

Regression Terminology

- Data consists of **pairs** (\mathbf{x}_n, y_n) , where y_n is the n'th output and \mathbf{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, regres-sands.

Linear Regression

- Assumes linear relationship between inputs and output.

- $y_n \approx f(\mathbf{x}_n) := w_0 + w_1 x_{n1} + \dots + w_D x_{nD}$
 $\hat{\mathbf{x}}_n^T \hat{\mathbf{w}}$ 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 outliers.

- Mean Squared Error:

$$\text{MSE}(\mathbf{w}) := \frac{1}{N} \sum_{n=1}^N [y_n - f_w(\mathbf{x}_n)]^2$$

not robust to outliers.

- Mean Absolute Error:

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

- 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 $\forall \mathbf{u}, \mathbf{v} \in \mathbb{R}^D, 0 \leq \lambda \leq 1$:

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

Stirctly convex if $\leq \Rightarrow <$

- 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:

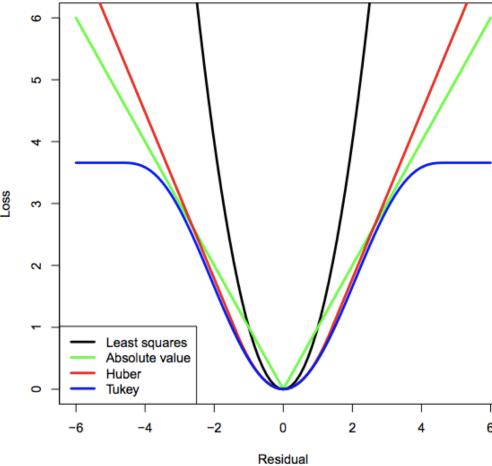
$$\begin{aligned} \text{MAE}(\mathbf{w}) &:= \frac{1}{N} \sum_{n=1}^N \mathcal{L}_n(\mathbf{w}), \mathcal{L}_n(\mathbf{w}) = |y_n - f_w(\mathbf{x}_n)| \\ \mathcal{L}_n(\lambda \mathbf{w}_1 + (1 - \lambda) \mathbf{w}_2) &\leq \lambda \mathcal{L}_n(\mathbf{w}_1) + (1 - \lambda) \mathcal{L}_n(\mathbf{w}_2) \\ |y_n - x_n^T (\lambda \mathbf{w}_1 + (1 - \lambda) \mathbf{w}_2)| &\leq \lambda |y_n - x_n^T \mathbf{w}_1| + (1 - \lambda) |y_n - x_n^T \mathbf{w}_2| \\ (1 - \lambda) \geq 0 &\Rightarrow (1 - \lambda) |y_n - x_n^T \mathbf{w}_2| = |(1 - \lambda) y_n - (1 - \lambda) x_n^T \mathbf{w}_2| \\ a = \lambda y_n - x_n^T \mathbf{w}_1, b = (1 - \lambda) y_n - (1 - \lambda) x_n^T \mathbf{w}_2 \\ a + b = y_n - x_n^T (\lambda \mathbf{w}_1 + (1 - \lambda) \mathbf{w}_2) \\ |a + b| \leq |a| + |b| &\Rightarrow \mathcal{L}_n(\mathbf{w}) \text{ convex} \Rightarrow \text{MAE}(\mathbf{w}) \text{ convex} \end{aligned}$$

- Huber loss:

$$\text{Huber}(e) := \begin{cases} \frac{1}{2} e^2 & , \text{if } |e| \leq \delta \\ \delta |e| - \frac{1}{2} \delta^2 & , \text{if } |e| > \delta \end{cases} \quad \text{convex, differentiable, and robust to outliers but setting } \delta \text{ is not easy.}$$

- Tukey's bisquare loss:

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



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.

$$\mathcal{L}(\mathbf{w}^*) \leq \mathcal{L}(\mathbf{w}) \quad \forall \mathbf{w} \text{ with } \|\mathbf{w} - \mathbf{w}^*\| < \epsilon$$

- Global minimum $\mathbf{w}^*, \mathcal{L}(\mathbf{w}^*) \leq \mathcal{L}(\mathbf{w}) \quad \forall \mathbf{w} \in \mathbb{R}^D$

Smooth Optimization

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

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

Gradient Descent

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

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

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:

$$\begin{aligned} f_w(x) = w_0 &\Rightarrow \mathcal{L}(w) = \frac{1}{2N} \sum_{n=1}^N (y_n - w_0)^2 = \nabla \mathcal{L} = \frac{\partial}{\partial w_0} \mathcal{L} = \frac{1}{2N} \sum -2(y_n - w_0) = (-\frac{1}{N} \sum y_n) + w_0 = w_0 - \bar{y} \end{aligned}$$

$$(min_w L(w) = w_0 - \bar{y} = 0 \Rightarrow w_0 = \bar{y})$$

$$w_0^{(t+1)} := (1 - \gamma) w_0^{(t)} + \gamma \bar{y}$$

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 $\mathbf{e} : \mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w}$ and MSE as follows:

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

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

$$\mathcal{L}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \mathcal{L}_n(\mathbf{w})$$

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

- Computational cost: $\Theta(D)$

- Cheap and unbiased estimate of the gradient!
 $E[\nabla \mathcal{L}_n(\mathbf{w})] = \frac{1}{n} \sum_{n=1}^N \nabla \mathcal{L}_n(\mathbf{w}) = \nabla \left(\frac{1}{N} \sum \dots \right) = \nabla \mathcal{L}(\mathbf{w})$ which is the true gradient direction.

Mini-batch SGD

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

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

- Randomly chosen a subset $B \subseteq [N]$ of the training examples. For each of these selected examples n , we compute the respective gradient $\nabla \mathcal{L}_n(\mathbf{w})$, 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

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

meaning that the function must always lie above its linearization.

Subgradients

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

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

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:

$$\mathcal{L}(\mathbf{w}) = \text{MAE}(\mathbf{w}) := \frac{1}{N} \sum_{n=1}^N |y_n - f_w(\mathbf{x}_n)|$$

For linear regression, its (sub)gradient is easy to compute using the chain rule. Compute it!

The subgradient is given by:

$$\partial \mathcal{L}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N g(e_n) \mathbf{x}_n$$

since $f_w(\mathbf{x}_n) = \mathbf{w}^\top \mathbf{x}_n$, then $\nabla f_w(\mathbf{x}_n) = \mathbf{x}_n$ where $e_n = y_n - f_w(\mathbf{x}_n)$.

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}

$$\mathbf{m}^{(t+1)} := \beta_1 \mathbf{m}^{(t)} + (1 - \beta_1) \mathbf{g} \quad (\text{momentum term})$$

$$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma \mathbf{m}^{(t+1)}$$

- momentum from previous gradients (acceleration)

Adam

- pick a stochastic gradient \mathbf{g}

$$\mathbf{m}^{(t+1)} := \beta_1 \mathbf{m}^{(t)} + (1 - \beta_1) \mathbf{g}$$

$$\mathbf{v}_i^{(t+1)} := \beta_2 \mathbf{v}_i^{(t)} + (1 - \beta_2) (\mathbf{g}_i)^2 \quad \forall i \quad (\text{Momentum term})$$

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

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

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

Constrained Optimization

- Sometimes, optimization problems come posed with additional constraints:

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

- 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)

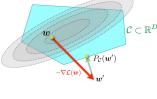
- Formal definition:

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

Projected Gradient Descent

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

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



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

Constrained → Unconstrained Problems

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

- 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)

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

Can't run GD because non-continuous objective.

- Penalize error. Example:

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

- ℓ_1 norm encourages sparsity which reduces memory: $P(\mathbf{w}) = \lambda \|\mathbf{w}\|_1$

- Linearized Penalty Functions (see Lagrange Multipliers)

Implementation Issues

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

2) Optimality:

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

2nd order: \mathcal{L} potentially non-convex, if $\nabla \mathcal{L}(\mathbf{w}^*) = 0 \& \nabla^2 \mathcal{L}(\mathbf{w}^*) \geq 0 \Rightarrow \mathbf{w}$ 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 $\gamma < \gamma_{\min}$, γ_{\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 → 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.:

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

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

Least Squares

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

Normal Equations

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

- Proof of convexity:

1) Simplest way: observe that \mathcal{L} is naturally represented as the sum (with positive coefficients) of the simple terms $(y_n - \mathbf{x}_n^\top \mathbf{w})^2$. 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}'

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

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

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): $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$
 \mathbf{U} and \mathbf{V} are orthogonal matrices, and \mathbf{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,

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

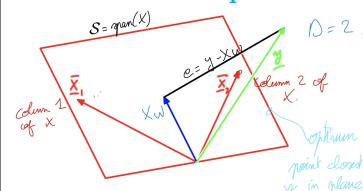
\mathbf{S} diagonal matrix with non-negative entries, $\mathbf{V}^\top \mathbf{v}$ vector.

