Iterative Approximate Cross Validation in High Dimensions

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Section 1

Background

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General Problem Setting

- Input space $\mathcal{X}$ and an output space $\mathcal{Y}$.
- Data is "generated" by a *true* distribution $P(\mathcal{X}, \mathcal{Y})$.
- Find a mapping $h : \mathcal{X} \to \mathcal{Y}$ (called a hypothesis).
- All possible combinations of input and output space are $\mathcal{D} = \{(X, Y) \in (\mathcal{X}, \mathcal{Y})\}$.

Risk

To measure the error (or loss) we make on a data point, define a function $\ell(h; D_i)$,

$$\ell(h; D) = \sum_{i=1}^{n} \ell(h; D_i) \text{ where } D_i = (X_i, Y_i).$$

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Risk

Define the **risk** of a hypothesis for the complete space of inputs and outputs as,

$$R(h) = \mathbb{E}_{\mathcal{X},\mathcal{Y}}[\ell(h; \mathcal{D})].$$

We define **empirical risk** of a hypothesis given data D as,

$$R_{\text{emp}}(h; D) = \ell(h; D).$$

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Regularised Empirical Risk

To restrict the hypothesis space, we define the formulation of **regularised empirical risk** as,

$$R_{\text{reg}}(h; D) = R_{\text{emp}}(h; D) + \lambda\pi(\theta).$$

$\pi : \mathbb{R}^p \to \mathbb{R}$ is a regulariser and $\lambda \in \mathbb{R}^+$ is controls the strength of regularisation.

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Leave One Out Cross Validation (LOOCV) is effective [1], but costly.

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Section 2

Literature Review

Approximate CV Methods

To reduce the computational cost LOOCV, we turn to Approximate Cross Validation (ACV).

LOOCV

The definition of leave-one-out (LOO) regularised empirical risk is,

$$R_{\text{reg}}(\theta; D_{-j}) = \sum_{i=1,\, i \neq j}^{n} \ell(\theta; D_i) + \lambda \pi(\theta)$$

where we leave out a point with index j for this experiment.

Methods for ACV

There are three main methods for ACV in the literature.

- Newton Step ("NS")
- Infinitesimal Jackknife ("IJ")
- Iterative Approximate Cross Validation ("IACV")

both NS and IJ are existing methods, and IACV is a new proposed method which we aim to adapt and extend.

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We present a short summary of the theory behind these approximations.

Newton Step

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For discussion, the standard notation we use for the NS method is,

$$\tilde{\theta}_{\mathsf{NS}}^{-i} = \hat{\theta} + \Big(H(\hat{\theta}; D) - \nabla_{\theta}^{2}\ell(\hat{\theta}; D_i)\Big)^{-1} \nabla_{\theta} R_{\mathsf{reg}}(\hat{\theta}; D_i)$$

The quality of the approximation depends heavily on the fact that $\hat{\theta} \approx \theta^{*}$.

Infinitesimal Jackknife

The general idea is again to perform a first-order Taylor expansion to approximate LOOCV, around the weights of a Jackknife.

The final form derived for this case is

$$\tilde{\theta}_{\mathsf{IJ}}^{-i} = \hat{\theta} + (H(\hat{\theta}; D))^{-1} \nabla_\theta R_{\mathsf{reg}}(\hat{\theta}; D_i)$$

with the same assumptions as in NS (loss and regularisation are continuously twice-differentiable, H is invertible and $\hat{\theta} \approx \theta^*$).

Iterative Approximate Cross Validation

Iterative Approximate Cross Validation (IACV) relaxes the assumptions of previous methods.

We solve the main learning task through updates,

$$\hat{\theta}^{(k)} = \hat{\theta}^{(k-1)} - \alpha_k \nabla_\theta R_{\text{reg}}(\hat{\theta}^{(k-1)}; D_{S_k})$$

for $S_k \subseteq [n]$ as a subset of indices and α_k.

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The LOO update excluding a point i is defined as,

$$\hat{\theta}_{-i}^{(k)} = \hat{\theta}_{-i}^{(k-1)} - \alpha_k \nabla_\theta R_{\text{reg}}(\hat{\theta}_{-i}^{(k-1)}; D_{S_k \setminus i})$$

this step is what we aim to approximate.

