Problem Set 2, EE 150/CS 148a, Winter 2025

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1. (10 points) Dropout

   (a) (5 points) Dropout Equivalence to ℓ_2 Regularization

   Show that OLS Regression with dropout is equivalent to Ridge Regression by proving that the expected squared loss with dropout is of the following form:

$$E[L(w)] = \|y - f(p)Xw\|^2 + g(p)\|\Gamma w\|^2$$

   where $f(p)$ and $g(p)$ are functions of p, and Γ is a diagonal matrix with the standard deviations of features in data matrix X.

Solution: The expected OLS loss is

$$\mathbb{E}[\mathcal{L}(w)] = ||y - \mathbb{E}[Xw]||^2 + \mathbb{E}[||\mathbb{E}[Xw] - Xw||^2].$$

In dropout, we zero out each weight randomly. Thus, the predictions of a OLS model with dropout can be written as

$$\hat{y} = XMw,$$

where M is a mask matrix of size $D \times D$ where D is the dimension of the weights. M is an indentity matrix with the i-th diagonal value being 0 if w_i is zeroed out for dropout. Thus, the expected loss for OLS with dropout is

$$\mathbb{E}[\mathcal{L}(w)] = ||y - \mathbb{E}[XMw]||^2 + \mathbb{E}[||\mathbb{E}[XMw] - XMw||^2].$$

We know $\mathbb{E}[M] = \frac{1}{1-p}I$, where I is a $D \times D$ identity matrix. This is because each value along the diagonal is an independent Bernoulli random variable with probability of p of being 0 and $1 - p$ to be 1.

Computing the bias via linearity of expectation,

$$||y - \mathbb{E}[XMw]||^2 = ||y - X\mathbb{E}[M]w||^2 = ||y - (1-p)Xw||^2.$$

To compute the variance, we first substitute the expected value of the prediction:

$$\sigma^2 = \mathbb{E}[||\mathbb{E}[XMw] - XMw||^2] = \mathbb{E}[||(1-p)Xw - XMw||^2].$$

Now, we expand the expression inside the outer expected value using its quadratic form:

$$\begin{aligned}
\sigma^2 &= ||(1-p)Xw - XMw||^2 \\
&= ((1-p)Xw)^T((1-p)Xw) - 2((1-p)Xw)^T(XMw) + (XMw)^T(XMw) \\
&= (1-p)^2 w^T X^T Xw - 2(1-p)w^T X^T XMw + w^T M^T X^T XMw.
\end{aligned}$$

Computing the expected value,

$$\begin{aligned}\sigma^2 &= \mathbb{E}\left[(1-p)^2 w^T X^T X w - 2(1-p) w^T X^T X M w + w^T M^T X^T X M w\right] \\ &= (1-p)^2 w^T X^T X w - 2(1-p) w^T X^T X \mathbb{E}[M] w + \mathbb{E}[w^T M^T X^T X M w] \\ &= (1-p)^2 w^T X^T X w - 2(1-p)^2 w^T X^T X w + (1-p) w^T X^T X w.\end{aligned}$$

In the above computation, the last expected value in the second line is simplifies as such because the expected value of the square of a Bernoulli r.v. is the expected value of just the regular Bernoulli r.v.

We know that Γ, the standard deviation matrix, is the diagonal matrix with elements being the square root of the sum of the variances in each column of covariance matrix of X. Thus, $||w^T X^T X w|| = ||\Gamma w||^2$. Substituting this in,

$$\sigma^2 = (1-p)^2 ||\Gamma w|^2 - 2(1-p)^2 ||\Gamma w|^2 + (1-p)||\Gamma w|^2 = p(1-p)||\Gamma w||^2.$$

Thus, we have

$$E[L(w)] = \|y - f(p) X w\|^2 + g(p)\|\Gamma w\|^2,$$

where $f(p) = 1 - p$ and $g(p) = p(1-p)$

(b) (5 points) Dropout Code Create a copy of the Dropout Colab Notebook and rename it to Dropout {first name last name}.ipynb. Follow the instructions to generate a Loss vs. Dropout Rate plot.

