Motivation: Structured Prediction

Classical supervised learning:

Input: P

Output: "P"
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Input: \( P \)

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Structured prediction:

Input: \( \text{Paris} \)

Output: "Paris"
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Structured prediction:

Input: Paris

Output: "Paris"

Other structure prediction tasks:

- Labelling all people/places in Wikipedia, finding coding regions in DNA sequences, labelling all voxels in an MRI as normal or tumor, predicting protein structure from sequence, weather forecasting, translating from French to English, etc.
Naive approaches to predicting letters $y$ given images $x$:

- **Multinomial logistic regression** to predict word:

  $$ p(y|x, w) = \frac{\exp(w^T_y F(x))}{\sum_{y'} \exp(w^T_{y'} F(x))}. $$
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This requires parameter vector $w_k$ for all possible words $k$. 

- For each letter:

  $$p(y_j|x_j, w) = \frac{\exp(w_{y_j}^T F(x_j))}{\sum_{y'_j} \exp(w_{y'_j}^T F(x_j))}.$$ 

This works if you are really good at predicting individual letters. But this ignores dependencies between letters.
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- What letter is this?
Motivation: Structured Prediction

- What letter is this?
  
  \[ \text{Y} \]

- What are these letters?
  
  \[ \text{Vancouver} \]
Conditional random fields model targets $y$ given inputs $x$ using

$$p(y|x, w) = \frac{\exp(w^T F(y, x))}{\sum_{y'} \exp(w^T F(y', x))} = \frac{\exp(w^T F(y, x))}{Z},$$

where $w$ are the parameters.

Examples of features $F(y, x)$:
- $F(y_j, x)$: these features lead to a logistic model for each letter.
- $F(y_{j-1}, y_j, x)$: dependency between adjacent letters ('q-u').
- $F(y_{j-1}, y_j, j, x)$: position-based dependency (French: 'e-r' ending).
- $F(y_{j-2}, y_{j-1}, y_j, j, x)$: third-order and position (English: 'i-n-g' ending).
- $F(y \in D, x)$: is $y$ in dictionary $D$?

CRFs are a ubiquitous tool in natural language processing: Part-of-speech tagging, semantic role labelling, information extraction, shallow parsing, named-entity recognition, etc.
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Typically train using $\ell_2$-regularized negative log-likelihood:

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Optimization Formulation and Challenge

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- Bad news: evaluating $\log p(y_i|x_i, w)$ and its gradient is expensive.
  - Chain-structures: run forward-backward on each example.
  - General features: exponential in tree-width of dependency graph.
  - A lot of work on approximate evaluation.

- This optimization problem remains a bottleneck.
Current Optimization Methods

- Lafferty et al. [2001] proposed an iterative scaling approach.
- Outperformed by **L-BFGS** quasi-Newton algorithm.


  - Has a **linear convergence rate**: $O(\log(1/\epsilon))$ iterations required.

- To scale to large $n$, we looked at stochastic gradient methods.  
  [Vishwanathan et al., 2006]

  - Iteration cost is independent of $n$.
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- These remain the strategies used by most implementations.  
  Many packages implement both strategies.

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L-BFGS vs. Stochastic Gradient

- **L-BFGS** has fast convergence but slow iterations.
- **SG** (decreasing $\alpha$) has slow convergence but fast iterations.
- **SG** (constant $\alpha$) has fast convergence but not to optimal.

(Using $\alpha_t = \alpha/(\delta + \sqrt{t})$ gives intermediate performance.)
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- Can we develop a method that outperforms these methods?
2007: summer project with Kevin Swersky on improving SG.

- **ASG**: averaged stochastic gradient with large step-sizes.
  
  [Polyak & Juditsky, 1992, Bach & Moulines, 2011]

  - Typically outperform non-averaged SG, doesn’t always beat L-BFGS.

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2010: methods with improved regret.

- **AdaGrad**: adaptive diagonal scaling.
  
  [Duchi et al., 2010]

  - Often improves performance over basic stochastic gradient.
  - Still has $O(1/\epsilon)$ rate and typically outperformed by **ASG**.
Comparison of Stochastic Gradient Methods

- Comparison of Pegasos, SG, ASG, and AdaGrad:

- ASG often outperforms SG and AdaGrad.
2008: proposed to explore *hybrid* methods in my PhD proposal:

![Graph showing the comparison between IRLS (Newton) and Stochastic Gradient methods for Logistic Regression classifier with L2-penalization using 100,000 training examples.]