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$$\nabla_\theta R_{\text{reg}}(\hat{\theta}_{-i}^{(k-1)}; D_{S_k \setminus i}) \approx \underbrace{\nabla_\theta R_{\text{reg}}(\hat{\theta}^{(k-1)}; D_{S_k \setminus i}) + \nabla_\theta^2 R_{\text{reg}}(\hat{\theta}^{(k-1)}; D_{S_k \setminus i}) \left(\tilde{\theta}_{-i}^{(k-1)} - \hat{\theta}^{(k-1)}\right)}_{\tilde{J}_{-i}^{(k)}}$$

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We swap a Jacobian for a Jacobian *and* a Hessian in the approximation step.

[2]Y. Luo, Ren, and Barber (2023)

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	IACV	Exact LOOCV
GD	$n(A_p + B_p) + np^2$	$n^2 A_p + np$
SGD	$K(A_p + B_p) + np^2$	$nKA_p + np$
ProxGD	$n(A_p + B_p + D_p) + np^2$	$n^2 A_p + nD_p + np$

where A_p is one evaluation of the Jacobian, B_p is one evaluation of the Hessian, D_p is one evaluation of the proximal operator and K is the size of the subset used for SGD [2].

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where A_p is one evaluation of the Jacobian, B_p is one evaluation of the Hessian, D_p is one evaluation of the proximal operator and K is the size of the subset used for SGD [2].

We can however parallelise calculations while keeping $\hat{\theta}^{(k-1)}$ fixed for a measurable speedup.

[2] Y. Luo, Ren, and Barber (2023)

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$$\mathsf{Err}_{\mathsf{Approx}} = \frac{1}{n}\sum_{i=1}^{n} \|\tilde{\theta}_{-i}^{(k)} - \hat{\theta}_{-i}^{(k)}\|_2^2$$

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The standard dataset $D = \{(X_i, Y_i)\}_{i=1}^n$ for $X_i \in \mathbb{R}^p$ and $Y_i \in \{0, 1\}$ is generated by

$$Y_i \sim \text{Bernoulli}\left(\frac{1}{1+\exp(-X_i^T\theta^*)}\right)$$

for $\theta^* \in \mathbb{R}^p$ with 5 non-zero entries.

We recreate the experiment shown in the paper ($n = 250, p = 20$) as a sanity check of the Python implementation.

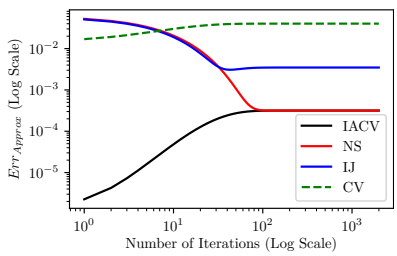

Figure 1: My implementation (run for less iterations).

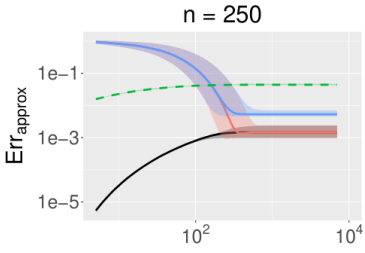

Figure 2: Experiment in the paper.

The 'baseline' we measure is using $\hat{\theta}^{(k)}$ as LOOCV estimates.

Gaps in the Literature

There are current gaps in the literature that we aim to address.

- Problems in high dimensions
- Lack of standard (or optimised) Python implementation of IACV
- No application of ACV to non GLM settings
- No attempt at applying ACV to models without a Hessian

Smooth Hinge Loss

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We therefore seek a smooth approximation which is twice-differentiable to model the same problem an apply ACV for a fast approximation of true risk.

The paper (J. Luo, Qiao, and Zhang 2021), introduces a Smooth Hinge Loss of the form

$$\psi_M(z;\sigma) = \Phi_M(v)(1-z) + \phi_M(v)\sigma,$$

where $v = (1-z)/\sigma$ and $\sigma > 0$ controls the *smoothness* of the loss.

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where $v = (1-z)/\sigma$ and $\sigma > 0$ controls the *smoothness* of the loss.