Solution: colab link

2. (10 points) Batch Normalization

(a) (5 points) BatchNorm Backpropagation Given $\frac{\partial L}{\partial Y}$, derive expressions for:

- $\frac{\partial L}{\partial \beta}$
- $\frac{\partial L}{\partial \gamma}$
- $\frac{\partial L}{\partial X}$

Solution:

$$Y_{ij} = \gamma_j \hat{X}_{ij} + \beta_j \implies Y_i = \gamma^T \odot \hat{X}_i + \beta \implies \frac{\partial Y_i}{\partial \beta^T} = 1 \implies \frac{\partial \mathcal{L}}{\partial \beta} = \sum_{i=1}^{N} \left(\frac{\partial \mathcal{L}}{\partial Y_i}\right)^T$$

$$Y_{ij} = \gamma_j \hat{X}_{ij} + \beta_j \implies Y_i = \gamma^T \odot \hat{X}_i + \beta \implies \frac{\partial Y_i}{\partial \gamma^T} = \hat{X}_i \implies \frac{\partial \mathcal{L}}{\partial \gamma} = \sum_{i=1}^{N} \left(\frac{\partial \mathcal{L}}{\partial Y_i} \odot \hat{X}_i\right)^T$$

$$Y_{ij} = \gamma_j \hat{X}_{ij} + \beta_j \implies Y_i = \gamma^T \odot X_i + \beta \implies \frac{\partial Y_i}{\partial \hat{X}_i} = \gamma^T \implies \frac{\partial \mathcal{L}}{\partial \hat{X}} = \frac{\partial \mathcal{L}}{\partial Y} \odot \begin{bmatrix} \gamma^T \\ \vdots \\ \gamma^T \end{bmatrix}$$

Now, we know that $\hat{X}_{ij} = (X_{ij} - \mu_j)/\sqrt{\sigma_j^2 + \epsilon}$. Since μ_j, σ_j^2 are both functions of X_{ij}, we need to apply quotient rule and chain rule:

$$\frac{\partial \hat{X}_{ij}}{\partial X_{ij}} = \frac{s_j(X_{ij} - \mu_j)' - (X_{ij} - \mu_j)s_j'}{s_j^2}.$$

Here, s_j is $\sqrt{\sigma_j^2 + \epsilon}$. Computing the gradients, we have

$$\begin{aligned}
\mu_j' &= \frac{1}{N} \\
s_j' &= \frac{1}{2\sqrt{\sigma_j^2 + \epsilon}} \cdot \frac{\partial}{\partial X_{ij}}(\sigma_j^2 + \epsilon) \\
&= \frac{1}{2s_j} \cdot \frac{\partial}{\partial X_{ij}} \cdot \frac{1}{N} \cdot \sum_{k=1}^{N} (X_{kj} - \mu_j)^2 \\
&= \frac{1}{2s_j} \cdot \frac{2}{N} \cdot \sum_{k=1}^{N} (X_{kj} - \mu_j) \cdot \frac{\partial}{\partial X_{ij}}(X_{kj} - \mu_j) \\
&= \frac{1}{2s_j} \cdot \frac{2}{N} \cdot \left(X_{ij} - \mu_j + \sum_{k=1}^{N} (X_{kj} - \mu_j) \cdot \left(-\frac{1}{N} \right) \right) \\
&= \frac{1}{Ns_j} \cdot (X_{ij} - \mu_j).
\end{aligned}$$

In the above calculation for s_j', the summation for $k = 1, \ldots, N$ cancels out because the sums of the difference with a mean is 0. The extra $X_{ij} - \mu_j$ term comes from the fact that when $k = i$, the partial derivative of $(X_{ij} - \mu_j)$ w.r.t. X_{ij} is $1 - \mu_j'$.

Thus, for $\hat{X}_{ij}$, the derivative is

$$\begin{aligned}
\frac{\partial \hat{X}_{ij}}{\partial X_{ij}} &= \frac{s_j(1 - \frac{1}{N}) - (X_{ij} - \mu_j) \cdot \frac{1}{Ns_j}(X_{ij} - \mu_j)}{s_j^2} \\
&= \frac{1}{s_j} - \frac{1 + \hat{X}_{ij}^2}{Ns_j}.
\end{aligned}$$

However, we still have to account for the role X_{ij} plays in $\hat{X}_{kj}, k \neq i$ since X_{ij} is used in μ_j, s_j for those terms as well.

$$\begin{aligned}
\frac{\partial \hat{X}_{kj}}{\partial X_{ij}} &= \frac{s_j(X_{kj} - \mu_j)' - (X_{kj} - \mu_j)s_j'}{s_j^2} \\
&= \frac{s_j\left(-\frac{1}{N}\right) - (X_{kj} - \mu_j) \cdot \frac{1}{Ns_j}(X_{ij} - \mu_j)}{s_j^2} \\
&= -\frac{1 + \hat{X}_{kj}\hat{X}_{ij}}{Ns_j}.
\end{aligned}$$