- Now find its minimum

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

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

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:

$$\mathbf{w}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Invertibility and Uniqueness

- $\mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{D \times D}$ invertible iff $\text{rank}(\mathbf{X}) = D$.

- Proof: assume $\text{rank}(\mathbf{X}) < D$. 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 $\text{rank}(\mathbf{X}^\top \mathbf{X}) < D$. 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., $\text{rank}(\mathbf{X}) < D$.

Rank Deficiency and Ill-Conditioning

- In practice, \mathbf{X} is often rank deficient.

- If $D > N$, we always have $\text{rank}(\mathbf{X}) < D$ (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

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

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

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

- 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 $\mathbf{y} = (y_1, \dots, y_N)$ given the input \mathbf{X} and the model \mathbf{w} is equal to

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

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

Defining cost with log-likelihood

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

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 → 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:

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

- 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)

$$\mathbf{w}_{\text{MLE}} \xrightarrow{p} \mathbf{w}_{\text{true}} \quad \text{in probability}$$

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

$$(\mathbf{w}_{\text{MLE}} - \mathbf{w}_{\text{true}}) \xrightarrow{d} \frac{1}{\sqrt{N}} \mathcal{N}(\mathbf{w}_{\text{MLE}} | \mathbf{0}, \mathbf{F}^{-1}(\mathbf{w}_{\text{true}}))$$

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

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

Regularization

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

L_2 -Regularization: Ridge Regression

- Standard Euclidean norm (L_2 - norm):

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

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

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

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

Explicit solution for \mathbf{w} :

$$\nabla = \nabla \mathcal{L} + \nabla \Omega = -\frac{1}{N} X^T (y - Xw) + \lambda 2w = 0 \Rightarrow \mathbf{w}_{\text{ridge}}^* = (\mathbf{X}^\top \mathbf{X} + \lambda' \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

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

Ridge Regression Fights Ill-Conditioning

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

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

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

- 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:

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

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 $\{\mathbf{w} : \|\mathbf{y} - \mathbf{Xw}\|^2 = \alpha\}$ 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 $\sum_i a_i w_i^2 = \alpha$ which is indeed the equation for an ellipsoid. In the general case, \mathbf{A} can be written as (using the SVD) $\mathbf{A} = \mathbf{U} \mathbf{B} \mathbf{U}^\top$, 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:

$$\mathbf{w}_{\text{lse}} \stackrel{(a)}{=} \arg \min_{\mathbf{w}} -\log p(\mathbf{y}, \mathbf{X} | \mathbf{w})$$

$$\stackrel{(b)}{=} \arg \min_{\mathbf{w}} -\log p(\mathbf{X} | \mathbf{w}) p(\mathbf{y} | \mathbf{X}, \mathbf{w})$$

$$\stackrel{(c)}{=} \arg \min_{\mathbf{w}} -\log p(\mathbf{X}) p(\mathbf{y} | \mathbf{X}, \mathbf{w})$$

$$\stackrel{(d)}{=} \arg \min_{\mathbf{w}} -\log p(\mathbf{y} | \mathbf{X}, \mathbf{w})$$

$$\stackrel{(e)}{=} \arg \min_{\mathbf{w}} -\log \left[\prod_{n=1}^N p(y_n | \mathbf{x}_n, \mathbf{w}) \right]$$

$$\stackrel{(f)}{=} \arg \min_{\mathbf{w}} -\log \left[\prod_{n=1}^N \mathcal{N}(y_n | \mathbf{x}_n^\top \mathbf{w}, \sigma^2) \right]$$

$$= \arg \min_{\mathbf{w}} -\log \left[\prod_{n=1}^N \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2} (y_n - \mathbf{x}_n^\top \mathbf{w})^2} \right]$$

$$= \arg \min_{\mathbf{w}} -N \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) + \sum_{n=1}^N \frac{1}{2\sigma^2} (y_n - \mathbf{x}_n^\top \mathbf{w})^2$$

$$= \arg \min_{\mathbf{w}} \frac{1}{2\sigma^2} \sum_{n=1}^N (y_n - \mathbf{x}_n^\top \mathbf{w})^2$$

- Ridge as MAP:

$$\mathbf{w}_{\text{ridge}} = \arg \min_{\mathbf{w}} -\log p(\mathbf{w} | \mathbf{X}, \mathbf{y})$$

$$\stackrel{(a)}{=} \arg \min_{\mathbf{w}} -\log \frac{p(\mathbf{y}, \mathbf{X} | \mathbf{w}) p(\mathbf{w})}{p(\mathbf{y}, \mathbf{X})}$$

$$\stackrel{(b)}{=} \arg \min_{\mathbf{w}} -\log p(\mathbf{y}, \mathbf{X} | \mathbf{w}) p(\mathbf{w})$$

$$\stackrel{(c)}{=} \arg \min_{\mathbf{w}} -\log p(\mathbf{y} | \mathbf{X}, \mathbf{w}) p(\mathbf{w})$$

$$= \arg \min_{\mathbf{w}} -\log \left[p(\mathbf{w}) \prod_{n=1}^N p(y_n | \mathbf{x}_n, \mathbf{w}) \right]$$

$$= \arg \min_{\mathbf{w}} -\log \mathcal{N}(\mathbf{w} | 0, \frac{1}{\lambda} \mathbf{I}) + \sum_{n=1}^N \mathcal{N}(y_n | \mathbf{x}_n^\top \mathbf{w}, \sigma^2)$$

$$= \arg \min_{\mathbf{w}} -\log \frac{1}{(2\pi\frac{1}{\lambda})^{D/2}} e^{-\frac{\lambda}{2} \|\mathbf{w}\|^2}$$

$$\times \sum_{n=1}^N \mathcal{N}(y_n | \mathbf{x}_n^\top \mathbf{w}, \sigma^2)$$

$$= \arg \min_{\mathbf{w}} \sum_{n=1}^N \frac{1}{2\sigma^2} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

- Ridge regression has a very similar interpretation.

Ridge Regression as MAP estimator

- We start with the posterior $p(\mathbf{w} | \mathbf{X}, \mathbf{y})$ 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 \mathcal{D} with range $\mathcal{X} \times \mathcal{Y}$

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

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

Generalization Error

- How accurate is f at predicting?

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

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

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

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

True	Risk
Expected	Error
Generalization	Loss

- Problem: $\mathcal{A}(S)$ 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: $L_S(f) \xrightarrow{|S| \rightarrow \infty} L_{\mathcal{D}}(f)$ but fluctuations!

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

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 $L_{\mathcal{D}}(f_S)$ i.e. overfitting

Generalization gap

- How far is the test from the true error?
- Claim: given a model f and a test set $S_{\text{test}} \sim \mathcal{D}$ i.i.d. (not used to learn f) and a loss $\ell(\cdot, \cdot) \in [a, b]$:

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

- 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

→ 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: $\mathcal{A}(S_{\text{train}}) = f_{S_{\text{train}}}$
- 3. Validate: $\mathbb{P}[L_{\mathcal{D}}(f_{S_{\text{train}}}) \geq L_{S_{\text{test}}}(f_{S_{\text{train}}}) + \sqrt{\frac{(a-b)^2 \ln(2/\delta)}{2|S_{\text{test}}|}}] \leq \delta$

⇒ 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: $\mathbb{E}[\Theta_n] = \mathbb{E}[\ell(y_n, f(x_n))] = L_{\mathcal{D}}(f)$
- What is the chance that the empirical loss $L_{S_{\text{test}}}(f)$ deviates from the true loss by more than a given constant? → concentration inequalities

Hoeffding inequality: a simple concentration bound

- Claim: Let $\Theta_1, \dots, \Theta_N$ 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? $L_{S_{\text{test}}}(f_{S_{\text{train}}, \lambda_k}) \approx L_{\mathcal{D}}(f_{S_{\text{train}}, \lambda_k})$?