The individual functions which make up the loss are,

$$\Phi_M(v) = \frac{1}{2}\left(1 + \frac{v}{\sqrt{1+v^2}}\right),$$
$$\phi_M(v) = \frac{1}{2\sqrt{1+v^2}}.$$

We then use this loss to define the main objective,

$$L(w; D, \sigma) = \frac{\lambda}{2}\|w\|_2^2 + \frac{1}{n}\sum_{i=1}^{n} \psi_M(Y_i w^T X_i; \sigma)$$

where λ controls the size of the margin.

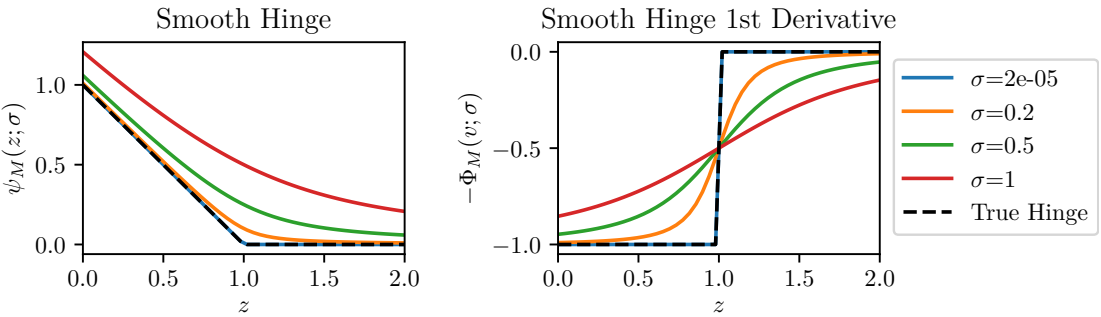

Figure 3: Smooth Hinge and its derivative for varying σ. Values for the original hinge loss are shown dotted.

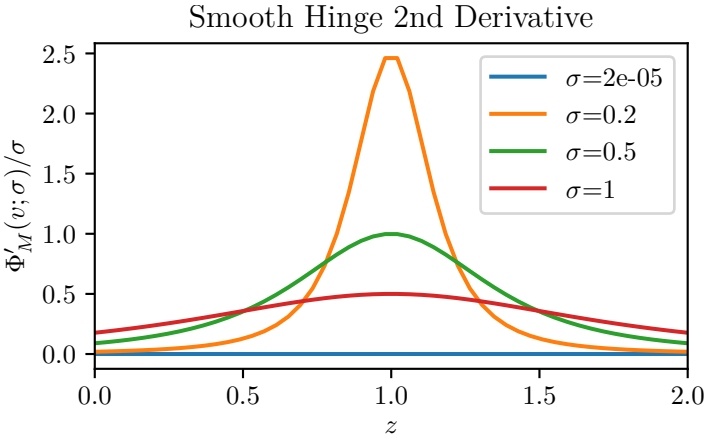

Figure 4: Second derivative of smooth hinge loss.

We can solve the Smooth SVM problem with GD and achieve results similar to solving SVM using QP (libsvm).

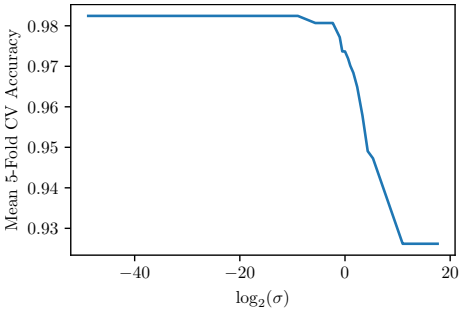

Figure 5: 5-Fold Accuracy of Smooth SVM solved using GD.

libsvm achieves a mean 97.88% accuracy on the same dataset (breast cancer binary classification from scikit-learn [3]).

[3] Pedregosa et al. (2011)

Section 3

Contributions

ACV Applied to Smooth Hinge

Previous attempts at applying ACV to problems without a Hessian are lacking. The Smooth SVM problem allows for ACV through its Hessian approximation.

