW_K \in \mathbb{R}^{T \times D_K}$, $W_K \in \mathbb{R}^{D \times D_K}$
- Queries : $Q = XW_Q \in \mathbb{R}^{T \times D_K}$, $W_Q \in \mathbb{R}^{D \times D_K}$
- W_Q, W_V, W_K are learned parameters.
- $Z = \text{softmax}\left(\frac{XW_Q W_K^T X^T}{\sqrt{D_K}}\right) XW_V$

Multi-Head Self-Attention

- Run H Self-Attention "heads" in parallel
- $Z_h = \text{softmax}\left(\frac{XW_{Q,h} W_{K,h}^\intercal X^\intercal}{\sqrt{D_K}}\right) XW_{V,h} \in \mathbb{R}^{T \times D_V}$



- $W_{V,h} \in \mathbb{R}^{D \times D_V}$, $W_{K,h} \in \mathbb{R}^{D \times D_K}$, $W_{Q,h} \in \mathbb{R}^{D \times D_K}$
- The final output is obtained by concatenating head-outputs and applying a linear transformation $Z = [Z_1, \ldots, Z_H]W_o$ where $W_O \in \mathbb{R}^{HD_V \times D}$ is learned via backpropagation

Positional Information

- Attention by itself does not account for the order of input
- incorporate a positional encoding in the network which is a function from the position to a feature vector $pos : \{1, ..., T\} \to \mathbb{R}^D$
- The most basic choice is to add a positional embedding W_{pos} corresponding to each token's position t to the input embedding. $W_{pos} \in \mathbb{R}^{D \times T}$ is learned via backpropagation along with the other parameters

MLP

- Mixing Information within Tokens
- Apply the same transformation to each token independently: $MLP(X) = \varphi(XW_1)W_2$
- $W_1, W_2 \in \mathbb{R}^{D \times D}$ learned via backprop

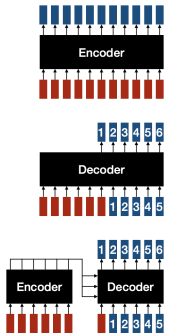
Output Transformations

- typically simple: linear transformation or a small MLP
- dependent on the task: Single output (e.g.,sequence-level classification): apply an output transformation to a special taskspecific input token or to the average of all tokens. Multiple outputs (e.g., per-token classification): apply an output transformation to each token independently

Vision Transformer Architecture

- Self-attention is more general than convolution and can potentially express it
- The receptive field is the whole image after just one self-attention layer
- ViTs require more data than CNNs due to their reduced inductive bias in extracting local features
- In many cases, the model attends to image regions that are semantically relevant for classification

Encoders & Decoders



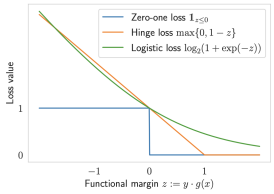
- Encoders (e.g., classification): They produce a fixed output size and process all inputs simultaneously
- Decoders (e.g., ChatGPT): Auto-regressively sample the next token as $x_{t+1} \sim sofimax(f(x_1, ..., x_t))$ and use it as new input token. Capable of generating responses of arbitrary length.
- Encoder-decoder (e.g., translation): First encode the whole input (e.g., in one language) and then decode to token by token (e.g., in a different language)

Adversarial ML

- We don't understand how NN models generalize and react to shifts in the distribution of data (i.e., distribution shifts)
- Classification problem: $(X, Y) \sim \mathcal{D}$, Y with range $\{-1, 1\}$
- Standard risk: average zero-one loss over X: $R(f) = \mathbb{E}_{\mathcal{D}}\left[1_{f(X) \neq Y}\right] = \mathbb{P}_{\mathcal{D}}\left[f(X) \neq Y\right]$ i.e. minimise proba of wrong prediction.
- Adversarial risk: average zero-one loss over small, worst-case perturbations of X: $R_\varepsilon(f) = \mathbb{E}_{\mathcal{D}}\left[\max_{\hat{x}, \|\hat{x} - X\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y}\right]$

Generating adversarial examples

- Task: given an input (x, y) and a model $f : \mathcal{X} \to \{-1, 1\}$ find an input $\hat{x}$ s.t.: a) $\|\hat{x} - x\| \leq \varepsilon$ b) the model f makes a mistake on it.
- Trivial case: x already missclassified → no action required
- General case: find $\hat{x}$ such that at $f(\hat{x}) \neq y$ and $||\hat{x} - x|| \leq \varepsilon$ i.e. $\hat{x} \in B_x(\varepsilon) \cap \{x' f(x') = -y\}$
- Optimization problem with respect to the inputs
- Problem: optimizing the indicator function is difficult: 1) The indicator function 1 is not continuous 2) The NN prediction f outputs discrete class values $\{-1, 1\}$
- Replace the difficult problem involving the indicator with a smooth problem $\max_{\hat{x}, \|\hat{x} - X\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y} \to \max_{\hat{x}, \|\hat{x} - X\| \leq \varepsilon} \ell(yg(\hat{x}))$
- decreasing, margin-based (i.e., dependent on $y * g(x)$) classification losses



White-Box attacks

- Solve $\max_{\hat{x}, \|\hat{x} - X\| \leq \varepsilon} \ell(yg(\hat{x}))$ knowing g
- $\nabla_x \ell(yg(x)) = y\ell'(yg(x)) \nabla_x g(x)$, with $y\ell'(yg(x)) \leq 0$ since classification losses are decreasing.
- Move in direction of $\propto -y \nabla_x g(x)$
- Interpretation $f(x) = \text{sign}(g(x))$: If $y = 1$ we want to decrease $g(x)$ and follow $-\nabla_x g(x)$. If $y = -1$ we want to decrease $g(x)$ and follow $\nabla_x g(x)$
- By using ℓ and not directly $yg(\hat{x})$ it will extend to multi-class classification and robust training.
- linearize the loss $\tilde{\ell}(x) := \ell(yg(x))$

$\max_{\|\hat{x} - x\| \leq \varepsilon} \tilde{\ell}(x)$
$\approx \max_{\|\hat{x} - x\| \leq \varepsilon} \tilde{\ell}(x) + \nabla_x \tilde{\ell}(x)^T (\hat{x} - x)$
$= \tilde{\ell}(x) + \max_{\|\hat{x} - x\| \leq \varepsilon} \nabla_x \tilde{\ell}(x)^T (\hat{x} - x)$
$= \tilde{\ell}(x) + \max_{\|\delta\| \leq \varepsilon} \nabla_x \tilde{\ell}(x)^T \delta$

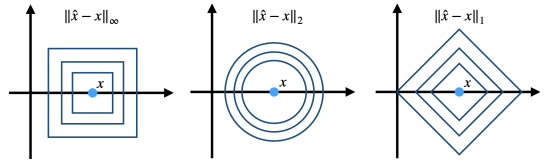
- We need to maximize the inner product under a norm constraint, i.e. find the optimal local update
- This is a simple problem for which we can get a closed-form solution depending on the norm used to measure the perturbation size $||\delta||$

One-step attack

- Solution for the ℓ_2 norm:
$\delta_2^\star = \varepsilon \cdot \frac{\nabla_x \tilde{\ell}(x)}{||\nabla_x \tilde{\ell}(x)||_2} = -\varepsilon y * \frac{\nabla_x g(x)}{||\nabla_x g(x)||_2} \Rightarrow$
$\hat{x} = x - \varepsilon y \cdot \frac{\nabla_x g(x)}{\|\nabla_x g(x)\|_2}$
- Solution for the ℓ_∞ norm called **Fast Gradient Sign Method**:
$\delta_\infty^\star = \varepsilon \cdot \text{sign}(\nabla_x \tilde{\ell}(x)) = -\varepsilon y \cdot \text{sign}(\nabla_x g(x)) \Rightarrow$
$\hat{x} = x - \varepsilon y \cdot \text{sign}(\nabla_x g(x))$

Multi-step attack

- These updates can be done iteratively and combined with a projection Π on the feasible set (i.e., balls ℓ_2 / ℓ_∞ here)
- Projected Gradient Descent (PGD attack)
- ℓ_2 norm:
$\delta^{t+1} = \Pi_{B_2(\varepsilon)}[\delta^t + \alpha \cdot \frac{\nabla \tilde{\ell}(x + \delta^t)}{\|\nabla \tilde{\ell}(x + \delta^t)\|_2}]$
$\Pi_{B_2(\varepsilon)}(\delta) = \begin{cases} \varepsilon \cdot \delta / \|\delta\|_2, & \text{if } \|\delta\|_2 \geq \varepsilon \\ \delta \text{ otherwise} \end{cases}$
- ℓ_∞ norm:
$\delta^{t+1} = \Pi_{B_\infty(\varepsilon)}\left[\delta^t + \alpha \cdot \text{sign}(\nabla \tilde{\ell}(x + \delta^t))\right]$,
$\Pi_{B_\infty(\varepsilon)}(\delta)_i = \begin{cases} \varepsilon \cdot \text{sign}(\delta_i), & \text{if } |\delta_i| \geq \varepsilon \\ \delta_i \text{ otherwise} \end{cases}$
- the gradients are computed by backprop w.r.t. inputs, not parameters!