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

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

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

- 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 $\sqrt{\ln(K)}$
⇒ 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 $K = 1$

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

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

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

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:

$$\text{For any } s \geq 0, \quad \mathbb{P} \left\{ \frac{1}{N} \sum_{n=1}^N \Theta_n \geq \varepsilon \right\} =$$

$$\mathbb{P} \left\{ s \frac{1}{N} \sum_{n=1}^N \Theta_n \geq s\varepsilon \right\}$$

$$= \mathbb{P} \left\{ e^{s \frac{1}{N} \sum_{n=1}^N \Theta_n} \geq e^{s\varepsilon} \right\}$$

$$\leq \mathbb{E} \left[e^{s \frac{1}{N} \sum_{n=1}^N \Theta_n} \right] e^{-s\varepsilon} \quad (\text{Markov inequality})$$

$$= \prod_{n=1}^N \mathbb{E} \left[e^{\frac{s\Theta_n}{N}} \right] e^{-s\varepsilon} \quad (\text{the r.v } \Theta_n \text{ are indep.})$$

$$= \mathbb{E} \left[e^{\frac{s\Theta}{N}} \right]^N e^{-s\varepsilon} \quad (\text{the r.v } \Theta_n \text{ are i.d.})$$

$$\leq e^{s^2(b-a)^2/(8N)} e^{-s\varepsilon} \quad (\text{Hoeffding lemma})$$

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

$$\mathbb{E}[e^{sX}] \leq e^{\frac{1}{8}s^2(b-a)^2} \text{ for any } s \geq 0$$

Proof outline:

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

Taking the expectation and recalling that $\mathbb{E}[X] = 0$, we get

$$\mathbb{E}[e^{sX}] \leq \frac{b}{b-a} e^{sa} - \frac{a}{b-a} e^{sb} \leq e^{s^2(b-a)^2/8}$$

⇒

$$\mathbb{E}_{S \sim \mathcal{D}, \varepsilon \sim \mathcal{D}_{\varepsilon}} [(f(x_0) + \varepsilon - f_S(x_0))^2] =$$

=

$$\text{Var}_{\varepsilon \sim \mathcal{D}_{\varepsilon}} [\varepsilon] + \mathbb{E}_{S \sim \mathcal{D}} [(f(x_0) - f_S(x_0))^2]$$

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

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

Cross-term:

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

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

$$= (f(x_0) - \mathbb{E}_{S' \sim \mathcal{D}} [f_{S'}(x_0)])^2$$

$$+ \mathbb{E}_{S \sim \mathcal{D}} [(\mathbb{E}_{S' \sim \mathcal{D}} [f_{S'}(x_0)] - f_S(x_0))^2]$$

Bias-Variance Decomposition

- We obtain the following decomposition into three positive terms:

$$\mathbb{E}_{S \sim \mathcal{D}, \varepsilon \sim \mathcal{D}_{\varepsilon}} [(f(x_0) + \varepsilon - f_S(x_0))^2]$$

$$= \text{Var}_{\varepsilon \sim \mathcal{D}_{\varepsilon}} [\varepsilon] \leftarrow \text{Noise variance}$$

$$+ (f(x_0) - \mathbb{E}_{S' \sim \mathcal{D}} [f_{S'}(x_0)])^2 \leftarrow \text{Bias}$$

$$+ \mathbb{E}_{S \sim \mathcal{D}} [(f_S(x_0) - \mathbb{E}_{S' \sim \mathcal{D}} [f_{S'}(x_0)])^2] \leftarrow \text{Var.}$$

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

→ To minimize the true error, we must choose a method that achieves low bias and low variance simultaneously

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

- 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: $L(f) = \mathbb{E}[\varepsilon^2]$
- It is not possible to predict the noise from the data since they are independent

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

- 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

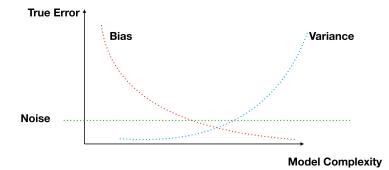
- If model complexity is low, bias is typically high
- If model complexity is high, bias is typically low

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

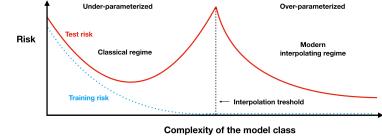
- Variance of the prediction function
- It measures the variability of predictions at a given point across different training set realizations

- 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):
⇒ Prediction: $f(x) = \text{sign}(x^\top w)$
- 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
⇒ 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
⇒ It will lead us to support vector machine (SVM) and logistic regression

Formalizing Binary Classification

- Setting: $(X, Y) \sim \mathcal{D}$ with ranges $\mathcal{X}, \mathcal{Y} = \{-1, 1\}$
- 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:
 $L_{\mathcal{D}}(f) = \mathbb{E}_{\mathcal{D}}[1_{Y \neq f(X)}] = \mathbb{P}_{\mathcal{D}}[Y \neq f(X)]$ (resp. classification error = probability of making an error)
- Goal: minimize $L_{\mathcal{D}}(f)$

Bayes classifier

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

Proof of the Bayes classifier

- Claim 1: $\forall x \in \mathcal{X}, f_*(x) \in \arg \min_{y \in \mathcal{Y}} \mathbb{P}(Y \neq y | X = x) \implies f_* \in \arg \min_{f: \mathcal{X} \rightarrow \mathcal{Y}} L_{\mathcal{D}}(f)$

$$L_{\mathcal{D}}(f) = \mathbb{E}_{X, Y} [1_{Y \neq f(X)}] = \mathbb{E}_X [\mathbb{E}_{Y|X} [1_{Y \neq f(X)} | X]] = \mathbb{E}_X [\mathbb{P}(Y \neq f(X) | X)] \geq \mathbb{E}_X [\min_{y \in \mathcal{Y}} \mathbb{P}(Y \neq y | X)] = \mathbb{E}_X [\mathbb{P}(Y \neq f_*(X) | X)] = \mathbb{E}_{X, Y} [1_{Y \neq f_*(X)}] = L_{\mathcal{D}}(f_*)$$
- Claim 2: $f_*(x) = \arg \min_{y \in \mathcal{Y}} \mathbb{P}(Y \neq y | X = x)$

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

Two classes of classification algorithms

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

Classification by empirical risk minimization

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

$$\min_{f: X \rightarrow Y} L_{\text{train}}(f) := \frac{1}{N} \sum_{n=1}^N 1_{f(x_n) \neq y_n} = \frac{1}{N} \sum_{n=1}^N 1_{y_n f(x_n) \leq 0}$$
- 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 $f: \mathcal{X} \rightarrow \mathcal{Y}$, learn $g: \mathcal{X} \rightarrow \mathbb{R}$ in a convex subset of continuous functions \mathcal{G} , and predict with $f(x) = \text{sign}(g(x))$. The problem becomes

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

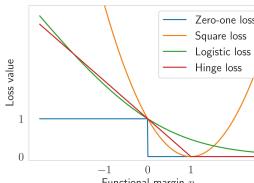
- Replace the indicator function by a convex $\phi: \mathbb{R} \rightarrow \mathbb{R}$ and minimize

$$\min_{g \in \mathcal{G}} \frac{1}{N} \sum_{n=1}^N \phi(y_n g(x_n))$$
 ϕ is a function of the functional margin $y_n g(x_n)$
⇒ This is a convex problem!