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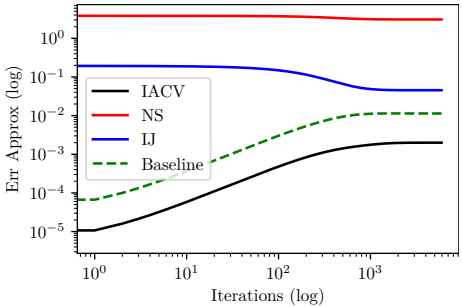

Figure 6: $\text{Err}_{\text{Approx}}$ for NS, IJ and IACV in the Smooth SVM problem ($\sigma = 0.5$ and $\lambda = 1$).

Why IACV?

- Less overall assumptions to satisfy.
- Accuracy before and at convergence. $\hat{w} \approx w^*$ not necessary.
- Per-iteration control of approximation.

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It's not that simple!

Main Result

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- **Assumption 1:** the LOO Hessian is well-conditioned.
- **Assumption 2:** the LOO Jacobian is bounded along the convergence path.
- **Assumption 3:** the LOO Hessian is $n\gamma-$Lipschitz.

The Smooth SVM problem satisfies Assumptions 2 and 3, though we need to find when Assumption 1 holds.

To investigate Assumption 1, we define the condition number. The LOO Hessian is provably positive-definite and symmetric, so we can use this bound.

Condition Number

For a positive-definite symmetric matrix $A \in \mathbb{R}^{n \times n}$, the condition number $\kappa(A)$ is defined as

$$\kappa(A) = \|A\|\|A^{-1}\| = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}.$$

We now present the main result.

Bound for LOO Hessian Condition Number

The condition number of the leave-one-out Hessian for the smooth SVM problem is bound by,

$$\kappa(\nabla_w^2 L(w; D_{-i}, \sigma)) \leq 1 + \frac{C}{\lambda\sigma} \cdot \frac{1}{2\sqrt{1 + \left(\frac{m_j}{\sigma}\right)^2}^3},$$

for $C = \|\tilde{X}^T \tilde{X}\|/(n-1)$ where $m_j = (1 - Y_j w^T X_j)$ is derived from the term

$$\max_j d_j = \max_j \Phi'_M((1 - Y_j w^T X_j)/\sigma)/\sigma.$$

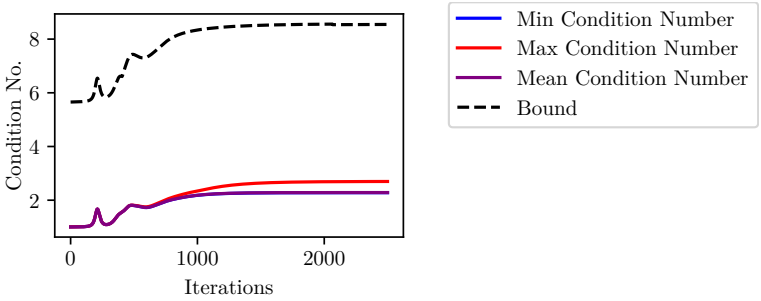

Figure 7: Bound along condition numbers across convergence path. ($\sigma = 0.1, \lambda = 1$)

To use this bound, we can find an optimal λ for a given σ for a well-conditioned LOO Hessian.

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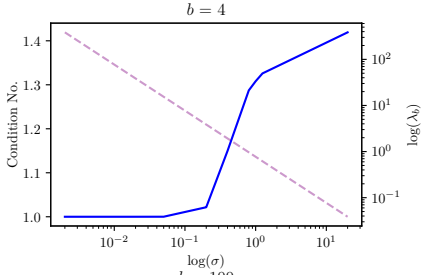
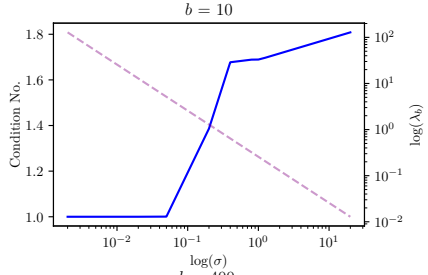
$$\lambda_b = \frac{C_f}{(b-1)\sigma} \cdot \frac{1}{2\sqrt{1 + \left(\frac{m^*}{\sigma}\right)^2}^3},$$

for a well-conditioned LOO Hessian. Here, $C_f = \|X^T X\|/(n-1)$ and m^* is a small constant close to 0.