Black-box attacks

- We don't know $g(x)$
- Obtaining a surrogate model can be costly and there is no guarantee of success
- Query-based methods often require a lot of queries (10k-100k), easy to restrict access for the attacker!

Query-based gradient estimation

- Score-based: we can query the continuous model scores $g(x) \in \mathbb{R}$. We can approximate the gradient by using the finite difference formula:
$\nabla_x g(x) \approx \sum_{i=1}^d \frac{g(x + \alpha e_i) - g(x)}{\alpha} e_i$
- Decision-based: we can query only the predicted class $f(x) \in \{-1, 1\}$, similar techniques can be adapted for the decision-based case.

Transfer Attacks

- Train a similar surrogate model $\hat{f} \approx f$ on similar data
- Model stealing (query f given some unlabeled inputs $\{x_n, f(x_n)\}_{n=1}^N$) can facilitate transfer attacks.

Adversarial training

- Adversarial training: the goal is to minimize the adversarial risk:
$\min_\theta R_\varepsilon(f_\theta) = \mathbb{E}_{\mathcal{D}}\left[\max_{\hat{x}, \|\hat{x} - X\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y}\right]$
- $\mathcal{D}$ unknown → approximate it with a sample average + classification loss is non-continuous → use a smooth loss ⇒
$\min_\theta \frac{1}{N} \sum_{n=1}^N \max_{\hat{x}_n, \|x_n - \hat{x}_n\| \leq \varepsilon} \ell(y_n g_\theta(\hat{x}_n))$
1) $\forall x_n$, $\hat{x}_n^\star \approx \arg\max_{||x_n - \hat{x}_n|| \leq \varepsilon} \ell(y_n g_\theta(\hat{x}_n))$
2) GD step w.r.t. θ using $\frac{1}{N} \sum_{n=1}^N \nabla_\theta \ell(y_n g_\theta(\hat{x}_n^\star))$

Advantages

- state-of-the-art approach for robust classification
- more interpretable gradients
- fully compatible with SGD

Disadvantages

- Increased computational time: proportional to the number of PGD steps
- Robustness-accuracy tradeoff: using too large ε leads to worse standard accuracy

Adversarial Example

$x \in \mathbb{R}^d, y \sim Bernoulli(\{-1, 1\}), Z_i \sim \mathcal{N}(0, 1)$
- Robust features: $x_1 = y + Z_1$
- Non-robust features: $x_i = y\sqrt{\frac{\log d}{d-1}} + Z_i$, $\forall i \in \{-1, 1\}$
- $d \to \infty \Rightarrow \uparrow$ adversarial risk and $\downarrow$ standard risk

- using the robust feature x_1:
MLE: $\arg\max_{\hat{y}\in\{\pm1\}} p(\hat{y} \mid x_1) =$
$\arg\max_{\hat{y}\in\{\pm1\}} \frac{p(x_1|\hat{y})p(\hat{y})}{p(x_1)} = \arg\max_{\hat{y}\in\{\pm1\}} p(x_1 \mid \hat{y})$
assuming $p(y=1) = p(y=-1)$
- Standard Risk: $\int_0^\infty \frac{1}{\sqrt{2\pi}} e^{-0.5(x+1)^2} dx \approx 0.16$
good but not perfect!
- using both robust and non-robust features:
MLE for all features $x_i = ya_i + Z_i$
$\arg\max_{\hat{y}\in\{\pm1\}} p(\hat{y} \mid x)$
$= \arg\max_{\hat{y}\in\{\pm1\}} \prod_{i=1}^d p(x_i \mid \hat{y})$
$= \arg\max_{\hat{y}\in\{\pm1\}} \sum_{i=1}^d \log p(x_i \mid \hat{y})$
$= \arg\max_{\hat{y}\in\{\pm1\}} \sum_{i=1}^d \log \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x_i - \hat{y}a_i)^2}$
$= \arg\min_{\hat{y}\in\{\pm1\}} \sum_{i=1}^d (x_i - \hat{y}a_i)^2$
$= \arg\min_{\hat{y}\in\{\pm1\}} \sum_{i=1}^d (x_i^2 - 2x_i\hat{y}a_i + \hat{y}^2 a_i^2)$
$= \arg\max_{\hat{y}\in\{\pm1\}} \hat{y} \sum_{i=1}^d x_i a_i$
$\hat{y}\sum_{i=1}^d x_i a_i = \hat{y}y(\sum_{i=1}^d a_i^2) + \hat{y}\sum_{i=1}^d a_i Z_i = \hat{y}y(1+\log(d)) + \hat{y}Z$ where $Z := \sum_{i=1}^d a_i Z_i \sim \mathcal{N}(0, 1+\log d)$
Scaling by $1/(1+\log d)$ the MLE results in:
$y\hat{y} + \hat{y}Z$ with $Z \sim \mathcal{N}(0, 1/(1+\log d))$
$d \to \infty, \hat{y}Z \to 0 \Rightarrow$ standard risk $R(f) \to 0$
- using the non-robust features improves standard risk!
- Adversarial risk:
The adversary can use tiny ℓ_∞ perturbations:
$\varepsilon = 2\sqrt{\frac{\log d}{d-1}}$ ($\to 0$ when) $d \to \infty$)
$\hat{x}_1 = \left(1 - 2\sqrt{\frac{\log d}{d-1}}\right) y + Z_1$, almost unaffected
$\hat{x}_i = -\sqrt{\frac{\log d}{d-1}} y + Z_i$, completely flipped
$R_\varepsilon(f) \approx 1 \Rightarrow$ tradeoff between accuracy and robustness.

Fairness criteria in classification

1. Use an algorithm to produce a score function $R = r(X)$
- Bayes optimal score
- Learned from labeled data, e.g., in logistic regression
2. Make binary decisions according to the threshold rule $D = 1_{R>t}$
- Assume R given and are interested in the decision process

Statistical classification criteria

- True positive rate: $\mathbb{P}(D=1 \mid Y=1)$
- False positive rate: $\mathbb{P}(D=1 \mid Y=0)$
- True negative rate: $\mathbb{P}(D=0 \mid Y=0)$
- False negative rate: $\mathbb{P}(D=0 \mid Y=1)$
- The choice of the threshold t in the decision rule D will depend on the classification criteria we pick

Sensitive attributes

- In many tasks, X can encode sensitive attributes of an individual
- Introduce additional random variable A encoding membership status in a protected class
- No fairness through unawareness: removing/ignoring sensitive attributes is not solving the problem
- Many features slightly correlated with the sensitive attribute can be used to recover the attribute
- If we remove the attribute, the classifier will still find a redundant encoding in terms of other features and we'll have learned an equivalent classifier

Three fundamental fairness criteria

- Idea: equalize different statistical quantities involving group membership A
- Most of the fairness criteria are properties of (A, Y, R) :
- Independence: $A \perp R$
- Separation: $A \perp R \mid Y$
- Sufficiency: $A \perp Y \mid R$

Independence: equal acceptance rate

- Implies, for any two groups a, b :
$\mathbb{P}(D=1 \mid A=a) = \mathbb{P}(D=1 \mid A=b)$
$\to$ The acceptance rate is the same in all groups: equal positive rate

Limitations of independence

- Does not rule out unfair practice. Let's imagine a company which
- hires with care (ie., makes good decisions) in a group a at some rate $p > 0$
- hires without care (i.e., makes poor decisions) in a group b with the same rate p
$\to$ acceptance in both groups is identical
$\to$ unqualified applicants are more likely to be selected in the group b
$\to$ members of the group b will appear to perform less well than those of a
It can happen on its own if there is less data in one group
A positive output can either be a false positive or a true positive
$\to$ we shouldn't be able to match true positives in one group with false positives in another

Separation: equal error rate

- Implies for all groups a, b :
$\mathbb{P}(D=1 \mid Y=0, A=a) = \mathbb{P}(D=1 \mid Y=0, A=b)$ (equal false positive rate)
$\mathbb{P}(D=0 \mid Y=1, A=a) = \mathbb{P}(D=0 \mid Y=1, A=b)$ (equal false negative rate)
- This is a post-hoc criterion: at decision time, we do not know who is a positive/negative instance
- It can be computed in retrospect, by collecting groups of positive and negative instances

Sufficiency:

- For all groups a, b and values r we have:
$\mathbb{P}(Y=1 \mid R=r, A=a) = \mathbb{P}(Y=1 \mid R=r, A=b)$
- Meaning: for predicting Y we do not need to know A if we have R

Calibration and sufficiency

- A score R is calibrated if $\mathbb{P}(Y=1 \mid R=r) = r$
$\to$ you can interpret your score as a probability
$\to$ a priori guarantee: score value r corresponds to positive outcome rate r
- The guarantee does not hold at the individual level
- Calibration by group: $\mathbb{P}(Y=1 \mid R=r, A=a) = r$
- Calibration by group implies sufficiency
- it is also possible to go from sufficiency to calibration

How to achieve fairness criteria

- Post-processing: adjust your learned classifier so that it becomes uncorrelated with the sensitive attribute A
- At training time: work the constraint into the optimization process
- Pre-processing: adjust your features so that they become uncorrelated with the sensitive attribute A : e.g., use deep learning to learn a representation of the data independent of A, while representing original data as well as possible - Zemel et al., 2015

Can we satisfy them simultaneously?