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

Losses for Classification

- Logistic loss → logistic regression
- Hinge loss → max margin classification



Good regressor ⇒ good classifier

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

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

$$L_{\mathcal{D}}^{\text{classif}}(f_\eta) - L_{\mathcal{D}}^{\text{classif}}(f^*) \leq 2\sqrt{L_{\mathcal{D}}^{\ell_2}(\eta) - L_{\mathcal{D}}^{\ell_2}(\eta^*)}$$
 Where $L_{\mathcal{D}}^{\text{classif}}(f_\eta) = \mathbb{E}_{\mathcal{D}}[1_{f(x) \neq Y}]$, $L_{\mathcal{D}}^{\ell_2}(f) = \mathbb{E}_{\mathcal{D}}[(Y - f(X))^2]$ and $\eta^* = \arg \min_{\eta} L_{\mathcal{D}}^{\ell_2}(\eta)$
⇒ 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 $S = \{(x_n, y_n)\}_{n=1}^N \in \mathcal{X} \times \{0, 1\}$

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:

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

Logistic Regression

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

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

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

Label prediction: quantize the probability:

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

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

- Interpretation:

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

Small $|x^\top w + w_0|$ corresponds to $p(1 | x)$ 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: $p(1 | x) = \sigma(w^\top x + w_0)$ 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:

$$\mathcal{L}(w) = p(\mathbf{y}, \mathbf{X} | w) = p(\mathbf{X} | w)p(\mathbf{y} | \mathbf{X}, w)$$

$$\begin{aligned} \mathbf{x}_{\perp \perp w} &= p(\mathbf{X} | \mathbf{x}, w) \\ p(\mathbf{y} | \mathbf{X}, w) &= \prod_{n=1}^N p(y_n | x_n, w) \\ &= \prod_{n: y_n=1} p(y_n = 1 | x_n, w) \\ &\quad \times \prod_{n: y_n=0} p(y_n = 0 | x_n, w) \\ &= \prod_{n=1}^N \sigma(x_n^\top w)^{y_n} [1 - \sigma(x_n^\top w)]^{1-y_n} \end{aligned}$$

The likelihood is proportional to:

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

Minimum of the NLL

$$\begin{aligned} -\log(p(\mathbf{y} | \mathbf{X}, w)) &= -\log \left(\prod_{n=1}^N \sigma(x_n^\top w)^{y_n} [1 - \sigma(x_n^\top w)]^{1-y_n} \right) \\ &= -\sum_{n=1}^N y_n \log \sigma(x_n^\top w) \\ &\quad + (1 - y_n) \log (1 - \sigma(x_n^\top w)) \\ &= \sum_{n=1}^N y_n \log \left(\frac{1 - \sigma(x_n^\top w)}{\sigma(x_n^\top w)} \right) - \log(1 - \sigma(x_n^\top w)) \\ &= \sum_{n=1}^N -y_n x_n^\top w + \log(1 + e^{x_n^\top w}) \\ \leftarrow 1 - \sigma(\eta) = \frac{1}{1 + e^\eta} \Rightarrow \frac{1 - \sigma(\eta)}{\sigma(\eta)} = e^{-\eta} \end{aligned}$$

We obtain the following cost function we will minimize to learn the parameter $w_* = \arg \min L(w) := \frac{1}{N} \sum_{n=1}^N -y_n x_n^\top w + \log(1 + e^{x_n^\top w})$

- 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 $y \in \{-1, 1\}$:

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

- 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

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

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

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

- 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) $\Rightarrow \log(1 + e^{x_n^\top w})$ 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 $\frac{\partial^2}{\partial w_i \partial w_j} L(w)$

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

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

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

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

It can be written under the matrix form:

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

where $S = \text{diag} [\sigma(x_1^\top w) (1 - \sigma(x_1^\top w))] \succcurlyeq 0$

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

How to minimize the convex function L ?

GD:

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

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

SGD:

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

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.

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

- 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

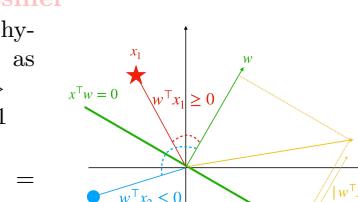
- Define a hyperplane as

$$\{x : w^\top x = 0\}$$

where $\|w\| = 1$

- Prediction:

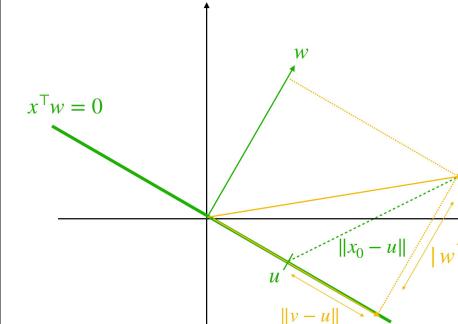
$$f(x) = \text{sign}(x^\top w)$$



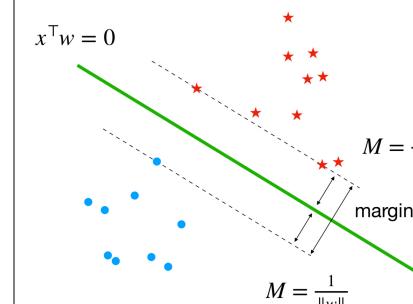
- Claim: The distance between a point x_0 and the hyperplane defined by w is $|w^\top x_0|$

- 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. $w^\top u = 0$



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:

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

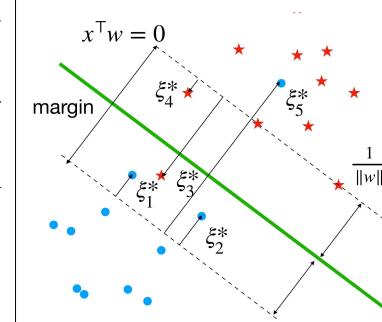
- Equivalent to:

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

- Also equivalent to:

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

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 ξ_1, \dots, ξ_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:

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

(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 $\xi_n = [1 - y_n x_n^\top w]_+$

Classification by risk minimization

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

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

- How: Through Empirical Risk Minimization (ERM):

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

ϕ represents the loss function of the functional

$$\text{margin } y_n x_n^\top w$$

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

Losses for Classification

Examples of margin-based losses ($\eta = yx^\top w$):

- 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: $Hinge(\eta) = [1 - \eta]_+$ 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:

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

- 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

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

- 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 $G(w, \alpha)$?

$$[z]_+ = \max(0, z) = \max_{\alpha \in [0,1]} \alpha z$$

$$- [1 - y_n x_n^\top w]_+ = \max_{\alpha \in [0,1]} \alpha_n (1 - y_n x_n^\top w)$$

- The SVM problem is equivalent to: $\min_w L(w) =$

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

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

Can min and max be interchanged?

$$\max_\alpha \min_w G(w, \alpha) \leq \min_w \max_\alpha G(w, \alpha)$$

- 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:

$$\min_w G(\alpha, w) \leq G(\alpha, w') \quad \forall w'$$

$$\max_\alpha \min_w G(\alpha, w) \leq \max_\alpha G(\alpha, w') \quad \forall w'$$

$$\max_\alpha \min_w G(\alpha, w) \leq \min_w \max_\alpha G(\alpha, w')$$

Application to SVM

- For SVM, the condition is met, allowing us to interchange min and max: $\min_w L(w) =$

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

- Minimizer computation:

$$\mathbf{Y} = \text{diag}(\mathbf{y})$$

$$\nabla_w G(w, \alpha) = -\frac{1}{N} \sum_{n=1}^N \alpha_n y_n x_n + \lambda w = 0 \Rightarrow w(\alpha) = \frac{1}{\lambda N} \sum_{n=1}^N \alpha_n y_n x_n = \frac{1}{\lambda N} \mathbf{X}^\top \mathbf{Y} \alpha$$

- Dual optimization problem:

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

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:

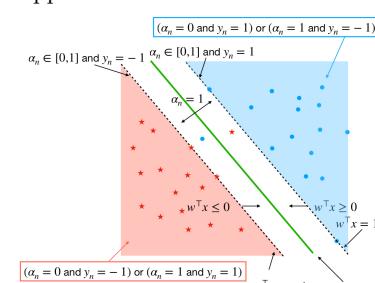
$$\max_{\alpha_n \in [0,1]} \alpha_n (1 - y_n x_n^\top w)$$

• 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 on 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 $\forall n, y_n x_n^\top w \geq 1$
- Soft SVM - relax the constraint for non-separable data

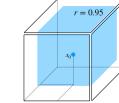
$$\min_w \frac{\lambda}{2} \|w\|^2 + \frac{1}{N} \sum_{n=1}^N [1 - y_n x_n^\top w]_+$$

• 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)



$\mathcal{X} = [0, 1]^d$

Curse of dimensionality

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

- Assume the data $x \sim \mathcal{U}([0, 1]^d)$

- 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 $r = 0.63$

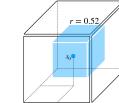
$d = 100 \rightarrow$ need to explore almost the whole box

- **Claim 2:** In high-dimension, data-points are far from each other.
- Consider N i.i.d. points uniform in the $[0, 1]^d$

$$\mathbb{P}(\exists x_i \in \square) \geq 1/2 \Rightarrow r \geq \left(1 - \frac{1}{2^{1/d}}\right)^{1/d}$$

- Proof: $\mathbb{P}(x \notin \square) = 1 - r^d$

$$\mathbb{P}(x_i \notin \square, \forall i \leq N) = \left(1 - r^d\right)^N$$



$\mathcal{X} = [0, 1]^d$

Generalization bound for 1-NN (I)