$b = 4$
Condition No.
$\log(\lambda_6)$
$\log(\sigma)$


$b = 10$
Condition No.
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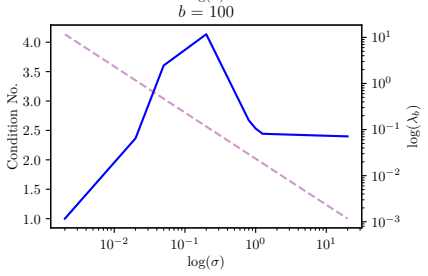
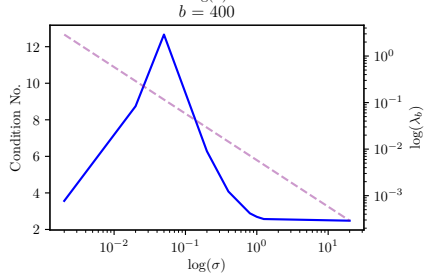

$b = 100$
Condition No.
$\log(\lambda_6)$
$\log(\sigma)$


$b = 400$
Condition No.
$\log(\lambda_6)$
$\log(\sigma)$

Does the bound work in improving IACV accuracy?

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Yes! This is an experiment run for $\sigma = 1 \times 10^{-10}$, picking an optimistic bound of $b = 1 \times 10^{10}$ when picking λ_b.

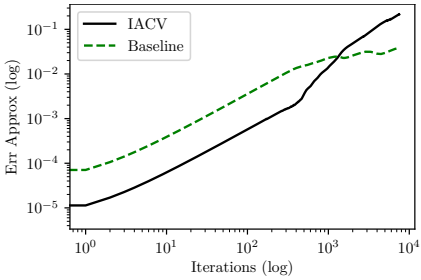

Figure 8: $\text{Err}_{\text{Approx}}$ when choosing $\lambda = 1$.

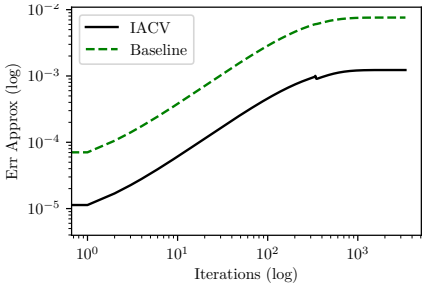

Figure 9: $\text{Err}_{\text{Approx}}$ when choosing $\lambda = \lambda_b$.

What do the condition numbers look like?

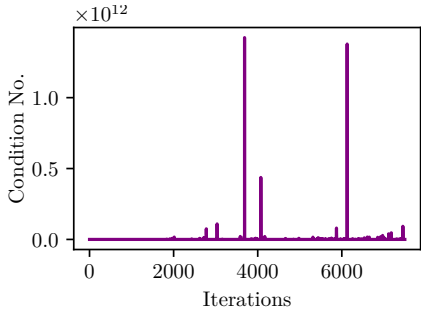

Figure 10: Condition number when choosing $\lambda = 1$.

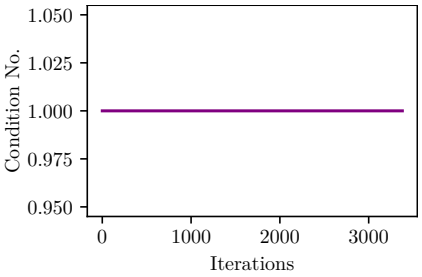

Figure 11: Condition number when choosing $\lambda = \lambda_b$.

Does choosing λ_b impact the overall quality of the model?

Does choosing λ_b impact the overall quality of the model?

Only slightly.

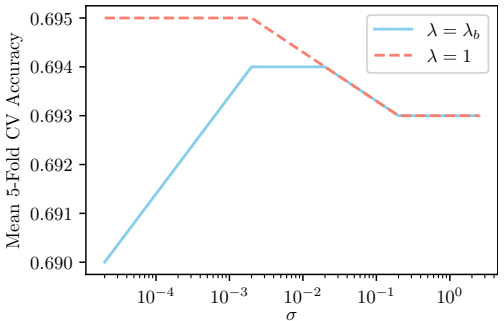

Figure 12: Accuracy for $\sigma = 0.1$ when picking $\lambda = 1$ and $\lambda = \lambda_b$.