Informal theorem: any of these three criteria are mutually exclusive - except in degenerate cases!

Recap

- ML models ultimately interact with the world, and their design should account for their impact. It's not only about the training.
- There is no fairness through unawareness. Naive data selection and ML techniques can perpetuate or introduce unwanted disparities. Careful preprocessing and post-processing are often necessary.
- We have examined statistical tools to formally reason about fairness criteria.

Incompatibility results: trade-offs are necessary I & II

1. Independence vs sufficiency: If A and Y are not independent, then sufficiency and independence cannot both hold
Proof: $A \perp R$ and $A \perp Y \mid R \Longrightarrow A \perp (Y, R) \Longrightarrow A \perp Y$
2. Independence vs separation: if A is not independent of Y and R is not independent of Y, then independence and separation cannot both hold
Proof: $A \perp R$ and $A \perp R \mid Y \Longrightarrow A \perp Y$ or $R \perp Y$

Proof of the second implication

- Claim: $A \perp R$ and $A \perp R \mid Y \Longrightarrow A \perp Y$ or $R \perp Y$
- Proof: $\mathbb{P}(R=r \mid A=a) = \sum_y \mathbb{P}(R=r \mid A=a, Y=y)\mathbb{P}(Y=y \mid A=a)$
Since $A \perp R$ and $A \perp R \mid Y$:
$\mathbb{P}(R=r) = \mathbb{P}(R=r \mid A=a) = \sum_y \mathbb{P}(R=r \mid Y=y)\mathbb{P}(Y=y \mid A=a)$
We also have
$\mathbb{P}(R=r) = \sum_y \mathbb{P}(R=r \mid Y=y)\mathbb{P}(Y=y)$
Thus
$\sum_y \mathbb{P}(R=r \mid Y=y)\mathbb{P}(Y=y \mid A=a) = \sum_y \mathbb{P}(R=r \mid Y=y)\mathbb{P}(Y=y)$
Since $Y \in \{0,1\}$ it implies
$\mathbb{P}(R=r \mid Y=0)\mathbb{P}(Y=0 \mid A=a) + \mathbb{P}(R=r \mid Y=1)\mathbb{P}(Y=1 \mid A=a) = \mathbb{P}(R=r \mid Y=0)\mathbb{P}(Y=0) + \mathbb{P}(R=r \mid Y=1)\mathbb{P}(Y=1)$
It directly implies
$\mathbb{P}(Y=0)(\mathbb{P}(R=r \mid Y=0) - \mathbb{P}(R=r \mid Y=1)) = \mathbb{P}(Y=0 \mid A=a)(\mathbb{P}(R=r \mid Y=0) - \mathbb{P}(R=r \mid Y=1))$
Therefore either $\mathbb{P}(Y=0) = \mathbb{P}(Y=0 \mid A=a)$ and $A \perp Y$
Or $\mathbb{P}(R=r \mid Y=0) = \mathbb{P}(R=r \mid Y=1)$ and $Y \perp R$

Incompatibility results: trade-offs are necessary III

3. Separation vs sufficiency: Assume all events in the joint distribution of (A, R, Y) have positive probability and assume A/Y. Then, separation and sufficiency cannot both hold
Proof: $A \perp R \mid Y$ and $A \perp Y \mid R \Longrightarrow A \perp (R, Y) \Longrightarrow A \perp R$ and $A \perp Y$

Unsupervised learning

- In unsupervised learning, our data consists only of features (or inputs) $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$, vectors in $\mathbb{R}^D$, and there are no outputs y_n available.
- Unsupervised learning seems to play an important role in how living beings learn. Variants of it seem to be more common in the brain than supervised learning.
- Two main directions in unsupervised learning are
- representation learning
- density estimation & generative models

Examples for Representation Learning

- Given ratings of movies and viewers, we use matrix factorization to extract useful features (see e.g. Netflix Prize). Maybe not unsupervised?
- Learning word-representations using matrix-factorizations, word2vec (Mikolov et al. 2013).
- Given voting patterns of regions across Switzerland, we use PCA to extract useful features (Etter et al. 2014).
- PCA Example 2: Genes mirror geography
- Dendrogram from agglomerative hierarchical clustering with average linkage to the human tumor microarray data.
- Clustering more than two million biomedical publications (Kevin Boyack et.al. 2011)

Unsupervised Representation Learning & Generation

How does it work?

Define a unsupervised or self-supervised loss function, for

- Compression & Reconstruction (e.g. Auto-Encoder)
- Consistency & Contrastive Learning (e.g. Noise-contrastive estimation)
- Generation (e.g. Auto-Encoder, Gaussian Mixture Model)

Examples:

(G = can be used as a generative model)

- Auto-Encoders (G): Invertible networks, learned compression, normalizing flows
- Representation Learning: e.g. images, text, time-series, video. Combining unsupervised representation learning (pre-training) with supervised learning
- Language Models & Sequence Models (G): text generation, or sequence continuation, BERT, video, audio & timeseries (auto-regressive, contrastive, ...)
- Generative Adversarial Networks (GAN) (G) see also predictability minimization
- Contrastive image-language pretraining (CLIP): learns a joint representation space for images and text using contrastive learning
- Diffusion models (G) new state-of-the-art in image generation; these models can be adapted to generate images from text prompts (e.g., DALL-E 2, Stable Diffusion, Midjourney)

Clustering

- Clusters are groups of points whose inter-point distances are small compared to the distances outside the cluster.
- Find "prototype" points $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K$ and cluster assignments $z_n \in \{1, 2, \ldots, K\}$ for all $n = 1, 2, \ldots, N$ data vectors $\mathbf{x}_n \in \mathbb{R}^D$.

K-means clustering

Assume K is known.

$\min_{\mathbf{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2$

s.t. $\boldsymbol{\mu}_k \in \mathbb{R}^D, z_{nk} \in \{0, 1\}, \sum_{k=1}^{K} z_{nk} = 1$,

where $\mathbf{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]^\top$

$\mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N]^\top$

$\boldsymbol{\mu} = [\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K]^\top$

K-means Algorithm

Initialize $\boldsymbol{\mu}_k \forall k$, then iterate:

1. For all n, compute $\mathbf{z}_n$ given $\boldsymbol{\mu}$.

$z_{nk} = \begin{cases} 1 \text{ if } k = \arg\min_{j=1,2,\ldots K} \|\mathbf{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 \text{ otherwise} \end{cases}$

$\rightarrow O(NKD)$

2. For all k, compute $\boldsymbol{\mu}_k$ given $\mathbf{z}$.Take derivative w.r.t. $\boldsymbol{\mu}_k$ to get:

$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk} \mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}} \rightarrow O(NKD)$

Convergence

Convergence to a local optimum is assured since each step decreases the cost (see Bishop, Exercise 9.1).

Coordinate descent

K-means is a coordinate descent algorithm, where, to find $\min_{\mathbf{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu})$, we start with some $\boldsymbol{\mu}^{(0)}$ and repeat the following:

$\mathbf{z}^{(t+1)} := \arg\min_{\mathbf{z}} \mathcal{L}\left(\mathbf{z}, \boldsymbol{\mu}^{(t)}\right)$

$\boldsymbol{\mu}^{(t+1)} := \arg\min_{\boldsymbol{\mu}} \mathcal{L}\left(\mathbf{z}^{(t+1)}, \boldsymbol{\mu}\right)$

Data Compression for images

- aka vector quantization.

Probabilistic model for K-means

$\log \prod_{n=1}^{N} p(x_n|\mu, z) = \log \prod_{n=1}^{N} \mathcal{N}(x_n|\mu_{k'}, I_0)$

$= \log \prod_{n=1}^{N} \prod_{k=1}^{K} \mathcal{N}(x_n|\mu_k, I_0)^{z_{nk}}$

$= \log \prod_{n=1}^{N} \prod_{k=1}^{K} c \cdot e^{-\frac{1}{2}||x_n - \mu_{nk}||^2 \cdot z_{nk}}$

$= -\sum_{n=1}^{N} \sum_{k=1}^{K} \frac{1}{2} ||x_n - \mu_k||^2 z_{nk} + c'$

$= -\mathcal{L}(\mu, z)$

K-means as a Matrix Factorization

$$\min_{\mathbf{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2 = \left\|\mathbf{X}^\top - \mathbf{M}\mathbf{Z}^\top\right\|_{\text{Frob}}^2$$

s.t. $\boldsymbol{\mu}_k \in \mathbb{R}^D$, $z_{nk} \in \{0, 1\}, \sum_{k=1}^{K} z_{nk} = 1$

Issues with K-means

1. Computation can be heavy for large N, D and K.
2. Clusters are forced to be spherical (e.g. cannot be elliptical unlike GMM).
3. Each example can belong to only one cluster ("hard" cluster assignments).