- Setup: $(X, Y) \sim \mathcal{D}$ over $\mathcal{X} \times \mathcal{Y} = [0, 1]^d \times \{0, 1\}$

- Goal: Bound the classification error:

$$L(f) = \mathbb{P}_{(X, Y) \sim \mathcal{D}}(Y \neq f(X))$$

- Baseline:

- Bayes classifier: minimizes L over all classifiers $f_s(x) = 1_{\eta(x) \geq 1/2}$ where $\eta(x) = \mathbb{P}(Y = 1 | X = x)$

Proof 1:

$$\eta(x) \geq 1/2 \iff \mathbb{P}(Y = 1 | X = x) \geq 1/2$$

$$\iff \mathbb{P}(Y = 1 | X = x) \geq \mathbb{P}(Y = 0 | X = x)$$

$$\iff 1 \in \arg \max_{y \in \{0,1\}} \mathbb{P}(Y = y | X = x)$$

$$\Rightarrow 1_{\eta(x) \geq 1/2} = \arg \max_{y \in \{0,1\}} \mathbb{P}(Y = y | X = x) = f_s(x)$$

- Bayes risk: represents the minimum probability of misclassification

$$L(f_s) = \mathbb{P}(f_s(X) \neq Y)$$

$$= \mathbb{E}_{X \sim D_X} [\min\{\eta(X), 1 - \eta(X)\}]$$

Proof 2:

$$\begin{aligned} L(f_s) &= \mathbb{E}_{(X, Y) \sim \mathcal{D}} [1_{f_s(X) \neq Y}] \\ &= \mathbb{E}_{X \sim \mathcal{D}_X} [\mathbb{E}_{Y \sim \mathcal{D}_{Y|X}} [1_{f_s(X) \neq Y} | X] 1_{\eta(X) \geq 1/2} + \mathbb{E}_{Y \sim \mathcal{D}_{Y|X}} [1_{f_s(X) \neq Y} | X] 1_{\eta(X) < 1/2}] \\ &= \mathbb{E}_{X \sim \mathcal{D}_X} [\mathbb{E}_{Y \sim \mathcal{D}_{Y|X}} [1_{\eta(Y) \neq 1} | X] 1_{\eta(X) \geq 1/2} + \mathbb{E}_{Y \sim \mathcal{D}_{Y|X}} [1_{\eta(Y) \neq 1} | X] 1_{\eta(X) < 1/2}] \\ &= \mathbb{E}_{X \sim \mathcal{D}_X} [\mathbb{P}(Y = 0 | X) 1_{\eta(X) \geq 1/2} + \mathbb{P}(Y = 1 | X) 1_{\eta(X) < 1/2}] \\ &= \mathbb{E}_{X \sim \mathcal{D}_X} [\min\{\eta(X), 1 - \eta(X)\}] \end{aligned}$$

Generalization bound for 1-NN (II)

- Assumption: $\exists c \geq 0, \forall x, x' \in \mathcal{X} :$

$$|\eta(x) - \eta(x')| \leq c \|x - x'\|_2$$

\Rightarrow Nearby points are likely to share the same label

- **Claim:** $\mathbb{E}_{S_{\text{train}}} [L(f_s)]$

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

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

- Interpretation:

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

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

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

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

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

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

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

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: $x = x'$

$$\mathbb{P}(Y' \neq Y) = \mathbb{E}[1_{Y' \neq Y} 1_{Y'=1} + 1_{Y' \neq Y} 1_{Y'=0}]$$

$$= \mathbb{P}(Y' = 1) \mathbb{P}(Y = 0) + \mathbb{P}(Y' = 0) \mathbb{P}(Y = 0)$$

$$= 2\eta(x)(1 - \eta(x))$$

$$\leq 2 \min\{\eta(x), 1 - \eta(x)\}$$

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

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

Proof (III)

• General case:

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

Proof (IV)

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

Bound on the geometric term (I)

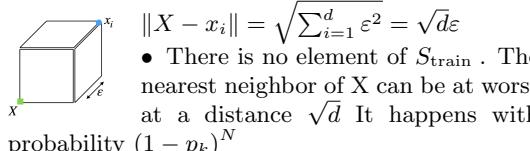
- Consider a fresh sample $X \sim \mathcal{D}$ and denote by $p_k = \mathbb{P}(X \in \text{Box}_k)$

- 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:



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

- 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)

$$\mathbb{E}[\|X - \text{nbh}(X)\|]$$

$$\leq \sum_k p_k \left[(1 - p_k)^N \sqrt{d} + (1 - (1 - p_k)^N) \sqrt{d}\varepsilon \right]$$

- 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 $p(y|x)$ by some $\hat{p}(y|x)$ These "plug-in" estimators are:

- $f(x) \in \arg \max \hat{P}(Y = y | x)$ for classification with the 0-1 loss $y \in \mathcal{Y}$
- $f(x) = \hat{E}[Y | x] = \int y \hat{p}(y | x) dy$ for regression with the square loss

- In the case of nearest neighbors:

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

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 $N \rightarrow \infty$, 1-NN is competitive with Bayes classifier

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

Equivalent formulations for ridge regression

- Objective:

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

- Solution:

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

- Alternative solution:

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

- 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 $Q = \frac{1}{N} \mathbf{X}$

Usefulness of the alternative form

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

1. Computational complexity:

- For the original formulation

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

- For the new formulation

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

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

2. Structural difference:

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

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

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 $\text{span}\{x_1, \dots, x_N\}$

- 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 $w = w_* - u$

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

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

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 :

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

- Claim: These two formulations are equivalent

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

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

- 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 $\phi: \mathbb{R}^d \rightarrow \mathbb{R}^{\tilde{d}}$ is used,

$$(x_n)_{n=1}^N \hookrightarrow (\phi(x_n))_{n=1}^N$$

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

- Problem: when $d \ll \tilde{d}$ 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:

$$y = \underbrace{\phi(x)^\top w_*}_{\text{Linear prediction in the feature space}} + \underbrace{\kappa(x, x')}_\text{Non linear prediction in the \mathcal{X} space}$$

$\kappa(x, x')$

$f_{W^*}(x)$

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

$$\kappa(x, x') = (x_1 x'_1 + x_2 x'_2 + x_3 x'_3)^2$$

- Feature map:

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

- Proof:

$$\begin{aligned} \kappa(x, x') &= \phi(x)^\top \phi(x') \\ \kappa(x, x') &= (x_1 x'_1 + x_2 x'_2 + x_3 x'_3)^2 \\ &= (x_1 x'_1)^2 + (x_2 x'_2)^2 + (x_3 x'_3)^2 + 2x_1 x_2 x'_1 x'_2 + 2x_1 x_3 x'_1 x'_3 + 2x_2 x_3 x'_2 x'_3 \\ &= (x_1^2, x_2^2, x_3^2, \sqrt{2}x_1 x_2, \sqrt{2}x_1 x_3, \sqrt{2}x_2 x_3)^\top (x_1^2, x_2^2, x_3^2, \sqrt{2}x_1 x'_2, \sqrt{2}x_1 x'_3, \sqrt{2}x_2 x'_3) \end{aligned}$$

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: $\phi(x) = e^{-x^2} \left(\dots, \frac{e^{k/2} x^k}{\sqrt{k!}} \dots \right)$

- Proof: $\kappa(x, x') = e^{-x^2 - x'^2 + 2x x'} = e^{-x^2} e^{-x'^2} \sum_{k=0}^{\infty} \frac{2^k x^k x'^k}{k!}$ (Taylor: $e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$)

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

- 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:

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

Proof 1:

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

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

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

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

Claim 2: Products of kernels are kernels:

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

Proof 2:

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

$$\begin{aligned} &= \phi_1(x)^\top \phi_1(x') \phi_2(x)^\top \phi_2(x') \\ \text{Let } \phi(x)^\top &= (\phi_1(x)_1 \phi_2(x)_1, \dots, \phi_1(x)_d \phi_2(x)_{d_2}, \dots, \phi_1(x)_{d_1} \phi_2(x)_1, \dots, \phi_1(x)_{d_1} \phi_2(x)_{d_2}) \in \mathbb{R}^{d_1 d_2} \text{ then} \\ \phi(x)^\top \phi(x') &= \sum_{i,j} (\phi_1(x))_i (\phi_2(x))_j (\phi_1(x'))_i (\phi_2(x'))_j \\ &= \sum_i (\phi_1(x))_i (\phi_1(x'))_i \sum_j (\phi_2(x))_j (\phi_2(x'))_j \\ &= \phi_1(x)^\top \phi_1(x') \phi_2(x)^\top \phi_2(x') = \kappa(x, x') \end{aligned}$$