To affirm the theory, we run a sensitivity study for both σ and λ. For the tests, we keep $\lambda = 1$ and $\sigma = 0.25$ fixed respectively.

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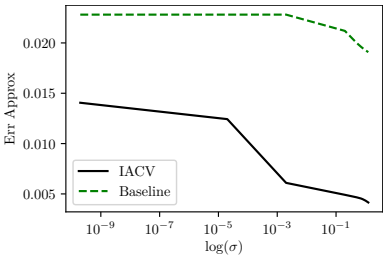


Figure 13: $\text{Err}_{\text{Approx}}$ for varying σ.

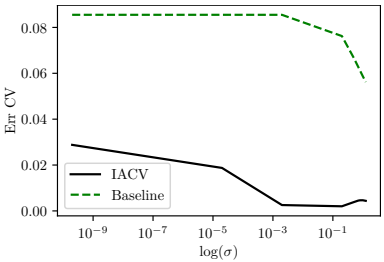


Figure 14: Err_{CV} for varying σ.

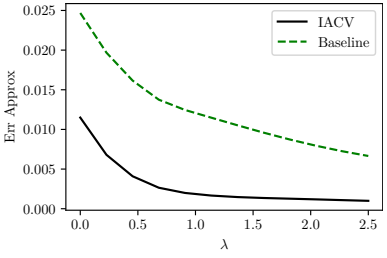


Figure 15: $\text{Err}_{\text{Approx}}$ for varying λ.

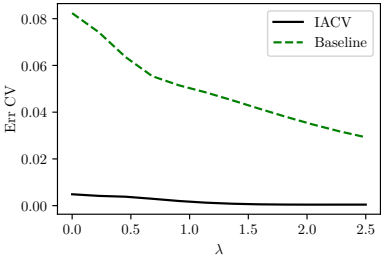


Figure 16: Err_{CV} for varying λ.

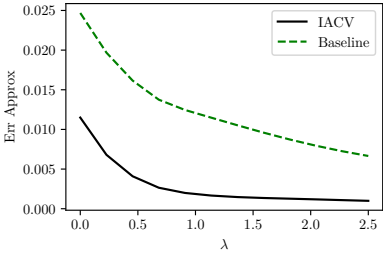


Figure 15: $\text{Err}_{\text{Approx}}$ for varying λ.

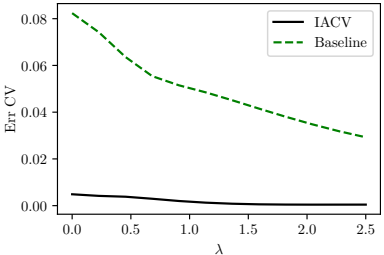
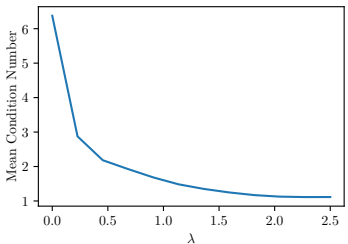


Figure 16: Err_{CV} for varying λ.



Python Implementation

How do we use it?

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```
self.approx_cv_obj = IACV(
    self.n,
    self.p,
    p_nabla,
    p_hess,
    p_nabla_single,
    p_hess_single,
    eta,
    calc_update=self.smooth_svm_calc_update,
)
```

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```
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    p_hess,
    p_nabla_single,
    p_hess_single,
    eta,
    calc_update=self.smooth_svm_calc_update,
)
```
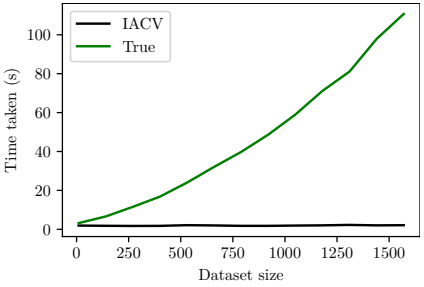

```
for t in range(n_iter):
    if approx_cv == True:
        if "IACV" in approx_cv_types:
            self.approx_cv_obj.step_gd(
                self.weights_, X, y, sav
            )
```

The underlying implementation uses JAX, making liberal use of vmap and jit to speed up runtime.