Gaussian Mixture Models

1) K-means forces spherical clusters, not elliptical.
2) In K-means, each example can only belong to one cluster

$\rightarrow$ Solved Gaussian Mixture Models.

Clustering with Gaussians

(1) resolved by using full covariance matrices $\boldsymbol{\Sigma}_k$ instead of isotropic covariances.

$p(\mathbf{X} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}, \mathbf{z}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \left[\mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right]^{z_{nk}}$

$\mu \in \mathbb{R}^{D \cdot K}$ $\Sigma \in \mathbb{R}^{D^2 \cdot K}$ $\mu \in \mathbb{R}^K$

Soft-clustering

(2) resolved by defining z_n to be a random variable, $z_n \in \{1, 2, \ldots, K\}$ that follows a multinomial distribution.

$z_{nk} = \begin{cases} 1 \text{ if assigned to k} \\ 0 \end{cases}, p\left(z_n = k\right) = \pi_k$

where $\pi_k > 0, \forall k$ and $\sum_{k=1}^{K} \pi_k = 1$

This leads to soft-clustering as opposed to having "hard" assignments.

GMM definition

$p(\mathbf{X}, \mathbf{z} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \prod_{n=1}^{N} p(\mathbf{x}_n \mid z_n, \boldsymbol{\mu}, \boldsymbol{\Sigma}) p(z_n \mid \boldsymbol{\pi})$

$= \prod_{n=1}^{N} \prod_{k=1}^{K} [\mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)]^{z_{nk}} \prod_{k=1}^{K} [\pi_k]^{z_{nk}}$

$\mathbf{x}_n :=$ observed data vectors, $z_n :=$ latent unobserved variables, unknown parameters $\boldsymbol{\theta} := \{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K, \boldsymbol{\pi}\}$

- Based on Bayes Rule (conditional probability)

Marginal likelihood

- GMM is a latent variable model with z_n being the unobserved (latent) variables. An advantage of treating z_n as latent variables instead of parameters is that we can marginalize them out to get a cost function that does not depend on z_n, i.e. as if z_n never existed.
- We get the following marginal likelihood by marginalizing z_n out from the likelihood:

$p\left(\mathbf{x}_n \mid \boldsymbol{\theta}\right) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$

- Deriving cost functions this way is good for statistical efficiency. Without a latent variable model, the number of parameters grows at rate $\mathcal{O}(N)$. After marginalization, the growth is reduced to $\mathcal{O}\left(D^2 K\right)$ (assuming $D, K \ll N$).

Maximum likelihood

- To get a maximum (marginal) likelihood estimate of $\boldsymbol{\theta}$, we maximize:

$\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$

- Non-convex cost
- Non-unique optima (permutations/renaming of the clusters)
- Unbounded: $\Sigma_k = \sigma_k \overrightarrow{1}$, $\sigma_k \in \mathbb{R}$

Expectation-Maximization Algorithm

- Computing maximum likelihood for Gaussian mixture model is difficult due to the log outside the sum.

$\max_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) := \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$

- EM algorithm uses an iterative two-step procedure where individual steps usually involve problems that are easy to optimize.

EM algorithm:

Start with $\boldsymbol{\theta}^{(1)}$ and iterate:

1. Expectation step: Compute a lower bound to the cost such that it is tight at the previous $\boldsymbol{\theta}^{(t)}$: $\mathcal{L}(\boldsymbol{\theta}) \geq \underline{\mathcal{L}}\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$ and $\mathcal{L}\left(\boldsymbol{\theta}^{(t)}\right) = \underline{\mathcal{L}}\left(\boldsymbol{\theta}^{(t)}, \boldsymbol{\theta}^{(t)}\right)$.
2. Maximization step: Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} \underline{\mathcal{L}}\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$.

Jensen's Inequatlity

- Log is convex $\rightarrow$ Concavity of log
- Given non-negative weights q s.t. $\sum_k q_k = 1$, the following holds for any $r_k > 0$:

$\log\left(\sum_{k=1}^{K} q_k r_k\right) \geq \sum_{k=1}^{K} q_k \log r_k$

The expectation step

$\log \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \geq \sum_{k=1}^{K} q_{kn} \log \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{q_{kn}}$ with equality when, $q_{kn} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}$

The maximization step

- Maximize the lower bound w.r.t. $\boldsymbol{\theta}$.

$\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \sum_{k=1}^{K} q_{kn}^{(t)} \left[\log \pi_k + \log \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right]$

- Differentiating w.r.t. $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k^{-1}$, we can get the updates for $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$.

$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \mathbf{x}_n}{\sum_n q_{kn}^{(t)}}$

$\boldsymbol{\Sigma}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} (\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)})^\top}{\sum_n q_{kn}^{(t)}}$

For π_k, we use the fact that they sum to 1. Therefore, we add a Lagrangian term, differentiate w.r.t. π_k and set to 0 , to get the following update:

$\pi_k^{(t+1)} := \frac{1}{N} \sum_{n=1}^{N} q_{kn}^{(t)}$

EM for GMM

Initialize $\boldsymbol{\mu}^{(1)}, \boldsymbol{\Sigma}^{(1)}, \boldsymbol{\pi}^{(1)}$ and iterate between the E and M step, until $\mathcal{L}(\boldsymbol{\theta})$ stabilizes.

1. E-step: Compute assignments $q_{kn}^{(t)}$:

$q_{kn}^{(t)} := \frac{\pi_k^{(t)} \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)}{\sum_{k=1}^K \pi_k^{(t)} \mathcal{N}\left(\mathbf{x}_n | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)}$

2. Compute the marginal likelihood (cost).

$\mathcal{L}\left(\boldsymbol{\theta}^{(t)}\right) = \sum_{n=1}^N \log \sum_{k=1}^K \pi_k^{(t)} \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)$

3. M-step: Update $\boldsymbol{\mu}_k^{(t+1)}, \boldsymbol{\Sigma}_k^{(t+1)}, \pi_k^{(t+1)}$.

$$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \mathbf{x}_n}{\sum_n q_{kn}^{(t)}}$$

$$\boldsymbol{\Sigma}_k^{(t+1)} := \frac{\sum_n q_{kn}^{(t)} \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)}\right)\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{(t+1)}\right)^\top}{\sum_n q_{kn}^{(t)}}$$

$$\pi_k^{(t+1)} := \frac{1}{N} \sum_n q_{kn}^{(t)}$$

- If we let the covariance be diagonal i.e. $\boldsymbol{\Sigma}_k := \sigma^2 \mathbf{I}$, then EM algorithm is same as K-means as $\sigma^2 \to 0$.

Posterior distribution

- show that $q_{kn}^{(t)}$ is the posterior distribution of the latent variable, i.e. $q_{kn}^{(t)} = p\left(z_n = k \mid \mathbf{x}_n, \boldsymbol{\theta}^{(t)}\right)$

$p(\mathbf{x}_n, z_n \mid \boldsymbol{\theta}) = p(\mathbf{x}_n \mid z_n, \boldsymbol{\theta}) p(z_n \mid \boldsymbol{\theta}) = p(z_n \mid \mathbf{x}_n, \boldsymbol{\theta}) p(\mathbf{x}_n \mid \boldsymbol{\theta})$

$\underbrace{p(A,B)}_{\text{joint}} = \underbrace{p(A|B)}_{\text{likelyhood}} \underbrace{p(B)}_{\text{prior}} = \underbrace{p(B|A)}_{\text{posterior}} \underbrace{p(A)}_{\text{marginal}}$

EM in general

- Given a general joint distribution $p(\mathbf{x}_n, z_n \mid \boldsymbol{\theta})$, the marginal likelihood can be lower bounded similarly. Compact EM: $\boldsymbol{\theta}^{(t+1)}$ $:= \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^N \mathbb{E}_{p(z_n|\mathbf{x}_n, \boldsymbol{\theta}^{(t)})}[\log p(\mathbf{x}_n, z_n \mid \boldsymbol{\theta})]$
- Another interpretation is that part of the data is missing, i.e. $(\mathbf{x}_n, z_n)$ is the "complete" data and z_n is missing. The EM algorithm averages over the "unobserved" part of the data.

Matrix Factorization

Given items (movies) $d = 1, 2, ..., D$ and users $n = 1, 2, ..., N$, we define X to be the $D \times N$ matrix containing all rating entries. That is, x_{dn} is the rating of n-th user for d-th item. Note that most ratings x_{dn} are missing, and our task is to predict them accurately.