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:

$$\forall N \geq 0, \forall (x_n)_{n=1}^N, \mathbf{K} = (\kappa(x_i, x_j))_{i,j=1}^N \geq 0$$

Proof of Mercer theorem

• If κ represents an inner product then it is symmetric and the kernel matrix is psd:

$$v^\top \mathbf{K} v = \sum_{i,j} v_i v_j \phi(x_i)^\top \phi(x_j) = \left\| \sum_i v_i \phi(x_i) \right\|^2$$

• Define $\phi(x) = \kappa(\cdot, x)$. Define a vector space of functions by considering all linear combinations $\{\sum_i \alpha_i \kappa(\cdot, x_i)\}$. Define an inner product on this vector space by

$$\langle \sum_i \alpha_i \kappa(\cdot, x_i), \sum_j \beta_j \kappa(\cdot, x'_j) \rangle =$$

$$\sum_{i,j} \alpha_i \beta_j \kappa(x_i, x'_j)$$

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): $y = f_{\text{NN}}(x) = f(x)^\top w$

Why Neural Networks?

- Classical machine learning:

• Relatively simple models on top of features handcrafted by domain experts

• Only works well when used with good hand-crafted 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

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

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

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 $p(1 | x) \geq 0.5$ or, equivalently, if $\sum_{i=1}^d x_i w_i \geq -b$

Two-Layer Neural Networks

(aka two-layer perceptron)

• Stack logistic regression units $\phi(x)_j = \sigma\left(\sum_{i=1}^d x_i w_{i,j} + b_j\right)$ (aka hidden units or neurons) in a hidden layer

• Aggregate the hidden units using a linear function $\phi(x)^\top w^{(2)}$

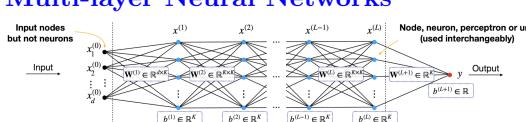
Pattern-matching perspective:

- 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

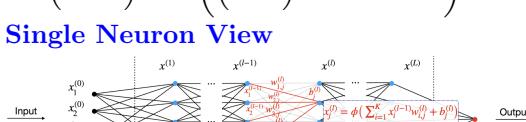


- Learnable Parameters: Weight matrices $\mathbf{W}^{(l)}$ and bias vectors $b^{(l)}$ for $1 \leq l \leq L+1$

- Each column of $\mathbf{W}^{(l)}$ corresponds to the weights of one perceptron

- Outputs of hidden layer l given by vector: $x^{(l)} = f^{(l)}(x^{(l-1)}) := \phi\left(\left(\mathbf{W}^{(l)}\right)^\top x^{(l-1)} + b^{(l)}\right)$

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 $\{b^{(l)}\}_{l \in [L]}$ and weights $\{\mathbf{W}^{(l)}\}_{l \in [L]}$ so we learn $\Rightarrow O(dK + K^2L) \approx O(K^2L)$ parameters
- The activation function ϕ we pick

- In practice: both L and K are large - over-parametrized 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 $y \in \{1, \dots, K\}$

$$\text{argmax}_{c \in \{1, \dots, K\}} h(x)_c$$

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

Popular activation functions

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

L₂ 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 $r > 0$, $\exists f_n$:

$$f_n(x) = \sum_{j=1}^n c_j \phi(x^\top w_j + b_j) + c_0$$

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 $f_n = c^\top \phi(W^\top x + b) + c_0$

L1 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:

$$\int_{|x| \leq r} |f(x) - f_n(x)| dx \leq \text{Something small}$$

$f : \mathbb{R} \rightarrow \mathbb{R}$ 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

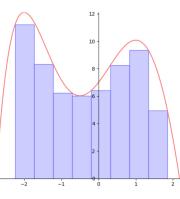
- Remarks:

- 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:

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

- ℓ_∞ -approximation result (Shekhtman, 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

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

where $\tilde{a}_1 = a_1, \tilde{b}_1 = b_1, a_i = \sum_{j=1}^i \tilde{a}_j$ 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

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

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

• For $x \in [0, r_1]$

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

$$\bullet \text{ For } x \in [r_1, r_2], r(x) = \tilde{a}_1 x + \tilde{b}_1 + (a_2 - a_1)(x - r_1)_+ = a_1 x + b_1 + (a_2 - a_1)(x - r_1) = a_2 x + b_1 - (a_2 - a_1)r_1$$

$$r'(x) = a_2 \text{ and } r(r_1) = q(r_1) \text{ as shown above} \\ \Rightarrow r(x) = q(x) \text{ for } x \in [r_1, r_2]$$

Proof by induction

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

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

$$r(x) = \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^m \tilde{a}_j (x - \tilde{b}_j)_+$$

$$= \tilde{a}_1 x + \tilde{b}_1 + \sum_{j=2}^i \tilde{a}_j (x - \tilde{b}_j)$$

$$= \sum_{j=1}^i \tilde{a}_j x + \tilde{b}_1 - \sum_{j=2}^i \tilde{a}_j \tilde{b}_j$$

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

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

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

- In Practice: Step size schedule, mini-batch, momentum, Adam

- Problem: With $O(K^2 L)$ 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

$$\bullet x^{(1)} = f^{(1)}(x^{(0)}) := \phi\left(\left(\mathbf{W}^{(1)}\right)^T x^{(0)} + b^{(1)}\right)$$

$$\bullet x^{(l)} = f^{(l)}(x^{(l-1)}) := \phi\left(\left(\mathbf{W}^{(l)}\right)^T x^{(l-1)} + b^{(l)}\right)$$

$$\bullet y = f^{(L+1)}(x^{(L)}) := \left(\mathbf{W}^{(L+1)}\right)^T x^{(L)} + b^{(L+1)}$$

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

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

Cost function

$$\mathcal{L} = \frac{1}{2N} \sum_{n=1}^N (y_n - f^{(L+1)} \circ \dots \circ f^{(2)} \circ f^{(1)}(x_n))^2$$

Chain rule

$$\mathcal{L}_n = \frac{1}{2} (y_n - f^{(L+1)} \circ \dots \circ f^{(l+1)} \circ \phi(z^{(l)}))^2$$

$$\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} = \sum_{k=1}^K \frac{\partial \mathcal{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}}$$

$$= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} \quad \text{since } \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = 0 \text{ for } k \neq j$$

$$= \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \cdot x_i^{(l-1)} \quad \text{since } z_j^{(l)} = \sum_{k=1}^K w_{k,j}^{(l)} x_k^{(l-1)} + b_j^{(l)}$$

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

Forward Pass

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

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

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

Backward pass (I)

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

Backward pass (II)

- Using $z_k^{(l+1)} = \sum_{i=1}^K w_{i,k}^{(l+1)} x_i^{(l)} + b_k^{(l+1)}$ = $\sum_{i=1}^K w_{i,k}^{(l+1)} \phi(z_i^{(l)}) + b_k^{(l+1)}$
- We obtain $\frac{\partial z_k^{(l+1)}}{\partial z_j^{(l)}} = \phi'(z_j^{(l)}) w_{j,k}^{(l+1)}$
- Thus $\delta_j^{(l)} = \sum_k \delta_k^{(l+1)} \phi'(z_j^{(l)}) w_{j,k}^{(l+1)}$
- $\delta^{(l)} = (\mathbf{W}^{(l+1)} \delta^{(l+1)}) \odot \phi'(z^{(l)})$

Backward pass (III)

Initialization (first derivative):

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

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

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

Computational complexity: $O(K^2L)$

Derivatives computation

- Using $z_m^{(l)} = \sum_{k=1}^K w_{k,m}^{(l)} x_k^{(l-1)} + b_m^{(l)}$:
- $\frac{\partial \mathcal{L}_n}{\partial b_j^{(l)}} = \sum_{k=1}^K \frac{\partial \mathcal{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial b_j^{(l)}} = \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial b_j^{(l)}} = \delta_j^{(l)}$
- $\frac{\partial \mathcal{L}_n}{\partial w_{i,j}^{(l)}} = \sum_{k=1}^K \frac{\partial \mathcal{L}_n}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial w_{i,j}^{(l)}} = \frac{\partial \mathcal{L}_n}{\partial z_j^{(l)}} \frac{\partial z_j^{(l)}}{\partial w_{i,j}^{(l)}} = \delta_j^{(l)} \cdot x_i^{(l-1)}$