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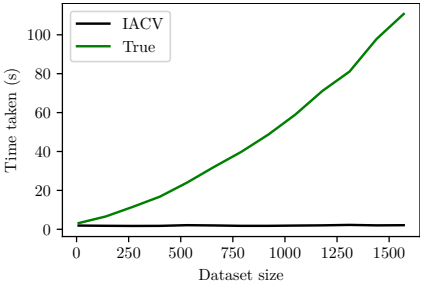
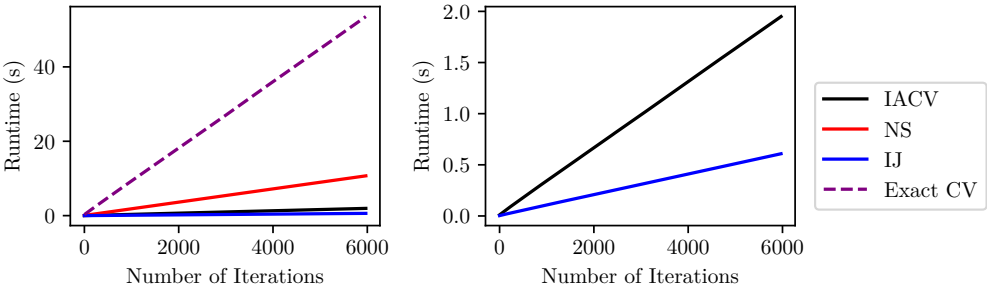
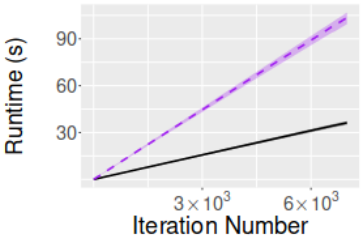


$$\tilde{\theta}_{-i}^{(k)} = \tilde{\theta}_{-i}^{(k-1)} - \alpha_k \left(\nabla_\theta R_{\text{reg}}(\hat{\theta}^{(k-1)}; D_{S_k \setminus i}) + \nabla_\theta^2 R_{\text{reg}}(\hat{\theta}^{(k-1)}; D_{S_k \setminus i}) \left(\tilde{\theta}_{-i}^{(k-1)} - \hat{\theta}^{(k-1)} \right) \right)$$

Improves on existing implementation by an order of magnitude.





Kernelising Smooth SVM

We can kernelise the smooth SVM by substituting $w = \phi(X) \cdot u$ for $u \in \mathbb{R}^n$,

$$L(u; D, \sigma) = \frac{\lambda}{2} u^T G u + \frac{1}{n} \sum_{i=1}^{n} \psi_M(Y_i G_i u; \sigma)$$

where G is the Gram matrix.

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where G is the Gram matrix.

This gives us non-linearity through the feature map $\phi : \mathbb{R}^p \to \mathbb{R}^d$ where $d > p$. **How does kernelisation impact IACV?**

The bound for the condition number in this case is,

$$\kappa(\nabla_u^2 L(u; D_{-i}, \sigma)) \leq \frac{\|\tilde{G}^{-1}\| \left(\lambda \|\tilde{G}\| + C_k B_k\right)}{\lambda}$$

where $C_k = \|\tilde{G}^T \tilde{G}\|/(n-1)$ and $B_k = 1/\left(2\sigma\sqrt{1 + (\frac{m^*}{\sigma})^2}^3\right)$.

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where $C_k = \|\tilde{G}^T \tilde{G}\|/(n-1)$ and $B_k = 1/\left(2\sigma\sqrt{1 + (\frac{m^*}{\sigma})^2}^3\right)$.

Assumptions 2 and 3 hold similar to the linear SVM case.

The condition number is much less sensitive to change based on σ and depends mostly on λ.

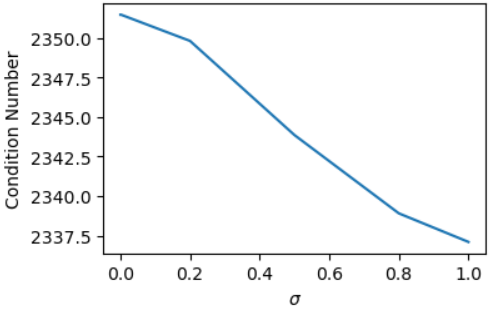


Figure 17: Kernel SVM.