Algorithm

$X \approx WZ^T$, $W \in \mathbb{R}^{D \times K}$, $Z \in \mathbb{R}^{N \times K}$ tall matrices $K << N, D$

$\min_{W,Z} \mathcal{L}(W, Z) := \frac{1}{2} \sum_{(d,n) \in \mathbb{Q}} [x_{dn} - (WZ^T)_{dn}]^2$

- We hope to "explain" each rating x_{dn} by a numerical representation of the corresponding item and user - in fact by the inner product of an item feature vector with the user feature vector.
- The set $\Omega \subseteq [D] \times [N]$ collects the indices of the observed ratings of the input matrix X.
- This cost is not jointly convex w.r.t. W and Z, nor identifiable as $(w^*, z^*) \Leftrightarrow (\beta w^*, \beta^{-1} z^*)$

Choosing K

- $\uparrow K \Rightarrow$ overfitting ($\Leftrightarrow \downarrow K \Rightarrow$ underfitting). For $K >> N, D \Rightarrow (W^*, Z^{*^T}) = (X, I) = (I, X)$

Regularization

$\frac{1}{2} \sum_{(d,n) \in \Omega} [x_{dn} - (WZ^T)_{dn}]^2 + \frac{\lambda_w}{2} ||W||_{\text{Frob}}^2 + \frac{\lambda_z}{2} ||Z||_{\text{Frob}}^2$ $\lambda_w, \lambda_z \in \mathbb{R} > 0$

Stochastic Gradient Descent

$$\mathcal{L} = \frac{1}{|\Omega|} \sum_{(d,n) \in \Omega} \underbrace{\frac{1}{2} [x_{dn} - (\mathbf{W}\mathbf{Z}^\mathsf{T})_{dn}]^2}_{f_{d,n}}$$

For one fixed element (d, n) of the sum, we derive the gradient entry (d', k) for W:

$\frac{\partial}{\partial w_{d',k}} f_{d,n}(W, Z) \in \mathbb{R}^{D \times K} =$

$$\begin{cases} -\left[x_{dn} - (\mathbf{W}\mathbf{Z}^T)_{dn}\right] z_{n,k} & \text{if } d' = d \\ 0 \text{ otherwise} \end{cases}$$

$\frac{\partial}{\partial z_{n',k}} f_{d,n}(W, Z) \in \mathbb{R}^{N \times K} =$

$$\begin{cases} -\left[x_{dn} - (\mathbf{W}\mathbf{Z}^T)_{dn}\right] w_{d,k} & \text{if } n' = n \\ 0 \text{ otherwise} \end{cases}$$

- cost: $\Theta(K)$ which is cheap!

Alternating Least Squares

- No missing entries:

$\frac{1}{2} \sum_{d=1}^D \sum_{n=1}^N \left[x_{dn} - \left(W\mathbf{Z}^\mathsf{T}\right)_{dn}\right]^2$
$= \frac{1}{2} \|\mathbf{X} - \mathbf{W}\mathbf{Z}^\mathsf{T}\|_{Frob}^2$

- We first minimize w.r.t. Z for fixed W and then minimize W given Z (closed form solutions):

$Z^\mathsf{T} := (\mathsf{W}^\mathsf{T}\mathsf{W} + \lambda_z \mathsf{I}_K)^{-1} \mathsf{W}^\mathsf{T}\mathsf{X}$

$\mathbf{W}^\mathsf{T} := (\mathbf{Z}^\mathsf{T}\mathbf{Z} + \lambda_w \mathbf{I}_K)^{-1} \mathbf{Z}^\mathsf{T}\mathbf{X}^\mathsf{T}$

- Cost: need to invert a $K \times K$ matrix
- With missing entries: Can you derive the ALS updates for the more general setting, when only the ratings $(d, n) \in \Omega$ contribute to the cost, i.e. $\frac{1}{2} \sum_{(d,n) \in \Omega} \left[x_{dn} - \left(\mathsf{W}\mathsf{Z}^\mathsf{T}\right)_{dn}\right]^2$

Compute the gradient with respect to each group of variables, and set to zero.

Text Representation

-Finding numerical representations for words is fundamental for all machine learning methods dealing with text data.

-Goal: For each word, find mapping (embedding) $w_i \mapsto \mathbf{w}_i \in \mathbb{R}^K$

Co-Occurence Matrix

-A big corpus of un-labeled text can be represented as the co-occurrence counts. n_{ij} := #contexts where word w_i occurs together with word w_j.

- Needs definition of Context e.g. document, paragraph, sentence, window and Vocabulary $\mathcal{V} := \{w_1, \ldots, w_D\}$
- For words $w_d = 1, 2, \ldots, D$ and context words $w_n = 1, 2, \ldots, N$, the co-occurence counts n_{ij} form a very sparse $D \times N$ matrix.

Learning Word-Representations

- Find a factorization of the cooccurence matrix!
- Typically uses log of the actual counts, i.e. $x_{dn} := \log(n_{dn})$.
- Aim to find $\mathbf{W}, \mathbf{Z}$ s.t. $\mathbf{X} \approx \mathbf{W}\mathbf{Z}^\top$

$\min_{\mathbf{W},\mathbf{Z}} \mathcal{L}(\mathbf{W}, \mathbf{Z}) :=$
$\frac{1}{2} \sum_{(d,n) \in \Omega} f_{dn} \left[x_{dn} - \left(\mathbf{W}\mathbf{Z}^\top\right) dn\right]^2$

where $\mathbf{W} \in \mathbb{R}^{D \times K}$, $\mathbf{Z} \in \mathbb{R}^{N \times K}$, $K \ll D, N$, $\Omega \subseteq [D] \times [N]$ indices of non-zeros of the count matrix $\mathbf{X}$, f_{dn} are weights to each entry.

GloVe

A variant of word2vec.

$f_{dn} := \min\{1, (n_{dn}/n_{\max})^\alpha\}$, $\alpha \in [0; 1]$ (e.g. $\alpha = \frac{3}{4}$)

Note: Choosing K; K e.g. 50, 100, 500

Training

- Stochastic Gradient Descent (SGD) ($\Theta(K)$ per step $\to$ easily parralelizable)
- Alternating Least-Squares (ALS)

Skip-Gram Model

- Uses binary classification (logistic regression objective), to separate real word pairs (w_d, w_n) from fake word pairs. Same inner product score = matrix factorization.
- Given w_d, a context word w_n is:

real = appearing together in a context window of size 5

fake = any word $w_{n'}$ sampled randomly: Negative sampling (also: Noise Contrastive Estimation)

Learning Representations of Sentences & Documents

- Supervised: For a supervised task (e.g. predicting the emotion of a tweet), we can use matrix factorization or CNNs. - Unsupervised:

Adding or averaging (fixed, given) word vectors,

Training word vectors such that adding/averaging works well

Direct unsupervised training for sentences (appearing together with context sentences) instead of words

Fast Text

Matrix factorization to learn document/sentence representations (supervised).

Given a sentence $s_n = (w_1, w_2, \ldots, w_m)$, let $\mathbf{x}_n \in \mathbb{R}^{|\mathcal{V}|}$ be the bag-of-words representation of the sentence.

$$\min_{\mathbf{W},\mathbf{Z}} \mathcal{L}(\mathbf{W}, \mathbf{Z}) := \sum_{s_n \text{ a sentence}} f\left(y_n \mathbf{W}\mathbf{Z}^\top \mathbf{x}_n\right)$$

where $\mathbf{W} \in \mathbb{R}^{1 \times K}, \mathbf{Z} \in \mathbb{R}^{|\mathcal{V}| \times K}$ are the variables, and the vector $\mathbf{x}_n \in \mathbb{R}^{|\mathcal{V}|}$ represents our n-th training sentence.

Here f is a linear classifier loss function, and $y_n \in \{\pm 1\}$ is the classification label for sentence $\mathbf{x}_n$.

Language Models

Selfsupervised training:

- Can a model generate text? train classifier to predict the continuation (next word) of given text
- Multi-class: Use soft-max loss function with a large number of classes D = vocabulary size
- Binary classification: Predict if next word is real or fake (i.e. as in word2vec)
- Impressive recent progress using large models, such as transformers

---

Self-supervised Learning

- Problem: Labelled data for supervised learning is often limited and expensive to acquire.
- Transfer learning: Fine-tune an existing model trained on a related task giving it a good internal representation of the input data. This can allow us to achieve high performance on the downstream task with significantly fewer labels. However, we still need supervision (labels) for the base task.
- Self-Supervised Learning: Use the input itself to generate supervisory signals. The base task is an artificial pretext task that requires learning useful features and structure in the input data.

In the pretext task we want to learn a model f : $f : \mathbf{x}_{\text{in}} \mapsto \mathbf{x}_{\text{out}}$

Where we use a transformation $g : \mathbf{x} \mapsto (\mathbf{x}_{\text{in}}, \mathbf{x}_{\text{out}})$ to create an input and a target from an (unlabelled) datapoint $\mathbf{x} \in \mathcal{X}$. Note that g often involves some randomness.