Combining the derivatives from $\hat{X}_{kj}$ and $\hat{X}_{ij}$ with the values of $\frac{\partial \mathcal{L}}{\partial \hat{X}_{ij}}$,

$$\frac{\partial \mathcal{L}}{\partial X_{ij}} = \frac{1}{s_j} \cdot \frac{\partial \mathcal{L}}{\partial \hat{X}_{ij}} - \frac{1}{Ns_j} \sum_{k=1}^{N} \frac{\partial \mathcal{L}}{\partial \hat{X}_{kj}} - \frac{\hat{X}_{ij} \sum_{k=1}^{N} \hat{X}_{kj} \cdot \frac{\partial \mathcal{L}}{\partial \hat{X}_{kj}}}{Ns_j}.$$

Not sure if the TA reading this is looking for the OG Batchnorm paper derivation, so here's the comparision: essentially, in the sum above, the first term is the derivative that comes from the contribution of X_{ij} to every $\hat{X}_{ij}$, the second term is from the contribution of X_{ij} to every time the mean is used to compute an element in column j for $\hat{X}$, and the last term is the contribution of X_{ij} to every time the variance is used to compute an element in column j in $\hat{X}$. To put this into matrix form (as a product of a Jacobian of sorts with the matrix of $\frac{\partial L}{\partial \hat{X}}$, which we will now denote D), notice that the matrix corresponding to the first term is $\frac{1}{s_j} \odot (ID)$, where I is the identity matrix, the second term can be written as $-\frac{1}{Ns_j} \odot (\mathbf{1}D)$, where $\mathbf{1}$ is the matrix of all ones, and the last term corresponds to $\frac{1}{Ns_j} \odot \hat{X} \odot \Big(\mathbf{1} \cdot (\hat{X} \odot D)\Big)$. Thus, our gradient for the input is

$$\frac{\partial \mathcal{L}}{\partial X} = \frac{1}{s_j} \odot (I \frac{\partial \mathcal{L}}{\partial Y} \odot [\gamma^T]) - \frac{1}{Ns_j} \odot (\mathbf{1} \frac{\partial \mathcal{L}}{\partial Y} \odot [\gamma^T]) - \frac{1}{Ns_j} \odot \hat{X} \odot \left(\mathbf{1}(\hat{X} \odot \frac{\partial \mathcal{L}}{\partial Y} \odot [\gamma^T])\right).$$

In the equation above, $[\gamma^T]$ is the $N \times D$ matrix with its rows being γ^T.

(b) (5 points) Batch Normalization Code Implement BatchNorm from scratch and verify that your implementation matches PyTorch's built-in BatchNorm function.

Solution: colab link
Holy shit it actually works I didn't think my formula was right since it was different from the batchnorm paper's.

3. (15 points) Layer Normalization

(a) (5 points) LayerNorm Backpropagation Given $\frac{\partial L}{\partial Y}$, derive expressions for:

- $\frac{\partial L}{\partial \beta}$
- $\frac{\partial L}{\partial \gamma}$
- $\frac{\partial L}{\partial X}$

Solution: There's no change for β and γ since the dimensions for those are still the same.

$$Y_{ij} = \gamma_j \hat{X}_{ij} + \beta_j \implies Y_i = \gamma^T \odot \hat{X}_i + \beta \implies \frac{\partial Y_i}{\partial \beta^T} = 1 \implies \frac{\partial \mathcal{L}}{\partial \beta} = \sum_{i=1}^{N} \left(\frac{\partial \mathcal{L}}{\partial Y_i}\right)^T$$

$$Y_{ij} = \gamma_j \hat{X}_{ij} + \beta_j \implies Y_i = \gamma^T \odot \hat{X}_i + \beta \implies \frac{\partial Y_i}{\partial \gamma^T} = \hat{X}_i \implies \frac{\partial \mathcal{L}}{\partial \gamma} = \sum_{i=1}^{N} \left(\frac{\partial \mathcal{L}}{\partial Y_i} \odot \hat{X}_i\right)^T$$

$$Y_{ij} = \gamma_j \hat{X}_{ij} + \beta_j \implies Y_i = \gamma^T \odot X_i + \beta \implies \frac{\partial Y_i}{\partial \hat{X}_i} = \gamma^T \implies \frac{\partial \mathcal{L}}{\partial \hat{X}} = \frac{\partial \mathcal{L}}{\partial Y} \odot \begin{bmatrix} \gamma^T \\ \vdots \\ \gamma^T \end{bmatrix}$$