Backpropagation algorithm

Forward pass:

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

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

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

Backward pass:

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

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

Compute the derivatives:

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

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

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

Batch Normalization

- Batch $B = (x_1, \dots, x_M)$ 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:

$$\bar{z}_n^{(l)} = \frac{z_n^{(l)} - \mu_B^{(l)}}{\sqrt{(\sigma_B^{(l)})^2 + \epsilon}} \quad (\text{Component-wise})$$

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

- 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 $\epsilon \approx 0$, the output is invariant to activation-wise affine scaling of $z_n^{(l)}$

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

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

- Estimate $\hat{\mu}^{(l)} = \mathbf{E}[\mu_B^{(l)}]$ and $\hat{\sigma}^{(l)} = \mathbf{E}[\sigma_B^{(l)}]$ 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 $30\times$)

Layer Normalization

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

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

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

- 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

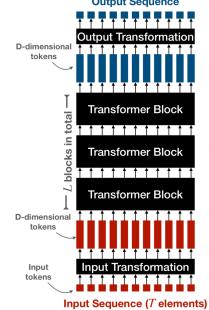
- Neural networks are trained with gradient-based methods such as SGD
- To compute the gradients, we use backpropagation, which involves the chain rule to efficiently calculate the gradients based on the network's intermediate outputs $z^{(l)}$ and $\delta^{(l)}$
- Proper parameter initialization should 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

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

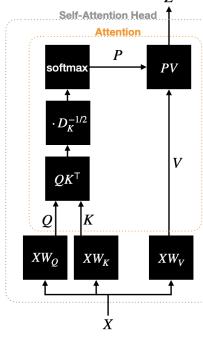
- Tokenization: split the input text into a sequence of input tokens (typically word fragments + some special symbols) according to some predefined tokenizer procedure:
- Convert each token ID $i \in \{1, \dots, N_{vocab}\}$ into a real-valued vector $\mathbf{w}_i \in \mathbb{R}^D$
- This can be seen as a matrix multiplication $\mathbf{W} \cdot \mathbf{e}_i = \mathbf{W}_{:,i} = \mathbf{w}_i$ (with $\mathbf{W} \in \mathbb{R}^{D \times N_{vocab}}$)
- \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: $z_i = \sum_{j=1}^{T_{in}} p_{ij} v_j$ 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 similar 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.
- $P = \text{softmax} \left(\frac{QK^T}{\sqrt{D_K}} \right)$ The softmax is applied

on each row independently. Scaling ensures uniformity at initialization and faster convergence

- 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.
- $Z = \text{softmax}\left(\frac{XW_QW_K^T X^T}{\sqrt{D_K}}\right) XW_V$



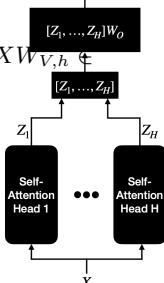
puts (e.g., per-token classification): apply an output transformation to each token independently

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 $x_{t+1} \sim \text{softmax}(f(x_1, \dots, x_t))$ 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)



Multi-Head Self-Attention

- Run H Self-Attention “heads” in parallel
- $Z_h = \text{softmax}\left(\frac{XW_{Q,h}W_{K,h}^T X^T}{\sqrt{D_K}}\right) XW_{V,h}$
- $W_{V,h} \in \mathbb{R}^{D \times D_V}, W_{K,h} \in \mathbb{R}^{D \times D_K}, W_{Q,h} \in \mathbb{R}^{D \times D_K}$
- The final output is obtained by concatenating head-outputs and applying a linear transformation $Z = [Z_1, \dots, Z_H]W_O$ 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 $\text{pos} : \{1, \dots, T\} \rightarrow \mathbb{R}^D$
- The most basic choice is to add a positional embedding W_{pos} corresponding to each token’s position t to the input embedding. $W_{\text{pos}} \in \mathbb{R}^{D \times T}$ 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 out-

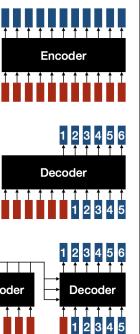
tinuous

- 2) The NN prediction f outputs discrete class values $\{-1, 1\}$

- Replace the difficult problem involving the indicator with a smooth problem $\max_{\hat{x}, \|\hat{x}-x\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y} \rightarrow \max_{\hat{x}, \|\hat{x}-x\| \leq \varepsilon} \ell(yg(\hat{x}))$
- 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.



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

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

$$\begin{aligned} \delta_\infty^* &= \varepsilon \cdot \text{sign}(\nabla_x \tilde{\ell}(x)) = -\varepsilon y \cdot \text{sign}(\nabla_x g(x)) \Rightarrow \\ \hat{x} &= x - \varepsilon y \cdot \text{sign}(\nabla_x g(x)) \end{aligned}$$

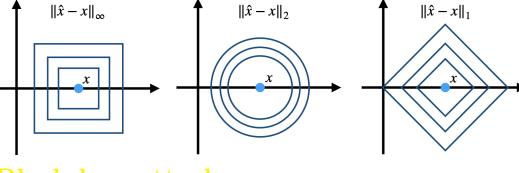
Multi-step attack

- 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:

$$\delta^{t+1} = \Pi_{B_\infty(\varepsilon)} [\delta^t + \alpha \cdot \text{sign}(\nabla \tilde{\ell}(x+\delta^t))],$$

$$\Pi_{B_\infty(\varepsilon)}(\delta)_i = \begin{cases} \varepsilon \cdot \text{sign}(\delta_i), & \text{if } |\delta_i| \geq \varepsilon \\ \delta_i & \text{otherwise} \end{cases}$$

- 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:
- $$\min_\theta R_\varepsilon(f_\theta) = \mathbb{E}_D [\max_{\hat{x}, \|\hat{x}-x\| \leq \varepsilon} 1_{f(\hat{x}) \neq Y}]$$
- D unknown → approximate it with a sample average + classification loss is non-continuous → use a smooth loss ⇒

$$\min_\theta \frac{1}{N} \sum_{n=1}^N \max_{\hat{x}_n, \|x_n - \hat{x}_n\| \leq \varepsilon} \ell(y_n g_\theta(\hat{x}_n))$$

$$1) \forall x_n, \hat{x}_n^* \approx \arg \max_{\|\hat{x}_n - x_n\| \leq \varepsilon} \ell(y_n g_\theta(\hat{x}_n))$$

$$2) \text{GD step w.r.t. } \theta \text{ using } \frac{1}{N} \sum_{n=1}^N \nabla_\theta \ell(y_n g_\theta(\hat{x}_n^*))$$

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

$x \in \mathbb{R}^d, y \sim \text{Bernoulli}(\{-1, 1\}), Z_i \sim \mathcal{N}(0, 1)$

- Robust features: $x_1 = y + Z_1$

- Non-robust features: $x_i = y\sqrt{\frac{\log d}{d-1}} + Z_i, \forall i \in \{-1, 1\}$

- $d \rightarrow \infty \Rightarrow \uparrow$ adversarial risk and \downarrow standard risk
- using the robust feature x_1 :

MLE: $\arg \max_{\hat{y} \in \{\pm 1\}} p(\hat{y} | x_1) =$

$\arg \max_{\hat{y} \in \{\pm 1\}} \frac{p(x_1 | \hat{y}) p(\hat{y})}{p(x_1)} = \arg \max_{\hat{y} \in \{\pm 1\}} p(x_1 | \hat{y})$
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 $x_i = ya_i + Z_i$

$\arg \max_{\hat{y} \in \{\pm 1\}} p(\hat{y} | x)$

$= \arg \max_{\hat{y} \in \{\pm 1\}} \prod_{i=1}^d p(x_i | \hat{y})$

$= \arg \max_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d \log p(x_i | \hat{y})$

$= \arg \max_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d \log \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x_i - \hat{y}a_i)^2}$

$= \arg \min_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d (x_i - \hat{y}a_i)^2$

$= \arg \min_{\hat{y} \in \{\pm 1\}} \sum_{i=1}^d (x_i^2 - 2x_i \hat{y}a_i + \hat{y}^2 a_i^2)$

$= \arg \max_{\hat{y} \in \{\pm 1\}} \hat{y} \sum_{i=1}^d x_i a_i$

$\hat{y} \sum_{i=1}^d x_i a_i = \hat{y}y(\sum_{i=1}^d a_i^2) + \hat{y} \sum_{i=1}^d a_i Z_i = \hat{y}y(1 + \log(d)) + \hat{y}Z$ 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 $Z \sim \mathcal{N}(0, 1/(1 + \log d))$

$d \rightarrow \infty, \hat{y}Z \rightarrow 0 \Rightarrow$ standard risk $R(f) \rightarrow 0$

- using the non-robust features improves standard risk!