Masked Language Modelling (MLM)

She [MASK] her coffee $\mapsto$ She drank her coffee

- (backward) Data generation: corrupt the data
- (forward) learning

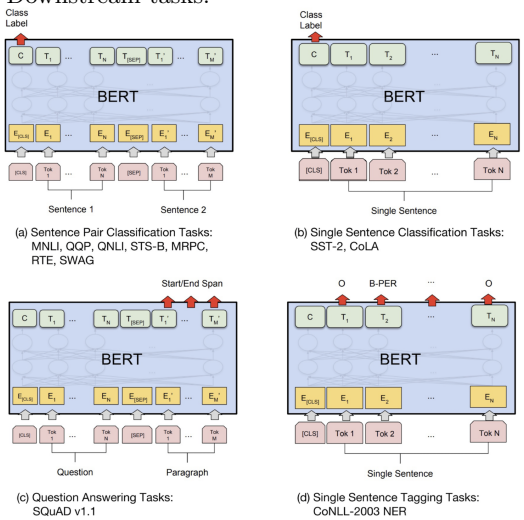
BERT

- (Bidirectional) Encoder Representations from Transformers is a well known family of language models based on the encoder-only transformer architecture and trained on masked language modelling.
- Encoder: Sees the whole sequence at once, every token can generally attend to every other token (both previous and later ones, hence bidirectional). Generates a fixed sized output, typically one token per input.

- Training Inputs: BERT is trained on input sequences consisting of two sentences and special tokens, for example:
[CLS] The cat is sleeping. [SEP] It's on the sofa. [SEP]
- [CLS] is a special classification token
- [SEP] is used to separate the two sentences.
- Around 15% of the standard tokens are selected to be replaced by [MASK].
- Occasionally the selected tokens are replaced by a random word or not replaced to reduce distribution shift for downstream tasks that do not have [MASK].
- Positional and segment encodings are added to the token embeddings.

BERT Training Objective:

• For each selected (replaced / masked) token: Predict the original token. Softmax cross-entropy loss over all possible tokens.
• For the [CLS] token: Predict whether the second sentence immediately follows the first sentence or not (binary classification).
- Downstream tasks:



(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG
(b) Single Sentence Classification Tasks: SST-2, CoLA
(c) Question Answering Tasks: SQuAD v1.1
(d) Single Sentence Tagging Tasks: CoNLL-2003 NER

• Classifying sentences or pairs (e.g. sentiment analysis): Use the [CLS] token.
• Word level classification (e.g. named entity recognition): Use the output for each token.
• Extracting a relevant passage (e.g. search): Use the individual outputs to define a span.

Next Token Prediction

-Language Modelling Task
- Predict the next token given previous tokens, e.g.: *She drank her* $\mapsto$ *coffee*
- Similar to Masked Language Modelling but is causal, we can only see previous words, not later ones. This makes it better suited for generating arbitrary length responses.

GPT

- Generative Pre-trained Transformers are a family of language models based on the decoder-only transformer architecture and trained on next token prediction. Most generative Large Language Models (LLMs) like GPT-4 and LLAMA are members of this family. They can be fine tuned for a variety of purposes, famously as chatbots / assistants (ChatGPT, Bard).

- Decoder: Each token can only attend to prior tokens (operates causally). Used autoregressively during inference, each generated output token is fed back into the model as an input to generate the following output token.

- Training Inputs: The training is simply done on token sequences with minimal changes e.g.: *[EOS] The cat is sleeping. It's on the sofa. [EOS]*

- [EOS] signifies the end of text and is used to separate unrelated chunks of text (but this can vary between implementations).

- Training Procedure: teacher forcing, where we don't use the model outputs as subsequent inputs (like in inference) but rather use the actual correct sequence. $\rightarrow$ allows training on all tokens in a sequence to happen in parallel rather than sequentially. We need to mask the attention to prevent tokens from attending to future tokens, preserving the causality needed for inference.

- loss for every token in the sequence corresponding to the prediction of the next token. This is a standard classification loss over the possible vocabulary (softmax cross-entropy). The total loss for a sequence is the mean loss over all tokens in the sequence.

- Downstream Tasks: Decoders are very general sequenceto-sequence models and can be adapted to most natural language tasks. GPTs have been fine tuned for various applications. The base models are also often capable of performing various tasks without further tuning.

In-Context Learning: new tasks with just a few examples of successful completion provided as inputs, without any model updates. The model uses patterns it has learned during its initial training to infer how to handle these new tasks. e.g. translation.

- Prompt engineering: search for an effective input (prompt) to achieve desired output behavior.

Joint Embedding Methods (Images)

Learn an encoder invariant to certain transformations on the data, e.g., to rotation rather than learning a model f :
$\mathbf{x}_{\text{in}} \mapsto \mathbf{x}_{\text{out}}$, learn $f : \mathcal{X} \rightarrow \mathbb{R}^d$ s.t. $f(\mathbf{x}_1) \approx f(\mathbf{x}_2)$ where $g : \mathbf{x} \mapsto (\mathbf{x}_1, \mathbf{x}_2)$ is a transformation that creates two views from the same input datapoint $\mathbf{x} \in \mathcal{X}$.
- g is usually a random function that applies multiple data augmentations, each with certain probability.
- Problem: constant f is a trivial encoder that is invariant!
- Solved by contrastive learning or non-contrastive methods with regularization, e.g.:
• BYOL: use two encoders f_1, f_2 where f_2 is the exponential moving average of f_1 and force $f_1(\mathbf{x}_1) \approx f_2(\mathbf{x}_2)$
• VicReg: force non-zero variances to avoid collapse but minimize the covariance to reduce information overlap.

Contrastive learning

- Push away representations of unrelated views from different data points!
- Given a positive pair $\mathbf{x}, \mathbf{x}^+$from the datapoint $\mathbf{x}$, and a negative view $\mathbf{x}^-$from a different datapoint $\mathbf{x}' \neq \mathbf{x}$: $\mathrm{s}\left(f(\mathbf{x}), f\left(\mathbf{x}^+\right)\right) > \mathrm{s}\left(f(\mathbf{x}), f\left(\mathbf{x}^-\right)\right)$, where the s function quantifies the similarity of two embeddings.

SimCLR

- A contrastive learning framework with optimized choices.
1. classification-like objective with N negative samples:

$$L(\mathbf{x}) = -\mathbb{E}\left[\log \frac{\exp\left(\mathrm{s}\left(f(\mathbf{x}), f\left(\mathbf{x}^+\right)\right)\right)}{\sum_{i=1}^{N} \exp\left(\mathrm{s}\left(f(\mathbf{x}), f\left(\mathbf{x}_i^-\right)\right)\right)}\right]$$

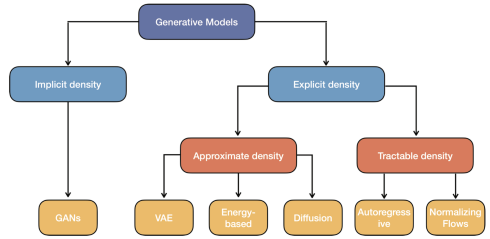
• maximize the score between $\mathbf{x}$ and $\mathbf{x}^+$,
• minimize the score between $\mathbf{x}$ and all $\mathbf{x}_i^-$.
2. use an additional projector to map the encoder output to the similarity (possibly lower-dimensional) space: $f(\mathbf{x}) = \underbrace{f_2}_{\text{projector}} \circ \underbrace{f_1}_{\text{encoder}} (\mathbf{x})$
• learn f_1 and f_2 jointly in an end-to-end fashion,
• use only f_1 for downstream tasks.
3. use cosine similarity with temperature scaling τ : $\mathrm{S}(\mathbf{e}_1, \mathbf{e}_2) = \frac{\langle \mathbf{e}_1, \mathbf{e}_2 \rangle}{\|\mathbf{e}_1\|_2 \|\mathbf{e}_2\|_2} / \tau$
4. How to $x \rightarrow x^+$? generate views with data augmentation:
e.g. Rotate $\{90°, 180°, 270°\}$, Crop, resize, Cutout, flip, Gaussian noise or blur, Color distort (drop or jitter), Sobel filtering
• stronger data augmentations than those used in supervised learning,
• random crop creates global to local ($B \rightarrow A$) views or adjacent view ($D \rightarrow C$) prediction tasks.

CLIP

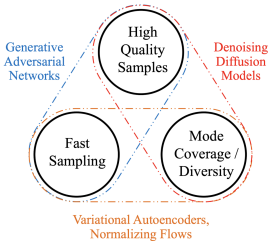
- Use captioned images to learn a joint multimodal embedding space.
- Objective: Maximize cosine similarity of caption and image embeddings while minimizing unrelated pairs.
- Few-shot learning: learn to classify new classes with only a few labelled examples. CLIP is able to zero-shot classify with the following text input: "A photo of [class]".