- Also rejected! “Too hard, focus on existing projects”.
Motivation for New Methods

- **Deterministic methods** requires $O(\log(1/\epsilon))$ with $O(N)$.
- **Stochastic methods** requires $O(1/\epsilon)$ iterations with $O(1)$.

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2010: **Hybrid** of L-BFGS and stochastic gradient.

- Key idea: control variance of gradient by growing batch size.
- $O(\log(1/\epsilon))$ rate but cheaper in early iterations.

**Hybrid** often outperforms L-BFGS, but not by very much.
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Can we have $O(1)$ cost and only $O(\log(1/\epsilon))$ iterations?
Online Exponentiated Gradient

- **OEG**: online exponentiated gradient.

- $O(\log(1/\epsilon))$ iterations for dual problem with $O(1)$ cost.
- In theory, the rate of deterministic with the cost of stochastic.

[Collin et al., 2008]
**Online Exponentiated Gradient**

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  - $O(\log(1/\epsilon))$ iterations for dual problem with $O(1)$ cost.
  - In theory, the rate of deterministic with the cost of stochastic.
  - Sometimes great and sometimes poor performance.

  ![Graph showing performance comparison between ASG, Hybrid, and OEG4](image)

- Best of hybrid vs. ASG vs. OEG is problem dependent.
- Fancier methods do not give consistent/significant improvement.
Recent new stochastic algorithms for minimizing finite sums,

\[
\min_w f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(x),
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requiring \(O(\log(1/\epsilon))\) iterations with \(O(1)\) cost.
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Stochastic average gradient (SAG): [Le Roux et al., 2012]

$$w^{t+1} = w^t - \alpha \frac{1}{n} \sum_{i=1}^{n} s_i^t,$$

where iteration sets $s_i^t = \nabla f_i(x^t)$ for random $i$ (o.w., $s_i^t = s_i^{t-1}$).
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Unlike EG, adaptive to strong-convexity.
### Comparison of Convergence Rates

Number of iterations to reach an accuracy of $\epsilon$:

<table>
<thead>
<tr>
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<th>Formula</th>
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Similar to deterministic methods, SAG can adapt to problem:

- SAG automatically adapts to local $\mu$ at solution.
- Practical implementations try to automatically adapt to $L$, too.

Strong empirical performance for independent classification.
SAG for Logistic Regression

Performance on logistic regression problems:

- SAG starts fast and stays fast.
Could this algorithm consistently outperform old CRF methods?
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First, we need to address that SAG requires storing $n$ gradients,

$$s_i^t = \lambda w^k - \nabla \log p(y_i|x_i, w^k),$$

for some previous $k$, which do not have a nice structure.
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- But requires extra evaluations of $\nabla \log p(y_i|x_i, w^t)$ per iteration.
The deterministic gradient update can be written:

\[ w^{t+1} = w^t - \alpha \lambda w^t + \frac{\alpha}{n} \sum_{i=1}^{n} \nabla \log p(y_i|x_i, w^t). \]
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A modified update where we don’t approximate the regularizer:

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The \( g_i^t \) have a nice structure, and regularizer update is efficient.
Consider a chain-structured CRF model of the form

\[ p(y|x, w) \propto \exp \left( \sum_{j=1}^{V} x_j^T w_{y_j} + \sum_{j=1}^{V-1} w_{y_j, y_{j+1}} \right). \]
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The gradient with respect to a particular vector $w_k$ is

$$\nabla_{w_k} \log p(y|x, w) = \sum_{j=1}^{V} x_j \left[ \mathbb{1}(y_j = k) - p(y_j = k|x, w) \right] .$$
Addressing the Memory Requirements

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\nabla w_k \log p(y|x, w) = \sum_{j=1}^{V} x_j \left[ \mathbb{I}(y_j = k) - p(y_j = k|x, w) \right].
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- The modified SAG algorithm needs to update the sum,

\[
\sum_{i=1}^{n} g_i^{t+1} = \sum_{i=1}^{n} [g_i^t] + g_i^{t+1} - g_i^t.
\]
Consider a chain-structured CRF model of the form

\[
p(y| x, w) \propto \exp \left( \sum_{j=1}^{V} x_j^T w_{y_j} + \sum_{j=1}^{V-1} w_{y_j, y_{j+1}} \right).
\]

The gradient with respect to a particular vector \(w_k\) is

\[
\nabla_{w_k} \log p(y|x, w) = \sum_{j=1}^{V} x_j \left[ \mathbb{I}(y_j = k) - p(y_j = k|x, w) \right].
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The modified SAG algorithm needs to update the sum,

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General pairwise graphical models require \( O(VK + EK^2) \).