- Adversarial risk:

The adversary can use tiny ℓ_∞ perturbations:

$\varepsilon = 2\sqrt{\frac{\log d}{d-1}}$ ($\rightarrow 0$ when) $d \rightarrow \infty$)

$\hat{x}_1 = (1 - 2\sqrt{\frac{\log d}{d-1}})y + Z_1$, 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.

Clustering

Clusters are groups of points whose inter-point distances are small compared to the distances outside the cluster.

The goal is to find "prototype" points $\mu_1, \mu_2, \dots, \mu_K$ and cluster assignments $z_n \in \{1, 2, \dots, K\}$ for all $n = 1, 2, \dots, N$ data vectors $x_n \in \mathbb{R}^D$.

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

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

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

Is this optimization problem easy?

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

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

2. For all k , compute $\boldsymbol{\mu}_k$ given \mathbf{z} .

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

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

Step 2: For all k , compute $\boldsymbol{\mu}_k$ given \mathbf{z} .

Take derivative w.r.t. $\boldsymbol{\mu}_k$ to get:

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^N z_{nk} \mathbf{x}_n}{\sum_{n=1}^N z_{nk}}$$

Hence, the name 'K-means'.

Summary of K-means

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

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

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

2. For all k , compute $\boldsymbol{\mu}_k$ given \mathbf{z} .

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^N z_{nk} \mathbf{x}_n}{\sum_{n=1}^N z_{nk}}$$

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:

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

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

Examples

K-means for the "old-faithful" dataset (Bishop's Figure 9.1)

(e) Iteration 0

(h) Iteration 2

(k) Iteration 3

(f) Iteration 1

(i) Iteration 2

(l) Iteration 4

(g) Iteration 1

(j) Iteration 3

(m) Iteration 4

Data compression for images (this is also known as vector quantization).

Probabilistic model for K-means

K-means as a Matrix Factorization

Recall the objective

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

$$= \|\mathbf{X}^\top - \mathbf{M}\mathbf{Z}^\top\|_{\text{Frob}}^2$$

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).

3. Each example can belong to only one cluster ("hard" cluster assignments).

Motivation

K-means forces the clusters to be spherical, but sometimes it is desirable to have elliptical clusters. Another issue is that, in K-means, each example can only belong to one cluster, but this may not always be a good choice, e.g. for data points that are near the "border". Both of these problems are solved by using Gaussian Mixture Models.

Clustering with Gaussians

The first issue is resolved by using full covariance matrices $\boldsymbol{\Sigma}_k$ instead of isotropic covariances.

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

Soft-clustering

The second issue is resolved by defining z_n to be a random variable. Specifically, define $z_n \in \{1, 2, \dots, K\}$ that follows a multinomial distribution.

$$p(z_n = k) = \pi_k \text{ where } \pi_k > 0, \forall k \text{ and } \sum_{k=1}^K \pi_k = 1$$

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

Gaussian mixture model

Together, the likelihood and the prior define the joint distribution of Gaussian mixture model (GMM):

$$p(\mathbf{X}, \mathbf{z} | \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})$$

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

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

Here, \mathbf{x}_n are observed data vectors, z_n are latent unobserved variables, and the unknown parameters are given by $\boldsymbol{\theta} := \{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K, \boldsymbol{\pi}\}$.

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.

Specifically, we get the following marginal likelihood by marginalizing z_n out from the likelihood: $p(\mathbf{x}_n | \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

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 $\mathcal{O}(D^2 K)$ (assuming $D, K \ll N$).

Maximum likelihood

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

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

Is this cost convex? Identifiable?

Bounded?

Motivation

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

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

Expectation-Maximization (EM) algorithm provides an elegant and general method to optimize such optimization problems. It uses an iterative two-step procedure where individual steps usually involve problems that are easy to optimize.

EM algorithm: Summary

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 $\boldsymbol{\theta}^{(t)}$:

$$\mathcal{L}(\boldsymbol{\theta}) \geq \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) \text{ and}$$

$$\underline{\mathcal{L}}(\boldsymbol{\theta}^{(t)}) = \underline{\mathcal{L}}(\boldsymbol{\theta}^{(t)}, \boldsymbol{\theta}^{(t)}).$$

2. Maximization step: Update $\boldsymbol{\theta}$:

$$\boldsymbol{\theta}^{(t+1)} = \arg \max_{\boldsymbol{\theta}} \underline{\mathcal{L}}(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}).$$

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

$$\log \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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

with equality when,

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

This is not a coincidence.

The maximization step

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

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

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:

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

Summary of EM for GMM

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

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

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

2. Compute the marginal likelihood (cost).

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

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

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

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

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

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 $\sigma^2 \rightarrow 0$.

Figure 1: EM algorithm for GMM

Posterior distribution

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

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

EM in general

Given a general joint distribution $p(\mathbf{x}_n, z_n | \boldsymbol{\theta})$, the marginal likelihood can be lower bounded similarly:

The EM algorithm can be compactly written as follows:

$$\boldsymbol{\theta}^{(t+1)} := \arg \max_{\boldsymbol{\theta}} \sum_{n=1}^N \mathbb{E}_{p(z_n | \mathbf{x}_n, \boldsymbol{\theta}^{(t)})} [\log p(\mathbf{x}_n, z_n | \boldsymbol{\theta})]$$

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) $d = 1, 2, \dots, D$ and users $n = 1, 2, \dots, N$, we define \mathbf{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

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

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

- 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 \mathbf{K}

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

Regularization

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

Stochastic Gradient Descent

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

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

$$\frac{\partial}{\partial w_{d', k}} f_{d, n}(W, Z) \in \mathbb{R}^{D \times K} = \begin{cases} -[x_{dn} - (WZ^T)_{dn}] z_{n, k} & \text{if } d' = d \\ 0 & \text{otherwise} \end{cases}$$

$$\frac{\partial}{\partial z_{n', k}} f_{d, n}(W, Z) \in \mathbb{R}^{N \times K} = \begin{cases} -[x_{dn} - (WZ^T)_{dn}] w_{d, k} & \text{if } n' = n \\ 0 & \text{otherwise} \end{cases}$$

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

Alternating Least Squares

- No missing entries:

$$\frac{1}{2} \sum_{d=1}^D \sum_{n=1}^N [x_{dn} - (WZ^T)_{dn}]^2 = \frac{1}{2} \|\mathbf{X} - \mathbf{WZ}^T\|_{\text{Frob}}^2$$

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

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

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

- 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. $\frac{1}{2} \sum_{(d, n) \in \Omega} [x_{dn} - (WZ^T)_{dn}]^2$

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-Occurrence 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 $\mathcal{V} := \{w_1, \dots, w_D\}$

- For words $w_d = 1, 2, \dots, D$ and context words $w_n = 1, 2, \dots, N$, the co-occurrence counts n_{ij} form a very sparse $D \times N$ matrix.

Learning Word-Representations

- Find a factorization of the cooccurrence matrix!

- Typically uses log of the actual counts, i.e. $x_{dn} := \log(n_{dn})$.

- Aim to find \mathbf{W}, \mathbf{Z} s.t. $\mathbf{X} \approx \mathbf{WZ}^T$

$$\min_{\mathbf{W}, \mathbf{Z}} \mathcal{L}(\mathbf{W}, \mathbf{Z}) :=$$

$$\frac{1}{2} \sum_{(d, n) \in \Omega} f_{dn} [x_{dn} - (\mathbf{WZ}^T)_{dn}]^2$$

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.

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

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

Training

- Stochastic Gradient Descent (SGD) ($\Theta(K)$ per step \rightarrow 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 $s_n = (w_1, w_2, \dots, w_m)$, let $\mathbf{x}_n \in \mathbb{R}^{|\mathcal{V}|}$ be the bag-of-words representation of the sentence.

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

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 $D = \text{vocabulary size}$
 - Binary classification: Predict if next word is real or fake (i.e. as in word2vec)
 - Impressive recent progress using large models, such as transformers
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