Generative Models

- Given data sample x
- Discriminative model predict *yarrow* conditional distribution $p(y \mid x)$.
- Generative models *arrow* distribution $p(x)$ defined over the datapoints x. Generative models categories: explicit (explicitly model the probability distribution) or implicit (generate samples according to p).
- Taxonomy:



- Implicit density models (GANs), high-quality, realistic samples, challenging to train (mode collapse model fails to capture the diversity of the data distribution)



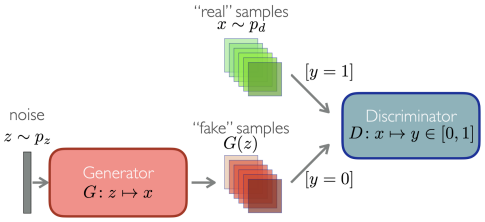
- Tractable density models, (Autoregressive models and Normalizing Flows), exact likelihood computation, (beneficial for tasks that require likelihood evaluation and interpretability). Autoregressive models generate data sequentially, slow in sampling. Normalizing Flows, more efficient sampling and inference (using invertible transformations), computationally intensive to train.
- Approximate models, (VAEs and Energy-based models). VAEs optimize a lower bound on the

likelihood *arrow* easier and more stable training than GANs but less sharp samples.

- Diffusion models *arrow* hybrid approach, iteratively convert noise into samples via a reverse Markov process, highquality images and audio, slow at sampling time.

- trade-off between sample quality, sampling speed, and diversity.

Generative Adversarial Networks



- two models: a generator G with paramters $\boldsymbol{\theta}$ and a discriminator D with parameters $\boldsymbol{\varphi}$.

- G learns to generate samples from the data distribution p_d, while D learns to distinguish between real and fake samples.

- Therefore, contrary to singleobjective minimization $f : \mathcal{X} arrow \mathbb{R}$, the optimization of a GAN is formulated as a differentiable two-player game where the generator G, and the discriminator D, aim at minimizing their own cost function $\mathcal{L}^{\boldsymbol{\theta}}$ and $\mathcal{L}^{\boldsymbol{\varphi}}$, respectively, as follows:

$$\boldsymbol{\theta}^\star \in \arg\min_{\boldsymbol{\theta}\in\Theta} \mathcal{L}^{\boldsymbol{\theta}}(\boldsymbol{\theta}, \boldsymbol{\varphi}^\star) \quad \boldsymbol{\varphi}^\star \in \arg\min_{\boldsymbol{\varphi}\in\Phi} \mathcal{L}^{\boldsymbol{\varphi}}(\boldsymbol{\theta}^\star, \boldsymbol{\varphi})$$

- When $\mathcal{L}^{\boldsymbol{\theta}} = -\mathcal{L}^{\boldsymbol{\varphi}}$ the game is called a zero-sum game and (2Player-Game) is a minmax problem.

1. The discriminator "distinguishes" real vs. fake samples:

p_z known "noise" distribution, e.g. $\mathcal{N}(0, 1)$

p_d the real data distribution

$D : x \mapsto y \in [0, 1]$, where y is an estimated probability that $x \sim p_d$

2. The generator aims at fooling the discriminator that its samples are real:

$G : z \mapsto x$, such that if $z \sim p_z$, then hopefully $x \sim p_d$

p_g the "fake" data distribution

3. Objective $\min_G \max_D \mathop{\mathbb{E}}_{x\sim p_d}[\log D(x)] + \mathop{\mathbb{E}}_{z\sim p_z}[\log(1 - D(G(z)))]$

- Loss for D : distinguish between $x \sim p_g$ and $x \sim p_d$ (binary classification):

$\mathscr{L}_D(G, D) = \max_D \mathop{\mathbb{E}}_{x\sim p_d}[\log D(x)] + \mathop{\mathbb{E}}_{z\sim p_z}[\log(1 - D(G(z)))]$

- Loss for G : fool D that $G(z) \sim p_d$:

$\mathscr{L}_G(G, D) = \min_G \mathop{\mathbb{E}}_{z\sim p_z}[\log(1 - D(G(z)))]$

$:= (\text{ in practice }) \max_G \mathop{\mathbb{E}}_{z\sim p_z}[\log(D(G(z)))]$

4. Theoretical Solution: The optimum is reached when $p_g = p_d$ and the optimal value is $-\log 4$

Alternating-GAN algorithm

- G : deep neural network $G(\mathbf{z}; \boldsymbol{\theta})$ with parameters $\boldsymbol{\theta}$

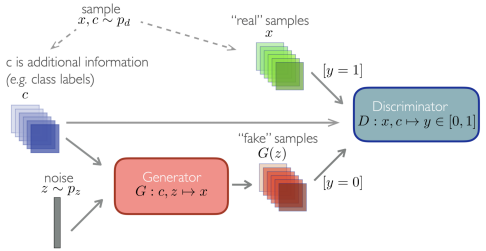
- D : deep neural network $D(\mathbf{x}; \boldsymbol{\varphi})$ with parameters φ

- In most GAN implementations G and D have different losses $\mathcal{L}^{\theta}$ and $\mathcal{L}^{\varphi a}$, resp.

Algorithm 1 *alternating*–GAN

Input: dataset $\mathcal{D}$, known distribution p_z, learning rate η, generator loss $\mathcal{L}^{\boldsymbol{\theta}}$, discriminator loss $\mathcal{L}^{\boldsymbol{\varphi}}$
Initialize: $D(\cdot; \boldsymbol{\varphi})$, $G(\cdot; \boldsymbol{\theta})$
for $t = 1$ **to** T **do**
  $\mathbf{x} \sim p_x$ {sample real data}
  $\mathbf{z} \sim p_z$ {sample noise from p_z}
  $\boldsymbol{\varphi} = \boldsymbol{\varphi} - \eta \nabla_{\boldsymbol{\varphi}} \mathcal{L}^{\boldsymbol{\varphi}}(\boldsymbol{\theta}, \boldsymbol{\varphi}, \mathbf{x}, \mathbf{z})$ {update D}
  $\mathbf{z} \sim p_z$ {sample noise from p_z}
  $\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}^{\boldsymbol{\theta}}(\boldsymbol{\theta}, \boldsymbol{\varphi}, \mathbf{z})$ {update G}
end for
Output: $\boldsymbol{\theta}, \boldsymbol{\varphi}$

Conditional GAN - (CGAN)

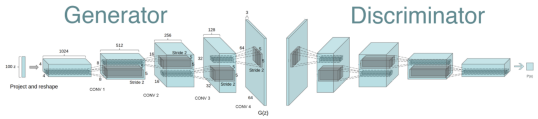


- Applications requiring conditional probability distribution (e.g. "in-painting", segmentation, predicting the next frame of a video etc.).

- In CGANs both the Generator and the Discriminator are conditioned during training by some additional information, typically the class labels (but could also be images e.g. auto-generated edges of an image, conditioning on non-occluded portion-so as to generate the occluded part of the image etc).

- When conditioning on the class labels, typically one-hot vector representation of the class labels is used (empirically shown to perform better).

GAN architectures for images

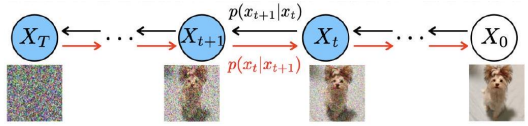


- Deep Convolutional GANs - DCGAN. Notably,

- G uses transposed convolutional layer (a.k.a. fractionally strided convolutions), also informally called "Deconvolution layers" (wrongfully).

- Simplest way to explain these is that they "swap" the forward and the backward passes of a convolution layer: the forward transposed convolution operation can be thought of as the gradient of some convolution with respect to its input, which is usually how transposed convolutions are also implemented in practice.

Diffusion models



- implementation in AI image generators like DALL-E 3, Stable Diffusion, and Midjourney.

- Unlike GANs, work by progressively adding noise to input data and training one single model to estimate the added noise and recover the data.

- Consider a Markov chain with $X_0 \sim p_0$ and a forward transition s.t. $X_{t+1} \sim p(\cdot \mid X_t)$ then we call **forward decomposition**:

$p(x_{0:T}) = p_0(x_0) \prod_{t=0}^{T-1} p(x_{t+1} \mid x_t)$

where at each step, the marginal distribution of X_t satisfies: $p(x_t) = \int p(x_t \mid x_{t-1}) p(x_{t-1}) \mathrm{d}x_{t-1}$

- backward transition can be obtained with Bayes' rule

$p(x_t \mid x_{t+1}) = p(x_{t+1} \mid x_t) p(x_t) / p(x_{t+1})$,

and we call **backward decomposition**:

$p(x_{0:T}) = p_T(x_T) \prod_{t=0}^{T-1} p(x_t \mid x_{t+1})$

- A generative model can be constructed sampling from $p(x_{0:T})$ using **ancestral sampling**:

Sample $X_T \sim p_T(\cdot)$ then: for $k = T - 1, \ldots, 0$: Sample $X_t \sim p(\cdot \mid X_{t+1})$

- We consider $p_0 = p_{\text{data}} \in \mathcal{P}(\mathbb{R}^d)$
- We chose the forward transition to be Gaussian $p(x_{t+1} \mid x_t) = \mathcal{N}(x_{t+1}; \alpha x_t, (1 - \ldots \alpha^2) \mathbb{I}_d)$
- The conditional $p(x_t \mid x_0)$ is also Gaussian $\mathcal{N}(x_t; \alpha^t x_0, (1 - \alpha^{2t}) \mathbb{I}_d)$
- The Markov chain converges to $p_{\text{ref}} = \mathcal{N}(x; 0, \mathbb{I}_d)$ for $T arrow \infty$.
- Therefore for T large enough $p_T(x) \approx p_{\text{ref}}(x)$
- To generate samples we use ancestral sampling replacing p_T with p_{ref}

- Key problem: the backward transition $p(x_t \mid x_{t+1})$ can't be computed, we need an approximation!