Unlike basic SAG, no dependence on number of features.
Traditional sources of frustration for stochastic gradient users:

1. Need to choose between slow convergence or oscillations.
2. Setting the sequence of step-sizes.
3. Deciding when to stop.
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These are easier to address in methods like SAG:

1. Faster convergence rates.
2. Allow a constant step-size ($\alpha = 1/L$).
3. Approximate the full gradient for deciding when to stop.
Practical issues: setting the step size and stopping

No manual step-size tuning, we approximate $L$ as we go:

- Start with $L = 1$. 

(Lipschitz approximation procedure from FISTA)

Decrease $L$ between iterations. (makes algorithm adaptive to local $L$)

Performance is better than using $1/L$ for global $L$.

Similar to choosing the optimal step-size.
Practical issues: setting the step size and stopping

No manual step-size tuning, we approximate $L$ as we go:

- Start with $L = 1$.
- If $\|f'_i(x)\|^2 \geq \delta$, increase $L$ until we satisfy:

$$f_i(x - \frac{1}{L} f'_i(x)) \leq f'_i(x) - \frac{1}{2L} \|f'_i(x)\|^2.$$ 

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- Similar to choosing the optimal step-size.
Comparison of SAG and state of the art methods.

- Comparison of SAG to existing methods.

- Sometimes better and sometimes worse than existing methods.

- Have we really made so little progress???
Maybe random sampling is too naive?

Can we instead do non-uniform sampling?
  
  Sample some training examples more often than others.
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Can we instead do non-uniform sampling?  
  Sample some training examples more often than others.  
Key idea:  
  Bias sampling towards examples whose gradients change quickly.  
  “If the gradient changes slowly, don’t sample it as often”.
Maybe random sampling is too naive?
Can we instead do **non-uniform sampling**?
  - Sample some training examples more often than others.

**Key idea:**
  - Bias sampling towards examples whose gradients change quickly.
  - “If the gradient changes slowly, don’t sample it as often”.

**Implemented by biasing sampling towards Lipschitz constants:**
  - High Lipschitz constant $\rightarrow$ gradient can change quickly.
Recent works show this improves various methods:


Does SAG converge with NUS?
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Does SAG converge with NUS?

- Not known, and seems hard to prove.
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Does SAG converge with NUS?

- Not known, and seems hard to prove.

We instead analyzed the SAGA variant with NUS.

[Defazio et al., 2014]

- Proved $O(\log(1/\epsilon))$ rate for any reasonable NUS method.
- Proved that rate is faster with Lipschitz sampling.
Still not practical.

- Global Lipschitz constants are hard to get.
- Even if you have them, it doesn’t help much.
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But it works better if you try to estimate local Lipschitz constant:

- We estimate each $L_i$ using similar Lipschitz approximation method.
- Adapts to the local distribution of $L_i$ at the solution.
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But it works better if you try to estimate local Lipschitz constant:
- We estimate each $L_i$ using similar Lipschitz approximation method.
- Adapts to the local distribution of $L_i$ at the solution.

Why should the local $L_i$ values work?
- For correctly-classified examples, $L_i$ is near zero.
- Algorithm focuses on incorrectly-classified examples.
Comparison of SAG-NUS to existing methods

- Comparison of SAG with NUS to existing methods:

- Similar or significantly better than best of previous methods.
Comparison of SAG-NUS to existing methods

- Test error:

(NUS did not improve performance of SG.)
We explored applying SAG to train CRFs.

- With a few modifications, the memory issue is not an issue.
- Allows adaptive step-size and has a stopping criterion.
- With NUS, substantially improves on state of the art.
- SAG4CRF code available on my webpage.
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Various extensions are possible:

- Could use non-smooth regularizers via proximal/ADMM versions.
- Faster methods may be possible via acceleration/Newton.
- Method should work with approximate inference.
- For conditional neural fields and variants like FCNs+CRFs:
  - Need SVRG to deal with the memory.