As for X, since it's analagous to the transposed version of batchnorm, if we sum from $j = 1 \dots D$, we should have the correct formulas for layernorm backprop. Notice that we also commute any matrix multiplications since we want it over the D dimension this time, not the N dimension.

$$\frac{\partial \mathcal{L}}{\partial X} = \frac{1}{s_i} \odot (\frac{\partial \mathcal{L}}{\partial Y} I \odot [\gamma^T]) - \frac{1}{Ns_i} \odot (\frac{\partial \mathcal{L}}{\partial Y} \mathbf{1} \odot [\gamma^T]) - \frac{1}{Ns_i} \odot \hat{X} \odot \left((\hat{X} \odot \frac{\partial \mathcal{L}}{\partial Y} \odot [\gamma^T])\mathbf{1}\right).$$

(b) (5 points) Layer Normalization Code Implement LayerNorm from scratch and verify correctness against PyTorch's built-in LayerNorm.

Solution: colab link

(c) (5 points) BatchNorm LayerNorm Puzzle Bob has access to Y from BatchNorm. How many elements in Z (LayerNorm output) does Bob know with certainty if X is symmetric?

Solution: For any γ, β, all of them. If the matrix is symmetric, then the mean and variance across the batch and feature dimensions are the same. Thus, the normalization without the affine transformation across the layer and batch dimensions are the same. Then, applying the affine transformation doesn't change anything since the outputs of the normalization are the same.

4. (40 points) Regularization, Optimizers, and Augmentation in MNIST

(a) (10 points) Regularization

1. Plot the distribution of weights of a newly initialized model. Let X be a random variable that is the value of a parameter chosen at random from our uninitialized model. Write an expression for the PDF of X. Why is it beneficial for the standard deviation of the initial distribution of a layer to decrease as layer width increases?
2. Plot the distribution of weights of a model trained using SGD. Qualitatively, what is the new distribution of weights?
3. Now plot the distribution of weights of a model trained using SGD and weight decay 0.01. Qualitatively, what changed about the distribution? In theory, why should this help a model's ability to generalize to unseen data?
4. ℓ_2 regularization on weights (not to be confused with ℓ_2 regularization on model outputs) and weight decay are often used interchangeably, but they are in fact distinct methods. Prove that for standard SGD, ℓ_2 regularization and weight decay are equivalent.
   Weight decay update:
   $$w_{t+1} \leftarrow w_t - (\nabla_w L + \lambda_{\text{weight decay}} w_t)$$
   ℓ_2 regularized update:
   $$w_{t+1} \leftarrow w_t - (\nabla_w L)$$
   where
   $$L = \lambda_{\ell_2} \sum_i w_i^2$$
5. Use your solution from part (d) to run SGD with ℓ_2 regularization with the ℓ_2 lambda that would make it equivalent to SGD with weight decay 0.01. How does the distribution of weights compare to part (c)?

Solution: colab
The distribution of new weights is the sum of multiple uniform distributions. The pdf is roughly

$$p(x) \approx \begin{cases} 0.03 & \text{if } x \in (-0.5, 0.5) \\ 0.14 & \text{if } x \in [-0.1, -0.05] \cup [0.05, 0.1] \end{cases}.$$

It makes sense for the the standard deviation of the initial distribution of a layer to decrease as layer width increases to make the next layer doesn't have an insanely high variance/standard deviation.

The distribution of weights trained with SGD is normal. In theory, this makes sense since naturally occuring data generally follows a uniform distribution.

ℓ_2 regularization and and weight decay are the same because the gradient of the sum of the squares of the weights is just the current weights times 2. Thus, the $\lambda_{\ell_2} = \frac{1}{2}\lambda_{\text{weight decay}}$. The distribution of the weights is the same.

(b) (15 points) Optimizers:

1. Derive the bias correction term $\frac{1}{1-\beta^t}$ for the Adam optimizer and show that it is necessary to un-bias the estimates for the first and second moments.
2. Explain why adding an ℓ_2 regularization penalty to the loss is problematic when using SGD with momentum. Discuss its effect when using RMSProp and Adam optimizers.
3. Explain how AdamW correctly penalizes weights in contrast with Adam.
4. Run the following and report the validation accuracies. Which two methods perform best? Why do the others perform worse?
   - Adam, default
   - Adam, ℓ_2 lambda=0.005
   - Adam, weight decay=0.01
   - AdamW, ℓ_2 lambda=0.005
   - AdamW, weight decay=0.01

Solution: The formula for the moment are

$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t$$
$$v_t = \beta_2 m_{t-1} + (1-\beta_2) g_t^2$$
.