- Using a Taylor expansion we can approximate the backward transition: $p(x_t \mid x_{t+1}) = p(x_{t+1} \mid x_t) \exp[\log p(x_t) - \log p(x_{t+1})] \approx \mathcal{N}(x_t; (2 - \alpha) x_{t+1} + (1 - \alpha^2) \underbrace{\nabla \log p(x_{t+1})}_{\text{Score}}, (1 - \alpha^2) \mathbb{I}_d)$

Denoising score matching

- The Stein Score is analytically intractable, but we can approximate it using a NN $s_\theta(x_t)$.

- Surprisingly, we can learn the score solving a simple regression problem via the Denoising Score Matching (DSM) loss: $\theta^\star = \arg\min_\theta \mathcal{L}(\theta) := \frac{1}{2} \mathbb{E}_{X_t}[\|\nabla \log p(X_t) - s_\theta(X_t)\|^2]$

- Problem still intractable: we do not have access to the marginal $p(x_t)$ at each step but we can manipulate it:

$$\begin{aligned}\mathcal{L}(\theta) &= \mathrm{C}_1 + \frac{1}{2}\mathbb{E}_{X_t}[\|s_\theta(X_t)\|^2] - \mathbb{E}_{X_t}[\nabla \log p(X_t)^\top s_\theta(X_t)] \\ &= \mathrm{C}_1 + \frac{1}{2}\mathbb{E}_{X_t}[\|s_\theta(X_t)\|^2] - \int \nabla \log p(X_t)^\top s_\theta(X_t) p(X_t) \mathrm{d}x_t\end{aligned}$$

- Using that $p(x_t) = \int p_0(x_0) p(x_t \mid x_0) \mathrm{d}x_0$ we get: $\nabla \log p(X_t) = \mathbb{E}_{X_0 \mid X_t}[\nabla \log p(X_t \mid X_0)]$

Substituding in the DSM-loss:

$$\begin{aligned}\mathcal{L}(\theta) &= \mathrm{C}_1 + \frac{1}{2}\mathbb{E}_{X_t}[\|s_\theta(X_t)\|^2] - \mathbb{E}_{X_0}\mathbb{E}_{X_t|X_0}[\nabla \log p(X_t \mid X_0)^\top s_\theta(X_t)] \\ &= \mathrm{C}_1 + \frac{1}{2}\mathbb{E}_{X_0}\mathbb{E}_{X_t|X_0}[\|s_\theta(X_t) - \nabla \log p(X_t \mid X_0)\|^2] \\ &\quad - \frac{1}{2}\underbrace{\mathbb{E}_{X_0}\mathbb{E}_{X_t|X_0}[\|\nabla \log p(X_t \mid X_0)\|^2]}_{\text{const.}} \\ &= \mathrm{C}_2 + \frac{1}{2}\mathbb{E}_{X_0}\mathbb{E}_{X_t|X_0}[\|s_\theta(X_t) - \nabla \log p(X_t \mid X_0)\|^2]\end{aligned}$$

- In practice we estimate all the scores simultaneously i.e. $s_{\theta^\star}(t, X_t)$ such that:

$\theta^* = \arg\min_\theta \frac{1}{2} \sum_{t=1}^T \mathbb{E}_{X_0}\mathbb{E}_{X_t|X_0}[\|s_\theta(t, X_t) - \nabla \log p(X_t \mid X_0)\|^2]$

- Recalling now our choice of forward transition for which $p(x_t \mid x_0) = \mathcal{N}(x_t; \alpha^t x_0, (1 - \ldots \alpha^{2t}) \mathbb{I}_d)$:

- $\nabla \log p(x_t \mid x_0) = -\frac{(x_t - \alpha^t x_0)}{(1 - \alpha^{2t})}$
- $X_t = \alpha^t X_0 + \sqrt{1 - \alpha^{2t}} \xi_t \xi_t \sim \mathcal{N}(0, \mathbb{I}_d)$
- $\nabla \log p(X_t \mid X_0) = -\frac{\xi_t}{\sqrt{1 - \alpha^{2t}}}$

- parameterize the score function as $s_\theta(t, X_t) = -\frac{\hat{\xi}_\theta(t, X_t)}{\sqrt{1 - \alpha^{2t}}}$ then the problem is equivalent to:

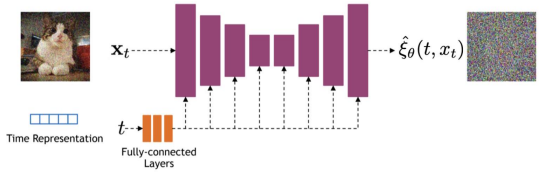
$\theta^\star = \arg\min_\theta \frac{1}{2} \sum_{k=1}^T \mathbb{E}_{X_0}\mathbb{E}_{X_t|X_0}[\|\hat{\xi}_\theta(t, X_t) - \xi_t\|^2]$

which has the illuminating interpretation of learning to predict the added noise ξ_t from the noised data X_t.

- Finally, we can generate new samples from the backward process by sampling $X_T \sim p_{\text{ref}}$ and using the approximation of the backward transition and the learned score to perform ancestral sampling:

$X_t = (2 - \alpha) X_{t+1} + (1 - \alpha^2) s_{\theta^\star}(t + 1, X_{t+1}) + \sqrt{1 - \alpha^2} \xi_{t+1} \quad \xi_{t+1} \sim \mathcal{N}(0, \mathbb{I}_d)$

Implementation



- Diffusion models often use a U-net architecture with ResNet blocks and self attention layers to represent the score function $\hat{\xi}_\theta(t, X_t)$.

- The time step can be represented with sinusoidal positional encodings as done for transformers or

with random Fourirer features.
- The time features are then fed to the residual blocks using either spatial addition or adaptive group normalization layers.

Training and Sampling

Algorithm 2 Training

Input: Data distribution p_0, α
Output: Learned parameters θ^*
Initialize: Parameters θ
repeat
  Sample initial data $X_0 \sim p_0$
  Sample time step $t \sim \text{Uniform}(\{1, \dots, T\})$
  Sample noise $\xi_t \sim \mathcal{N}(0, \mathbb{I}_d)$
  Update θ using gradient descent step on:
  $\nabla_\theta \frac{1}{2} \mathbb{E}_{X_0} \mathbb{E}_{X_t|X_0} \left[\| s_\theta(t, \alpha^t X_0 + \sqrt{1-\alpha^{2t}} \xi_t) - \xi_t \|^2 \right]$
until convergence

Algorithm 3 Sampling

Input: Learned parameters θ^*, p_{ref}, α
Output: Generated sample X_0
Sample $X_T \sim p_{\text{ref}}$
for $t = T-1$ **to** 0 **do**
  Sample noise $\xi_{t+1} \sim \mathcal{N}(0, \mathbb{I}_d)$:
  $X_t = (2-\alpha) X_{t+1} + (1-\alpha^2) s_{\theta^*}(t+1, X_{t+1}) + \sqrt{1-\alpha^2} \xi_{t+1}$
end for
Return x_0

Exponential moving average

- The training of the U-net via Denoising Score Matching can be very unstable.
- To regularize it, usually an exponential moving average of the weights is used along the training:
$\bar{\theta}_{n+1} = (1-\beta)\bar{\theta}_n + \beta\theta_n$
where β regulates the rate of forgetting of the initial conditions.

Conditional training

- for diffusion models, conditioning is done by adding an additional input to the score function such that a conditional score is learned:
$\theta^\star = \arg\min_\theta \frac{1}{2} \sum_{k=1}^T \mathbb{E}_{X_0,Y} \mathbb{E}_{X_t|X_0} [\| s_\theta(t, X_t^Y; Y) - \nabla \log p(X_t^Y \mid X_0^Y) \|^2]$
- conditioning is fed into the network in a similar way than the time features

Applications of GANs and Diffusion Models

Image generation and editing, art creation, data augmentation, adversarial examples, drug discovery, protein structure prediction, anomaly detection, weather forecasting, video generation, voice synthesis and modification, restoration of old photographs and artworks, fashion design, architectural visualization, gaming, virtual reality and augmented reality, language translation and interpretation, financial modeling.