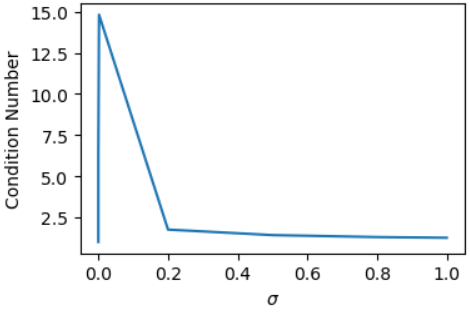


Figure 18: Linear SVM.

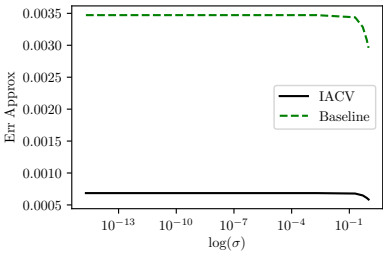


Figure 19: $\text{Err}_{\text{Approx}}$ for varying σ.

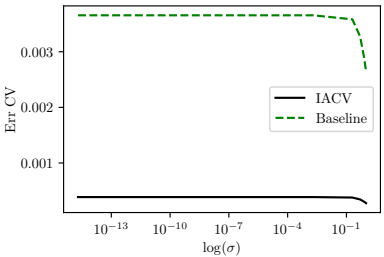


Figure 20: Err_{CV} for varying σ.

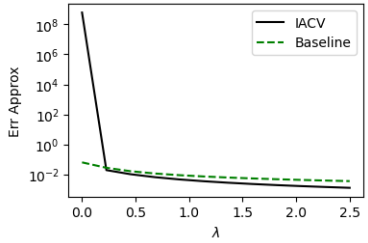


Figure 21: $\text{Err}_{\text{Approx}}$ for varying λ.

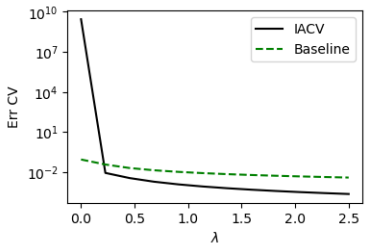
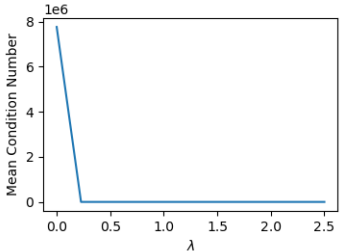


Figure 22: Err_{CV} for varying λ.



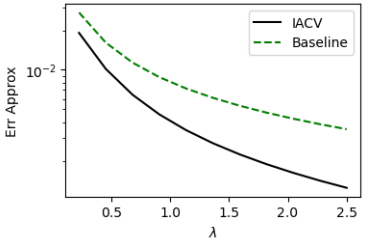


Figure 23: $\text{Err}_{\text{Approx}}$ for varying λ.

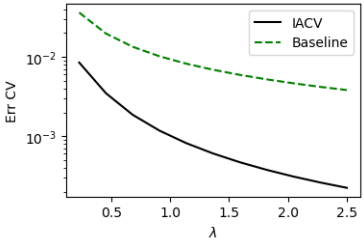
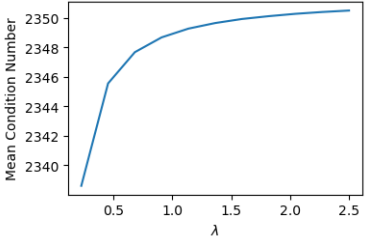


Figure 24: Err_{CV} for varying λ.



Section 4

Conclusion & Further Work

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Unfortunately, the original goal of applications to high dimensional problems was not fruitful.

In this thesis, we've explored ACV (specifically IACV) in a setting where an explicit Hessian does not exist without smoothing by applying it to Smooth SVM.

Conclusion & Further Work

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In this thesis, we've explored ACV (specifically IACV) in a setting where an explicit Hessian does not exist without smoothing by applying it to Smooth SVM.

- Analysis of IACV on similar smoothed problems
  - Smoothed ReLU
- IACV in a non-convex setting
- Is IACV is high dimensions feasible?

Section 5

Bibliography

Bibliography

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