Rewriting this non-recursively as a sum of terms,

$$m_t = (1-\beta_1) \sum_{i=1}^{t} \beta_1^{t-i} g_i$$
$$v_t = (1-\beta_2) \sum_{i=1}^{t} \beta_2^{t-i} g_i^2$$
.

Taking the expecvted value,

$$\mathbb{E}[m_t] = \mathbb{E}\left[(1-\beta_1) \sum_{i=1}^{t} B_1^{t-i} g_i\right]$$
$$\mathbb{E}[v_t] = \mathbb{E}\left[(1-\beta_2) \sum_{i=1}^{t} \beta_2^{t-i} g_i^2\right]$$
.

As the model converges, g_i becomes more stable and $g_i \to \mathbb{E}[g]$, the expected value becomes

$$\mathbb{E}[m_t] = (1-\beta_1)\sum_{i=1}^{t} B_1^{t-i}\mathbb{E}[g]$$
$$\mathbb{E}[v_t] = (1-\beta_2)\sum_{i=1}^{t} \beta_2^{t-i}\mathbb{E}[g^2]$$

.

Since we can estimate the expected values related to the gradients as constants, we can take them out and sum the geometric series:

$$\begin{aligned}\mathbb{E}[m_t] &= (1-\beta_1)\frac{1-\beta_1^t}{1-\beta_1}\mathbb{E}[g] \\ &= (1-\beta_1^t)\mathbb{E}[g] \\ \mathbb{E}[v_t] &= (1-\beta_2)\frac{1-\beta_2^t}{1-\beta_2}\mathbb{E}[g^2] \\ &= (1-\beta_2^t)\mathbb{E}[g^2].\end{aligned}$$

m_t and v_t are supposed to be moving averages of the gradient and gradient squared, but clearly their expected value is biased by a factor of $(1-\beta_1^t)$ and $(1-\beta_2^t)$. Thus, to unbias them, we need to multiply them by $\frac{1}{1-\beta_1^t}$ and $\frac{1}{1-\beta_2^t}$.

Adding ℓ_2 regularization penalty to the loss whne using SGD with momentum, RMSProp, and Adam is problematic because the penalty term creates a gradient that is not related to the training error when these optimizers calculate the moving average for momentum. AdamW correctly penalizes weights because separates the calculation for weight decay from loss by simply removing a scalar factor of the weights during the update rule instead of using the ℓ_2 penalty term.

Colab

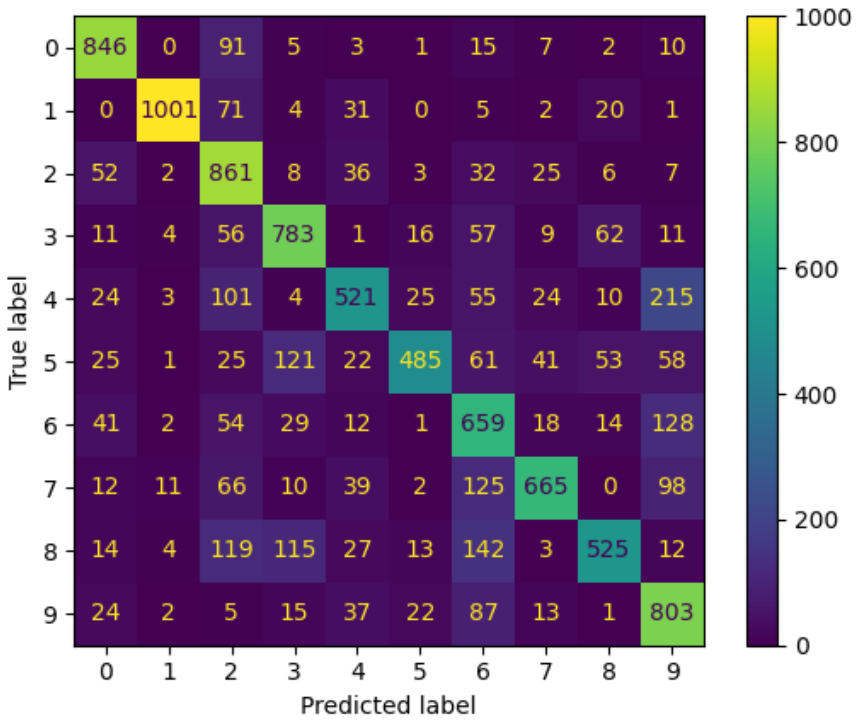
Using Adam with no weight decay or regularization worked best, but using AdamW with weight decay worked the best since AdamW accounts for momentum when using weight decay. AdamW does this by performing the weight decay updated and the momentum update separately, not by backpropagating the weight decay term as a gradient of the loss. Thus, the gradient from the L2 loss is not factored in when it computes the momentum.

(c) (15 points) Data Augmentation:

1. Implement methods for common image transformations: rotations, translations, blurring, scaling, shear, and Gaussian noise addition.
2. Display the effects of each augmentation using one example for each digit (0-9). Ensure augmented images remain recognizable.
3. Evaluate augmentation effects on performance:
   - Train a model on the small dataset and note validation accuracy.
   - Apply different augmentation strengths and train models to report:
     - Augmentation that decreases accuracy by $\leq 1\%$.
     - Augmentation that decreases accuracy by $1-3\%$.
     - Augmentation that decreases accuracy by $\geq 3\%$.
4. Investigate rotation range impact by setting $(-180, 180)$ and analyze misclassifications via a confusion matrix.

5. Develop a method to randomly apply augmentations to scale the dataset to 50,000 images. Train models and report validation accuracy for:
   - Small dataset (5,000 images).
   - Small dataset copied 10 times (50,000 images).
   - Augmented dataset (50,000 images).
   - Original dataset (50,000 images).

Solution: colab



The most misclassified numbers are 4 and 9, with 6 and 9 being the second most misclassified (I'm summing up the matrix with its transpose and subtracting diagonal).

5. (25 points) Word2Vec

   (a) (10 points) Implement CBOW Implement and train the Continuous Bag of Words (CBOW) model on the Shakespeare dataset.

   Solution: colab link

   (b) (15 points) Semantically Similar Clusters Find clusters of words that exhibit semantic similarity based on trained embeddings.

   Solution:

   - **my** (1.0), **his** (0.34), **your** (0.33), **thy** (0.31), **lawrence'** (0.28), **our** (0.27), **the** (0.26), **sicilian** (0.26), **hastings'** (0.24), **her** (0.23)
   - **brother** (1.0), **nunnery** (0.26), **son** (0.24), **sheepshearing** (0.22), **brother's** (0.21), **crutch** (0.21), **sons** (0.21), **beck** (0.2), **cow** (0.2), **daughter** (0.2)

- **slay** (1.0), **kill** (0.27), **submit** (0.27), **expose** (0.25), **railed** (0.25), **fade** (0.25), **practise** (0.25), **dardanius** (0.24), **guide** (0.24), **according** (0.24)
- **shall** (1.0), **will** (0.28), **blithe** (0.26), **longed** (0.26), **should** (0.25), **if't** (0.23), **may** (0.23), **can** (0.22), **would** (0.22), **tumbled** (0.22)
- **people** (1.0), **ground** (0.28), **forum** (0.26), **members** (0.24), **multitudes** (0.23), **ambassadors** (0.22), **wing** (0.22), **disciplines** (0.22), **lights** (0.21), **complaint** (0.21)
- **senator** (1.0), **bout** (0.26), **fisherman** (0.25), **soldier** (0.25), **citizen** (0.25), **witch** (0.24), **watch** (0.22), **singly** (0.21), **gentleman** (0.21), **exploits** (0.21)
- **prevail** (1.0), **attain** (0.29), **detain** (0.29), **peruse** (0.29), **meddle** (0.28), **mix'd** (0.27), **oaks** (0.26), **o'ertake** (0.26), **befall** (0.26), **surrender** (0.25)
- **man** (1.0), **man"** (0.29), **squire** (0.26), **carcass** (0.26), **snail** (0.25), **pig** (0.24), **sincerity** (0.24), **breeder** (0.24), **ducat** (0.24), **woman** (0.23)
- **horse** (1.0), **mare** (0.27), **crutch** (0.25), **club** (0.23), **sword** (0.23), **beaver** (0.22), **bounties** (0.22), **tribe** (0.21), **reference** (0.21), **team** (0.21)
- **dishonest** (1.0), **wiser** (0.29), **wight** (0.29), **wellfavoured** (0.29), **recount** (0.28), **drench** (0.27), **respite** (0.27), **ides** (0.26), **sentry** (0.25), **cutpurse** (0.25)